ADVERTIMENT. La consulta d'aquesta tesi queda condicionada a l'acceptació de les següents condicions d'ús: La difusió d'aquesta tesi per mitjà del servei TDX (www.tesisenxarxa.net) ha estat autoritzada pels titulars dels drets de propietat intel·lectual únicament per a usos privats emmarcats en activitats d'investigació i docència. No s'autoritza la seva reproducció amb finalitats de lucre ni la seva difusió i posada a disposició des d'un lloc aliè al servei TDX. No s'autoritza la presentació del seu contingut en una finestra o marc aliè a TDX (framing). Aquesta reserva de drets afecta tant al resum de presentació de la tesi com als seus continguts. En la utilització o cita de parts de la tesi és obligat indicar el nom de la persona autora.

ADVERTENCIA. La consulta de esta tesis queda condicionada a la aceptación de las siguientes condiciones de uso: La difusión de esta tesis por medio del servicio TDR (www.tesisenred.net) ha sido autorizada por los titulares de los derechos de propiedad intelectual únicamente para usos privados enmarcados en actividades de investigación y docencia. No se autoriza su reproducción con finalidades de lucro ni su difusión y puesta a disposición desde un sitio ajeno al servicio TDR. No se autoriza la presentación de su contenido en una ventana o marco ajeno a TDR (framing). Esta reserva de derechos afecta tanto al resumen de presentación de la tesis como a sus contenidos. En la utilización o cita de partes de la tesis es obligado indicar el nombre de la persona autora.

WARNING. On having consulted this thesis you're accepting the following use conditions: Spreading this thesis by the TDX (www.tesisenxarxa.net) service has been authorized by the titular of the intellectual property rights only for private uses placed in investigation and teaching activities. Reproduction with lucrative aims is not authorized neither its spreading and availability from a site foreign to the TDX service. Introducing its content in a window or frame foreign to the TDX service is not authorized (framing). This rights affect to the presentation summary of the thesis as well as to its contents. In the using or citation of parts of the thesis it's obliged to indicate the name of the author

Towards Integrated Management of the Supply Chain for Enterprise Sustainability

Towards Integrated Management of the Supply Chain for Enterprise Sustainability

José Miguel Laínez Aguirre
Industrial Engineer

A Thesis presented for the degree of
Doctor of Philosophy

Directed by Prof. Dr. Lluis Puigjaner and Dr. Antonio Espuña

Escola Tècnica Superior d'Enginyeria Industrial de Barcelona
Universitat Politècnica de Catalunya

November 2009

Copyright © 2009 by José Miguel Laínez Aguirre

A mis padres, Miguel y Odilia, con insondable amor

Ta mémoire et tes sens ne seront que la nourriture de ton impulsion créatrice. Quant au monde, quand tu sortiras, que sera-t-il devenu? En tout cas, rien des apparences actuelles.

from *J*eunesse IV
Les illuminations, Arthur Rimbaud (1854-1891)

Summary

Market trends have made enterprises change the way of doing business. Globalization makes accessible a wide range of globally dispersed potential suppliers and customers. For competitive customer service now the market demands environmentally friendly products, a good portfolio mix, rapid development of new products, high quality and reliability, after-sales services, among others. In order to fulfill such requirements firms depend more and more on their supply chains (SC). Indeed, nowadays competition is not longer among individual firms, but among SCs. The process system engineering community has been conscious of this shift and has thus devoted research efforts on devising SC and enterprise-wide modeling and optimization strategies. Likewise, from another stand point, the European chemical industry has realized the necessity of SC improvement in order to remain competitive in the global market.

Supply Chain Management (SCM) is intended to maximize financial returns by synchronizing material, cash and information flows across interconnected entities (e.g., suppliers, manufactures, distributors) that seek to provide goods or services to consumers. Lately, it has been recognized the necessity for *integrated* SCM solutions which incorporate and synchronize decisions from several business functions and different hierarchical levels. Current changing and uncertain market environment and internal business concerns make it even more difficult to synchronize all the activities taking place along all SC echelons. Hence, it would be desirable that SC objectives and plans were developed considering market and internal operations uncertainty explicitly, revised periodically and eventually modified following the uncertainty disclosure.

The aim of this thesis is to contribute to the *centralized* integrated SCM. The centralized approach to SCM considers that there exists a central entity that it is able to control the activities of the whole business.

After an overview of SCM and analysis of existing approaches, the second part of this thesis is focused on the development of models which con-

sider the variety of business functionalities decisions. This part explores how business performance can be improved by integrating strategic SCM with financial, marketing and product development planning. The following section is devoted to topics related to pure strategic and tactical SC operations. It is investigated how a more appropriate representation of production processes can be achieved at the SC level. This is done so as to explore any kind of material flows (i.e., raw materials, intermediates, final products) among any pair of supply chain components (e.g., suppliers, manufactures, distribution centers, customers) when optimally re/designing a SC network. This feature allows later integrating scheduling into the SC design - planning. This part is also concerned with the environmentally conscious design of SCs.

The fourth part is focused on uncertainty considerations. A model predictive control whose control algorithm is a stochastic formulation is proposed to face uncertainty and dynamics in SCM. Here, it is shown how incidences can be better resolved by approaching them from a SC perspective. This part also presents a novel and promising graph based approach to deal with scheduling under exogenous uncertainty. The S-graph framework is enhanced to address a two stage stochastic scheduling considering demand as uncertain. One of the advantages of this approach is that the search space does not increase with the number of considered scenarios. Such a feature reduces the computational cost required to solve this kind of problems which is one of the major challenges in this field, thus constituting a robust alternative to existing schedulers to become eventually the best option in integrated SCM.

The last contribution concerns the integration of hierarchical decision levels. The fifth part examines the implications of considering scheduling decisions when designing a SC network. It is shown how capacity is the core factor that allows the integration of hierarchical levels. This part emphasizes that an optimistic performance, due to capacity overestimation, is obtained if scheduling is not consider into the SC design formulation. Significant performance reductions can be found when the SC is actually deployed. This is particularly significant in batch processes where changeover times, cleaning times, idle times commonly appear. An integrated approach prevents this capacity overestimation by considering scheduling decisions. Moreover, it is demonstrated how capacity permits low level supervisory control integration. Such integration allows updating SC capacity and adequately resolving equipment disruptions or breakdowns.

Resumen

Las tendencias del mercado han hecho que las empresas cambien su forma de hacer negocios. La Globalización ha permitido a las empresas tener la posibilidad de acceder a distintos proveedores y mercados globalmente dispersos. Actualmente para mantener un servicio al cliente competitivo, el mercado reclama productos amigables con el medio ambiente, un amplio portafolio de productos, rápido desarrollo de nuevos productos, alta calidad y fiabilidad, entre otros. Para cumplir con tales requisitos, las empresas dependen cada vez más de su Cadena de Suministros (CS). De hecho, la competencia en el mercado ya no es únicamente entre empresas, sino entre CS. La comunidad científica, específicamente, la de Ingeniería de Sistemas de Procesos, es consciente de este cambio y ha dedicado esfuerzos a la concepción de estrategias para el modelado y optimización de CS. Asimismo, la industria química Europea reconoce necesaria la mejora de la Gestión de la Cadena de Suministros (GCS) para mantenerse competitiva en un mercado global.

La GCS trata de maximizar los retornos financieros sincronizando los flujos de materiales, información y efectivo existentes entre las distintas entidades que se encuentran interconectadas con el objetivo de proveer un bien o servicio al mercado. Recientemente, también se reconoce la necesidad de una *Gestión Integrada de la Cadena de Suministros* (GICS), la cual consiste en la sincronización de otras funciones del negocio y de diferentes niveles jerárquicos de decisión. El actual entorno dinámico de los negocios y de las propias operaciones de la CS hacen difícil la coordinación de las actividades de los componentes de la CS. Por tanto, es importante que los objetivos y planes sean desarrollados considerando explícitamente la incertidumbre del mercado y de las propias tareas de fabricación y que sean revisados periódicamente.

El propósito de esta tesis es contribuir al desarrollo de estrategias para la GICS. La tesis contempla CS *centralizadas*, es decir, se considera que existe una entidad central que es capaz de controlar las actividades de toda la CS.

Después de una revisión de conceptos y de las estrategias existentes para abordar la GICS, la tesis se enfoca en el desarrollo de modelos que incluyen decisiones de diferentes funcionalidades del negocio. Esta parte explora cómo puede mejorarse el comportamiento de la CS si conjuntamente con la gestión estratégica de la CS se integran decisiones asociadas con finanzas, marketing y desarrollo de nuevos productos. A continuación la tesis se dedica a temas puramente relacionados con la gestión estratégica y táctica de las operaciones de la CS. Se investiga cómo obtener una representación más apropiada de los procesos productivos a nivel de CS. De esta manera se exploran todo tipo de flujo de materiales (Ej., materia prima, producto en proceso) entre cualquier par de componentes de la CS cuando se optimiza el diseño de la red. Esta característica después permite integrar el diseño y planificación de CS con la programación de operaciones (PO). En esta parte se considera también el diseño de CS considerando su impacto ambiental asociado.

La cuarta parte está dedicada a la consideración de la incertidumbre. Para ello se propone un control predictivo (MPC) que incorpora como algoritmo de control un modelo estocástico. Se muestra como las incidencias pueden resolverse de mejor manera cuando se tiene en cuenta una visión completa de la CS en la búsqueda de posibles soluciones. Además se desarrolla una extensión del método para PO S-graph para abordar problemas bajo incertidumbre. Esta propuesta posee la particularidad que el tamaño del espacio de búsqueda no crece con el número de escenarios considerados. Dicha característica permite reducir los tiempos de solución, lo cual es uno de los principales desafíos en esta área, constituyendo así una alternativa a programadores actuales y eventualmente la mejor opción para la GICS.

La última contribución de esta tesis está relacionada con la integración de los distintos niveles de decisión. Se muestra como la capacidad es el factor clave para llevar a cabo esta integración. Se examinan las implicaciones de considerar la PO cuando se diseña una CS. En esta parte se hace hincapié en la errónea sobreestimación de la capacidad que se obtiene cuando la PO no es incluida en el diseño de CS. Reducciones significativas del rendimiento pueden darse cuando la CS es puesta en marcha. Este punto es aún más significativo para los procesos batch en los cuales aparecen usualmente tiempos muertos y tiempos de preparación de máquinas. Una estrategia integrada impide la sobreestimación de la capacidad al tener en cuenta la programación detallada de operaciones. Aún más, se demuestra como la capacidad permite la integración del módulo de control de bajo nivel con la CS por medio de la formulación de la PO. Dicha integración permite actualizar la capacidad real y resolver adecuadamente interrupciones y fallos en los equipos.

Acknowledgments

Undoubtedly, the learning and research represented by this thesis would have not been possible without the support of my family, my friends and colleagues. I do owe my deepest gratitude to all of you. I am truly indebted to Prof. Puigjaner and Toni for their mentorship and encouragement along these last four years. Finally, I would like to thank the financial support received from the "Generalitat de Catalunya" (Comissionat per a Universitats i Recerca del Departament d'Innovació, Universitats i Empresa) to carry out this thesis.

Agradecimientos

Indudablemente, el aprendizaje e investigación representados por esta tesis no hubiese sido posible sin el apoyo de mi familia, mis amigos y compañeros. A todos ustedes les debo y expreso mi más profunda gratitud. Estoy definitivamente en deuda con el Prof. Puigjaner y con Toni por todos sus conocimientos, consejos, experiencia, y motivación a lo largo de estos últimos cuatro años. Finalmente, quisiera agradecer la financiación recibida de la "Generalitat de Catalunya" (Comissionat per a Universitats i Recerca del Departament d'Innovació, Universitats i Empresa) para la realización de esta tesis.

Contents

Part III Operations Strategic and Tactical Issues

Part IV Treatment of Uncertainty

List of Tables

List of Figures

Part I

Overview

Chapter 1

Introduction

1.1 Introductory perspective and motivation

The European Union (EU) has the second largest chemical industry in the world. According to the European Chemical Industry Council (2009), the EU accounted for 29.5%, worth 537 billion €, of the total global chemical sales in 2007. Of the thirty largest chemical companies in the world, twelve are headquartered in Europe representing around 10% of world chemical sales. Moreover, chemicals account for 26% of the total EU manufacturing trade surplus. With regard to employment, approximately 29000 European chemical and pharmaceutical companies engage a total staff of about 1.9 million which is 6% of the overall workforce in the EU manufacturing industry. What is more, Figure 1.1 shows that the chemical industry is a key supplier of practically every sector of the European economy. Thus, it is considered that one job in the chemical industry creates two jobs outside of it. Owing to this, it is claimed the competitiveness of all these other sectors is partially dependent on the efficient supply of chemical products. Altogether, the chemical industry clearly makes a significant contribution to the EU economy.

Nevertheless, it is noteworthy that the share for the global market held by European companies is diminishing. The EU chemical industry has lost its traditional first place in the world ranking in favor of Asia. This fact is a result of the rapid expansion of the chemical industry mainly in India and China. This has also caused the European customer base to erode as chemicals large users relocate their production to lower labor cost countries in Middle and Far East. The EU chemical industry still has a positive trade balance with all regions, although for Asia it should be noticed that the trade surplus is very

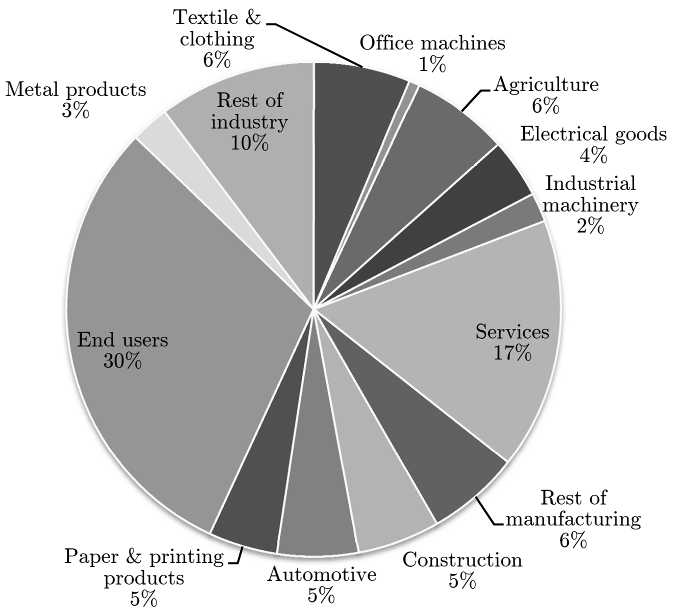


Figure 1.1: Consumption structure of EU chemical industry (CEFIC, 2009)

small and is diminishing over time. Furthermore, the Trade Competitiveness Indicator (TCI), an indicator that compares the trade balance to the total trade of a region, reveals a deteriorating competitiveness of the EU chemicals industry. Since 2003 to 2008, the TCI declined from 25% to 17%. This shows that European chemical imports are growing faster than exports. Such a trend is experienced by other industrial sectors as well (World Trade Organization, 2008).

The European Chemical Industry Council (CEFIC) and the European Petrochemical Association (EPCA) have recognized that to remain competitive in export markets and minimize import penetration into the European chemical market, enterprises producing chemicals must continue reducing their costs. As the scope for further reductions related to equipment technology is limited, given the size and age of European plants, performance improvements should come from an enhanced Supply Chain Management (McKinnon, 2004). Hence, in order to preserve its condition and persist as a vital sector in the European economy, the chemical companies are depending on the performance of their global Supply Chain (SC) networks.

Many proposals have emerged from the chemical industry for SC improvement. One of them is the necessity of improving the degree of functional coordination, it has been noticed that closer coordination between logistics and other functional units can improve overall business performance. In addition, it has been proposed the relocation of production capacity in the long term as a manner to significantly enhance chemical industry efficiency. Undoubtedly,

Figure 1.2: A supply chain network

both abovementioned proposals pose the challenge of developing efficient tools and methodologies so as to obtain innovative solutions for the operation and design of chemical SCs. From another standpoint, the Process System Engineering (PSE) community also recognizes that an optimum management of the SC offers a key opportunity for preserving and improving firm's value (Grossmann, 2004).

Certainly, there exists a economic trend that is changing the nature of business enterprise. Nowadays businesses are increasingly *boundaryless*, meaning that internal functional barriers are being removed in favor of horizontal process management; externally, the gap between vendors, distributors, customers and the firm is gradually closing (Christopher, 2005). As result of realizing this shift, academics as well as practitioners are focusing efforts on developing holistic frameworks which are capable of supporting the cross-functional decision making process required to remain competitive under the current complex and dynamic business environment (Jung, Blau, Pekny, Reklaitis, & Eversdyk, 2004; Wan, Pekny, & Reklaitis, 2005; Guillén-Gosálbez, Pina, Espuña, & Puigjaner, 2005c; Guillén-Gosálbez, Badell, Espuña, & Puigjaner, 2006a; Hugo & Pistikopoulos, 2005; Kouvelis & Rosenblatt, 2000).

1.2 Supply chain management

The concept of SC refers to the network of interdependent entities (e.i., retailers, distributors, transporters, storage facilities and suppliers) that constitutes the processing and distribution channels of a product from the sourcing of its raw materials to its delivery to the end consumer as illustrated in Figure 1.2.

Subsequently, Supply Chain Management (SCM) can be defined as the management of material, information and financial flows through a SC that aims at producing and delivering goods or services to consumers (Tang, 2006). The main objectives are to achieve the desired consumer satisfaction levels and the maximum financial returns by synchronizing and coordinating the SC members activities. The need for such coordination grows out of several trends in the marketplace. One of them is the so-called Globalization which has led to the availability of a vast set of alternative sources of materials and other inputs as well as a wider set of potential customers. This evidently expands the SCM scope to embrace the consideration of international issues. In addition, customers' changing expectations regarding value of goods and services, combined with advances in technology and the availability of information, have driven the formation of these "new forms" of networks (Handfield & Nichols, 1999).

1.2.1 Integrated supply chain management

Since its appearance in the nineties, the conception of SCM has evolved from the primary idea that was to align the forecasting, distribution, and manufacturing processes. Nevertheless, the original mission and essence which is to break down "walls" still remains and continue expanding (Hameed, 2007).

Recently, the term Integrated Supply Chain Management has been formally coined in the work of Varma, Reklaitis, Blau, and Pekny (2007). They noted that Integrated SCM should encompass in an unified manner strategic and tactical decisions such as raw material procurement contracts, routing to plant sites, capacity planning and lead time management, routing of finished products, warehouse positioning, network inventory management and marketing strategies.

In this thesis, Integrated SCM is understood as an enhanced concept that attempts to break down "walls" by integrating the decision making across three dimensions:

- Diverse geographically distributed facilities and organizations;
- Different hierarchical levels of decision-making (strategic, tactical and operational);
- Various business functionalities (e.g., operations, finances, R&D, marketing, environmental management).

Furthermore, as stated by Blanchard (2004) business environment current trends need to be pondered when developing a SC decision support system. Specifically, SC managers need to consider the dynamics of a rapidly changing market environment, such as variability in demand, cancellations and returns, as well as the dynamics of internal SC operations, such as processing times, production capacity pitfalls and the availability of materials. Evidently, market dynamics and uncertainty and internal business operations make it difficult

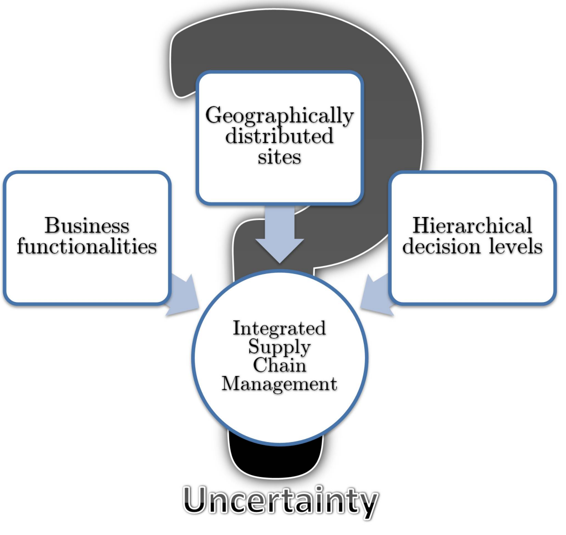


Figure 1.3: Dimensions of integrated supply chain management

to synchronize the activities of all SC echelons; this causes significant deviations from previous objectives and plans. Therefore, for a SC to be efficiently managed it is important to systematically review variability and to explicitly take it into account in decision making. These actions search for a flexible response to changes in the business environment, increase the decisions accuracy and robustness, and improve business performance. For these reasons, an integrated framework should include the explicit consideration of SC uncertainties and dynamics.

The research goal posed in the PSE community is to integrate all these aspects into a model which would ultimately serve as the core of a SC decision support system.

It is also important to mention that Enterprise Wide Modeling and Optimization (EWMO) has emerged as a new promising research field. Likewise, one of its key features is the integration of the information and decision making among the various functions that comprise the SC of a company and across different decision levels as well. Shapiro (2006) recognizes that SCM might be considered as an equivalent term for describing EWMO. However, in EWMO the emphasis is on the manufacturing facilities with a major focus being their planning, scheduling and control which often requires specific knowledge of process engineering (Grossmann, 2005). Here, the Integrated SCM application is devoted to the chemical process industry for which it is necessary to recall particular knowledge of process engineering as it occurs in EWMO. For the purposes of this thesis, EWMO and Integrated SCM are considered as equivalent terms.

1.3 Supply chain modeling

In general terms, modeling is the attempt of devising an approximate representation of a system with the goal of providing predictions of the system's performance measures of interest. Such a representation is called a *model*. A model is designed to capture certain behavioral aspects of the modeled system–those that are of interest to the analyst–in order to gain knowledge and insight into the system's behavior (Morris, 1967). Particularly, SC models enable us to investigate and discover potential satisfactory alternatives for managing the SC.

1.3.1 Organizational structure

SC entities such as raw material suppliers, manufactures, distributors, retailers can be managed as a single organization or they can be treated as independent organizations. Following this differentiation three managing approaches may appear in a SC, namely, centralized, semi-centralized, and decentralized.

Centralized This approach considers the existence of a central entity owning a global visibility on all nodes comprising the SC. Under this approach, it is assumed that the central entity can access all the information regarding the parameters that describe the characteristics and status of each SC members. The central entity uses this information to smooth out the pressure among SC members, and an attempt is made to optimize the entire SC.

Decentralized This approach considers that decisions are made separately by each SC member or groups of them. Since SCM does not mean ownership of other organizations, decentralized approaches attempt to influence decision making and impact system-wide performance (Vonderembse *et al.*, 2006).

Semi-centralized This approach is a hybrid of the two previous ones. Intermediate cases fall into this category.

In order to develop a SC model, firstly, the SC organizational structure is being dealt with should be determined. Obviously, the SC organizational structure conditions the model's scope and the elements to be contemplated.

1.3.2 Model elements

Min and Zhou (2002) outline some key elements which should be pondered for developing SC models, namely, (i) SC drivers, (ii) SC decisions, and (iii) SC restraints.

SC drivers This element refers to the SC goals setting and performance. The major driving forces behind a SC are customer satisfaction, economic incentives, efficiency and risk. Customer satisfaction is the degree to which customers meet their requirements with the product received. Typical customer oriented metric are the lateness, tardiness, response time, fill rate and customer service level. Economic drivers show how profitable a SC is. Examples of this type of metrics are total cost, profit, net present value (NPV), return-on-investment (ROI), among others. Efficiency measures reflect how well SC resources are utilized. Makespan and total idle time belong to this group. Finally, risk is a complementary metric that shows the probability of achieving a predefined performance level.

SC decisions SC performance is an outcome of the decisions made in order to synchronize the materials, information and cash flows along the SC partners. The decisions encompassed in a SC model depend on its scope. However, some of them are listed next.

- *Location* They involve determining where to place new SC facilities.
- *Capacity changes* These type of decisions determine where, when and what amount to expand or reduce SC capacity (i.e., equipment technology or workforce).
- *Flows magnitude* They determine the volume of purchasing, production and distribution of each material.
- *Allocation* They involve allocating resources to SC tasks (i.e., assignment, sequencing, and timing).
- *External links* These decisions define which external suppliers should be utilized or phased out. They also include outsourcing decisions.
- *Inventories* They determine the inventory control policies and safety stock levels.

SC restraints This set represents the SC restrictions. They determine the feasibility of the different management alternatives. This restrictions include: mass balances; SC capacity constraints; technological constraints (e.g., product recipes, product sequencing, unstable and perishable materials); budgeting limitations; suppliers' capacity; market demand and competition, customer satisfaction requirements, among others.

1.4 Research scope and objectives

Modern enterprises are global networks comprising several distinct SC echelons. Chemical enterprises are supported not only by production operations but also

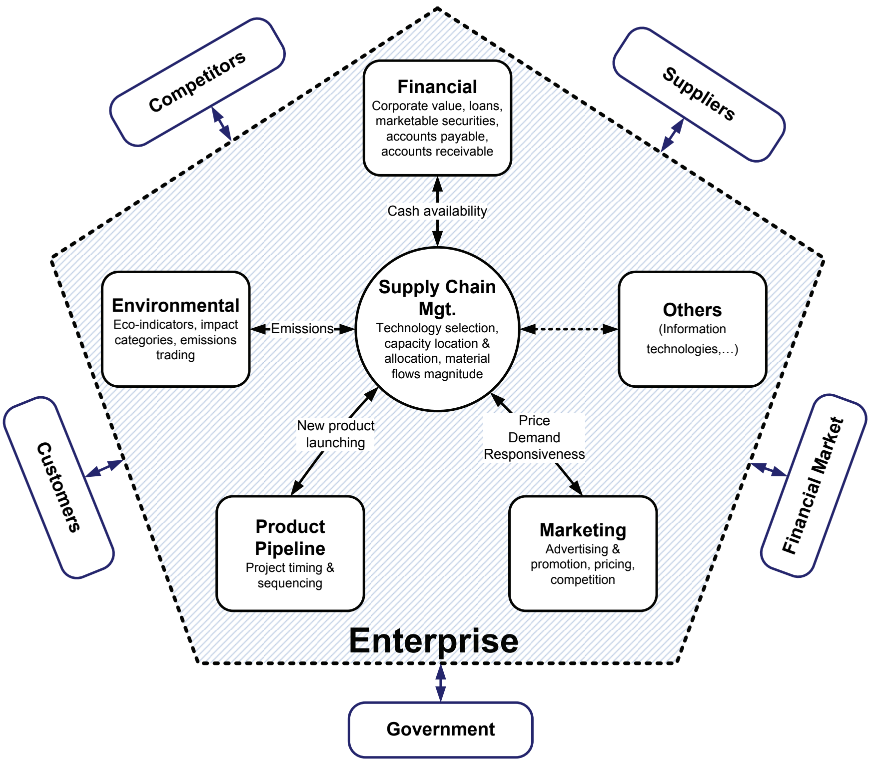


Figure 1.4: Schematic of an integrated SC model

by product R&D as well as by strategic functions such as financial planning and marketing. With the aim of maximizing growth and creation of firms value, companies need these functional components to be well coordinated by an integrated model. This fact can enhance capabilities of adapting and responding to uncertainties arising from internal processes as well as external environment.

Decisions within organizations ought to be carried out quantitatively understanding the trade-offs among the risks and benefits that imply the different available options. Despite the fact of being necessary, there has not still been proposed any integrated and unified model to provide such quantitative support for decision making, which will allow optimizing enterprise resources (e.g., materials, cash, personnel) utilization (see Fig. 1.4). In general, the main aim of this thesis is to contribute to the development of *integrated* mathematical programming models for *centralized* SCs considering the specific characteristics of chemical related sectors. This general aim can be broken down to four more specific objectives that would together achieve the overall goal of this thesis as follows:

- To develop and demonstrate the benefits of SC models that integrate different business functionalities and hierarchical decision levels.

- To formulate SC models that encompass a better description of production processes and SC members connectivity.
- To propose strategies for decision making under uncertainty that systematically review variability and explicitly take it into account.
- To apply solution strategies that allow reducing the computational burden required to tackle SC problems.

1.5 Thesis outline

The general structure of this thesis has been devised bearing in mind the dimensions of integrated SCM previously discussed. Figure 1.5 represents schematically the outline of this document.

In addition to the previous introduction, Part I presents in Chapter 2 a State-of-the-Art review which finally allows identifying some integrated SCM trend and challenges. Then, the methods and tools utilized throughout this thesis are briefly explained in Chapter 3.

The main body of this thesis has been divided in four parts. Part II deals with business functionalities integration in order to bring a systemic view of strategic SCM. With this purpose, Chapter 4 deals with the design and retrofit of SCs and proposes a novel framework to address this problem. The proposed framework consists in incorporating financial considerations at the strategic decision-making level and adopts the firm's corporate value as the objective to be maximized. Later on, this model is extended in the following two chapters. Chapter 5 presents an integrated model which also incorporates simultaneously R&D decisions. The model considers the endogenous uncertainty associated with product test outcomes during the development process. To end this part, a mathematical model that incorporates marketing decisions is presented in Chapter 6.

Part III focuses on purely operations strategic and tactical issues. In Chapter 7, a novel flexible formulation approach which translates a recipe representation to the SC environment is proposed to solve the challenging design-planning problem of SC networks. By extending the previous model, Chapter 8 addresses the optimization of SC planning and design considering economical and environmental issues. The model performs an environmental impact mapping along the comprising SC nodes and activities. Here, environmental metrics are also considered as objectives to be optimized.

Next, Part IV tackles uncertainty in SC problems. In Chapter 9, an MPC methodology is proposed which comprises as control algorithm the stochastic version of the strategic model presented in Chapter 4. Chapter 10 presents a novel approach to deal with scheduling problems under uncertainty. In this chapter a graph-theoretic approach, S-graph, is enhanced so that stochastic

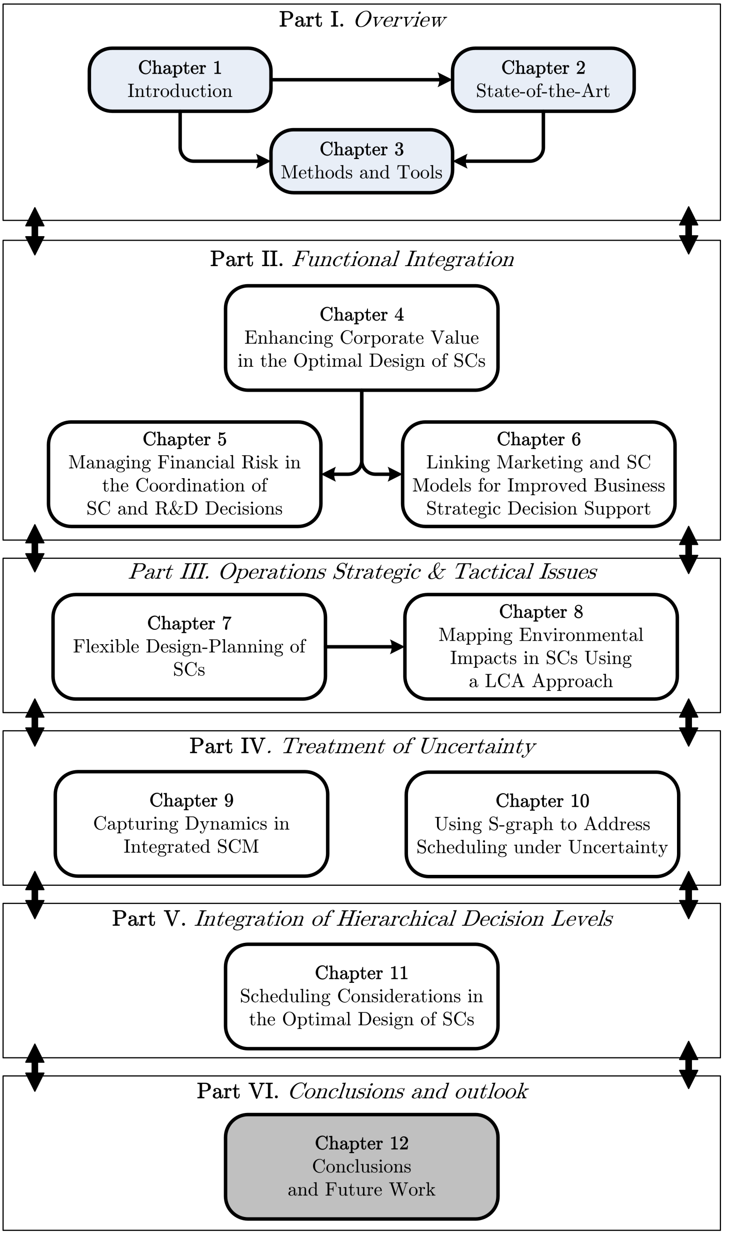


Figure 1.5: Thesis outline

scheduling problems can be handled. Next, Part V addresses the integration of hierarchical decision levels. Here, Chapter 11 shows the integration of the SC design-planning model with a scheduling formulation so that decision levels integration is achieved. The model developed in Chapter 7, which is a translation of a classical scheduling recipe representation to the SC context, and the framework proposed in Chapter 9 are combined in this chapter. The impact of considering scheduling aspects of process operations in the design of a SC network is evaluated.

Finally, Chapter 12 summarizes the thesis contribution and draws concluding remarks for future work.

Chapter 2

State-of-the-Art

2.1 Introduction

Different classifications have been proposed so far for SC problems approaches. For instance, Beamon (1998) suggests to catalog SC design and analysis problems into four categories, according to the nature of the inputs and the objective of the approach. The approaches are classified then as deterministic, stochastic, economic and simulation models. Shah (2005) proposes another classification which is divided in three categories: SC infrastructure design; SC analysis and policy formulation; and SC planning and scheduling. As it can be noticed, there are many possible classification criteria in order to group the methodologies that have been applied for SCM. What is more, all these categories may overlap among them. For the purposes of this thesis, a brief description concerning the techniques and tools utilized to solve the different problems arising in integrated SCM is done in next section. Afterward, the approaches developed so far are categorized following the integrated SCM dimensions established in section 1.2:

- The decision level at which the problem may be ascribed (e.g., strategic, tactical);
- The functional areas which are included in the modeling (e.g., finances, environmental issues), and
- The uncertainty treatment (e.g., stochastic programming, predictive control).

2.2 Solution approaches

Different tools and techniques have been deployed to support decision making processes. A general taxonomy distinguishes between transactional and analytical systems. Transactional systems are just concerned with the acquisition, processing and communication of data over the enterprise. Otherwise, analytical tools introduce some *intelligence* to evaluate different alternatives available to solve the addressed problems. Furthermore, analytical tools can be classified into descriptive and normative approaches.

It is noteworthy that the way in which computer aided systems for enterprise decision support have evolved has caused some problems and inefficiencies in SCM. In the last decade, Enterprise Resource Planning (ERP) became popular. Essentially, a ERP system is a multi-module application which is integrated with a relational database and can serve all departments within an enterprise. Certainly, ERPs are not enough as their main core is a not flexible non redundant database that centrally organizes transactional information.Due to the lack of software capable of linking transactional and analytical modeling systems, the material logic of the pioneer MRP system (Orlicky, 1975) still remains as the kernel of most of the current commercial ERPs. Additionally, analytical systems has not incorporated the multi-functional planning models required to optimize the combined effects of the different variables involved in the problem. Under this scenario, organizations ability to respond to the market changes in a efficient manner is being hampered. Indeed, integrated analytical systems which are instanced automatically from transactional systems data are required to open new ways of making satisfactory overall decisions.

2.2.1 Normative approaches

The normative category involve those approaches whose main goal is optimization: mathematical programming models and heuristic techniques.

According to the Mathematical Programming Society[1], in a mathematical programming or optimization problem, one seeks to minimize or maximize a real function of real or integer variables, subject to constraints on the variables. Optimization problems are made up of three basic components: (i) an objective function which one aims to minimize or maximize (e.g., in the area of PSE it is usual to maximize the profit or minimize the total cost); (ii) a set of variables which affect the value of the objective function (e.g., the amounts of different resources used or the time spent on each activity); and (iii) a set of constraints that allow the variables to take on certain values but exclude others. The term mathematical programming refers to the study of these problems, their mathematical properties, and the development and implementation of algorithms to solve these problems.

Most realistic optimization problems require the simultaneous optimization of more than one objective. In these and most other cases, it is unlikely that

[1] *http://www.mathprog.org/*

the different objectives would be optimized by the same variable value choices. Hence, some trade-off between the criteria is needed to ensure a satisfactory solution. The Multi-Objective (MO) optimization is suitable for this kind of problems. It gives a set of Pareto optimal solutions rather than an exclusive unique value. The MO optimization enables the efficient integration of a number of issues regarding different enterprise functionalities. Many methodologies have been proposed for treating MO optimization problems (Miettinen, 1999). Among them are the weighted-sum method, the ϵ-constraint method, and the goal-programming method. These methods are based on the conversion of the objectives vector into a scalar objective and are the most widely used in process engineering (Azapagic & Clift, 1999a; Zhou, Min, & Gen, 2002; Chen, Wang, & Lee, 2003; Cheng, Subrahmanian, & Westerberg, 2004). In addition, multi-parametric programming can be used to deal with multi-objective optimization in a more rigorous manner (Papalexandri & Dimkou, 1998; Guillén-Gosálbez & Grossmann, 2009).

On the other hand, heuristics are rules or algorithms that obtain a good feasible solution to a given problem, but they do not guarantee optimality. Lagrangian heuristics and meta-heuristics fall into this category. Lagrangian heuristics consist in iterative methods that try to build feasible solutions from the solution provided by the Lagrangian relaxation of an optimization problem. This process is usually repeated until the gap between the best upper bound and the best lower bound stands below a certain value (see section 3.8.1). Meta-heuristics (e.g., genetic algorithms, simulated annealing, tabu search, scatter search, ants colony) are solution methods that orchestrate an interaction between local improvement procedures and higher level strategies to create a process capable of escaping from local optima and performing a robust stochastic search of a solution space (Glover & Kochenberger, 2003). While meta-heuristics have proved to be very effective in combinatorial problems, their optimality and convergence are not certified; there is no systematic procedure for obtaining good bounds on the attainable optimum values of the objective function (Pekny & Reklaitis, 1998). Significant research in this field is devoted to incorporate meta-heuristics within mathematical programming techniques.

2.2.2 Descriptive approaches

Descriptive approaches, among them simulation and forecasting, intend to give some information in order to understand the nature of the system but without using specific algorithms for doing improvements.

Forecasting techniques are concerned with approaches for determining what the future holds[2]. The field of forecasting includes the study and application of judgment as well as of statistical methods such as time series analysis and regression. In SCM forecasting has been typically used to predict raw material costs and future demand of products.

[2] *http://www.forecastingprinciples.com/*

In simulation, a model of a system is created so as to describe some process involving individual entities such as persons, products or messages. The components of the model try to reproduce, with varying degrees of accuracy, the actual operations of the real components of the process. Most likely, the system will have time-varying inputs and time-varying outputs that are affected by uncertain events. Moreover, the flow of entities through the system is controlled by logic rules that derive from the operating rules and policies associated with the process being modeled (Jensen & Bard, 2003). Because the simulation model generally acts just as a function evaluator, which operates as a meritorious reproduction of its real-world counterpart, complex nonlinear relationships may be incorporated without significantly increasing computation times. In that sense, simulation is much less restricted than optimization models. Using simulation one can duplicate real systems with a high level of accuracy. Due to this capacity for detail, simulation has become a very popular method for SC analysis (Perea-López, Grossmann, Ydstie, & Tahmassebi, 2001; Jung *et al.*, 2004; Wan *et al.*, 2005; Mele, Espuña, & Puigjaner, 2006b). Its ability to model uncertain events with arbitrary probability distributions and systems that have a variety of interacting processes is particularly appealing.

Recently, the agent paradigm is being applied as a simulation tool to solve process engineering problems in which coordination of multiple entities is required (Han, Douglas, & Stephanopoulos, 1995; Maguire, Struthers, Scott, & Paterson, 1998; Yang & Yuan, 1999; McGreavy, Wang, Lu, Zhang, & Yang, 1996; Eo, Chang, Shin, & Yoon, 2000). A software agent is an autonomous, multi-threaded object, which is able to communicate with other agents, to react to changes in its environment, and to take initiative based on pre-specified goals (Wooldridge & Jennings, 1995).

SCM problems are distributed in nature, and require extensive coordinated decision-making. Thus, a multi-agent system is a suitable tool to tackle this kind of problems. For instance, Goodwin, Keskinocak, Murthy, Wu, and Akkiraju (1999) present a framework for providing decision support for an online exchange. The authors use a multi-agent system to find matches of demand and supply on the exchange and provide the user with the best set of transactions that is found. The match is selected based on the user discretion. Sauter, Parunak, and Goic (1999) present an architecture called Agent Network for Task Scheduling (ANTS), inspired by insect colonies and humans. Agents represent elements in the SC and within a factory. Each firm in turn is viewed as a small SC, thus the interface between agents within a firm is similar to those between different firms. This helps an easy integration of the SC elements. Agents also represent the resources of the firm. Each agent has a committed capacity profile, which shows its time-varying load. In case a new task has to be scheduled, each agent bids for that task with a bid that is inversely proportional to the committed capacity of the agent. Thus, resources are allocated to tasks without resorting to rescheduling the entire SC.

Simulation based optimization

Historically, one of the disadvantages of simulation is that it is not an optimization technique. Typically, a relatively small number of system configurations are simulated and the one that *appears* to give the "best" performance is chosen. However, simulation models can be coupled with meta-heuristics in order to provide them with improvement capabilities. In this scheme, which is known in literature as simulation based optimization, the simulator acts as a function evaluator and the meta-heuristic method uses the simulation results to search a set of parameters (i.e., decision variables) that improve the simulation outputs (i.e., objective function). The main drawbacks of this combined approach are the high computational effort required to obtain a consistent solution and the quality sensitiveness of the solution to the choice of the meta-heuristic and the corresponding parameter settings.

In order to alleviate the computational burden of simulation of complex systems, a surrogate model can be created to replace individual replications. Surrogate models or meta-models are functional relationships between the input variables and the performance measure. Surrogate models are tuned to mimic the underlying simulation model as closely as needed over a representative search space. SCM applications of simulation based optimization and surrogate models can be found in the works of Jung *et al.* (2004); Wan *et al.* (2005); and Mele, Espuña, and Puigjaner (2006a).

This thesis is focused on the analytical approaches developed to support decision making in SC problems.

2.3 Literature review

The criteria selected to catalog the approaches developed so far are specifically associated with the characteristics of the SC problem that is being addressed. Figure 2.1 shows schematically this classification. All those approaches that focus on the process operations side and neglect the interrelationship of business functional areas are categorized according to the hierarchical decision level criteria. Then, it has been considered appropriated to emphasize those approaches which merge functionalities by grouping them in accordance with that criterion. Finally, those approaches which deal with uncertainties are revised.

2.3.1 Hierarchical decision making levels

In integrated SCM, the dimension of hierarchical decision levels deals with issues related to temporal integration in that they involve coordinating decisions across different timescales. In practice, it is usually helpful to use the time dimension to establish hierarchical order to planning. The hierarchical planning approach was first presented in the work of Hax and Meal (1975). A framework for a hierarchical decision making in which the aggregate results of capacity planning provide constraints for detailed scheduling decisions was presented.

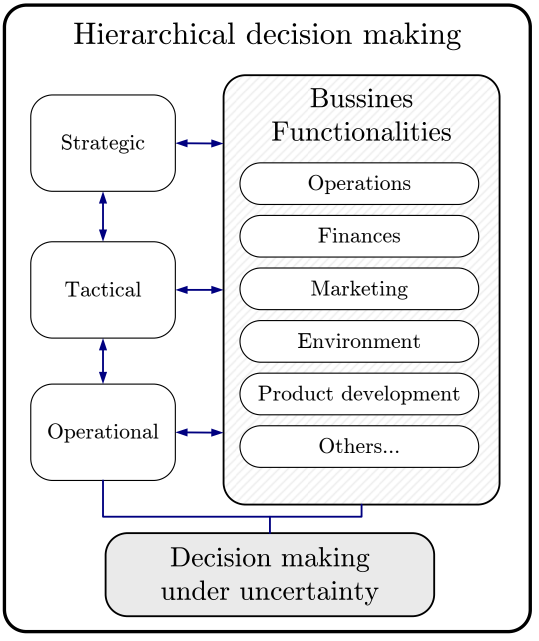


Figure 2.1: Classification of supply chain management approaches

The authors selected such an approach since an optimization for the entire system could not be developed using the analytic methods and data processing capabilities available at that time. Today's computing capabilities and optimization techniques progress together with the more horizontal management of firms create an appealing scenario for attempting integrated approaches for SCM.

Under a hierarchical-sequential scheme, first, long-term or strategic planning affects the achievement of goals over sourcing and investment decisions. Long-term plans generally concern the enterprise infrastructure and links with "external" organizations. Once implemented, plans cannot be easily altered at this level since their implementation is typically capital intensive and time consuming. In terms of organizational structure they are usually under the control of shareholders and/or upper level management personnel. Intermediate time periods require tactical planning. Tactical or middle term planning results in decisions related to the magnitude of material flows across the manufacturing/distribution network that is established by the strategic level. Finally, short term or operational planning is characterized by those many decisions that must be made at the shop floor for the daily or weekly activities.

The need to support decision making and improve operations over all levels of planning has lead to the development of several hierarchical modeling approaches. A sample of these works is provided in next sections.

Strategic level

The SC strategic level determines the network through which production and distribution serve the marketplace. The intent of the SC network design problem is typically to determine the optimal sourcing, manufacturing and distribution network for the new and existing product lines of a company (e.g., expansion or contraction of the business, introduction of new products, new strategic suppliers). The most common approach is to formulate a large-scale Mixed Integer Linear Program (MILP) that captures the relevant fixed and variable operating costs for each facility and each major product family. The fixed costs are usually associated with the investment and/or overhead costs for opening and operating a facility, or with placing a product family in a facility. The variable costs include not only the manufacturing, procurement and distributions costs, but also the tariffs and taxes that depend on the network design. The network design problem focuses on the design of two or three major echelons in the SC for multiple products. Due to the nature of the problem being solved, network design is typically solved every two to five years (Graves & Willems, 2003). The strategic plan is developed at an aggregated level of time, products and resources.

The SC design problem has its origins in the location problem which has been a subject of study in Operations Research since the 1950's. However, it was first structured in a solvable MILP form by Balinski (1965). An early example of a production-distribution network optimization study in the process industries is given by Brown, Graves, and Honczarenko (1987) who consider the biscuit division of Nabisco. Their model involves the opening or closing of plants, and the assignment of production to plants.

Papageorgiou, Rotstein, and Shah (2001) present a MILP to support strategic supply chain decision-making for pharmaceutical industries. The formulation include the selection of the product development and introduction strategy together with long-term capacity planning and investment strategy.

Cakravastia, Toha, and Nakamura (2002) develop an analytical model of the supplier selection process in designing a SC network. The assumed objective is to minimize the level of customer dissatisfaction, which is evaluated by two performance criteria: price and delivery lead time. The overall model operates at two levels of decision-making: the operational level and the strategic level. The operational level concerns decisions related to optimizing the manufacturing and logistical activities of each potential supplier in order to meet the customer's requirements. At the strategic level, all the bids from potential suppliers are evaluated and the final configuration of the SC is determined. Bansal, Karimi, and Srinivasan (2008) report a MILP formulation to fulfill the logistics needs of a global enterprise in terms of Third Party Logistic (3PL) contracts and in-house execution. They represent tasks as logistics recipes and superstructures, similar to the ones used by the scheduling model presented in Sundaramoorthy and Karimi (2005). The goal is to obtain the 3PLs contracts that serve the total needs of a company and with the minimum cost.

Kallrath (2002) describes a tool for simultaneous strategic and operational planning in a multi-site production network. He aims to optimize the total net profit of a global network, where key decisions include: operating modes of equipment in each time period, production and supply of products, minor changes to the infrastructure (e.g., addition and removal of equipment from sites) and raw material purchases and contracts. The standard material balance equations are adjusted to account for the fact that transportation times are much shorter than the period durations. Production plans were developed which resulted in cost savings of several millions of US dollars. Similarly, Sousa, Shah, and Papageorgiou (2008) develop a two-level sequential approach for SC design and operational planning. A feedback integration methodology is presented in order to reduce the gap between the strategic and planning stage. Their approach is illustrated using a case study from a multinational agrochemicals company. Recently, Al-Qahtani and Elkamel (2009) develop a mathematical programming tool for the simultaneous design of an integrated network of refineries and petrochemical processes. The model establishes the design of an optimal petrochemical process network from a range of process technologies to satisfy a given demand. A polyvinyl chloride complex is used to illustrate the economic potential and trade-offs involved in the optimization of the network. The objective is to minimize the annualized cost over a given time horizon.

Lasschuit and Thijssen (2004) describe a Linear Programming (LP)/ Non-Linear Programming (NLP) based branch and bound algorithm for the strategic and global planning of a network of manufacturing plants. The objective is to minimize total SC costs using the toolset known as Global Manufacturing and logistics Optimization System/Network analysis and Supply chain optimization System (GMOS/NetSim).

Ryu and Pistikopoulos (2005) propose a SC design model which can use three different operating policies, namely: cooperation (one market-one plant), coordination (one product-one plant) and competition (free commission). A MILP formulation is used to addressed this problem. They conclude that the optimal policy depends on the market conditions of each case.

The flexible process networks framework (Bok, Grossmann, & Park, 2000) is extended to tackle SC design problems by You and Grossmann (2008). They address SC design optimization considering responsiveness and NPV as the objectives to be maximized. The authors quantitatively analyze how network configurations may have an effect on the responsiveness to market changes.

Ferrio and Wassick (2008) present an approach which is aimed to the re-design of existing SC networks. Their model consists in a single period network design MILP model for multi-product SCs considering three echelons (processing plants, distribution centers and customers). Direct shipping and product flows among plants and/or distribution centers are taken into account, but the potential linkages must be predefined. Naraharisetti, Karimi, and Srinivasan (2008) present a MILP approach for SC redesign considering the alternative of disinvestments. They illustrate the financial impact of ignoring disinvestment and/or relocation decisions for a multinational corporation case study.

Mele, Guillén-Gosálbez, Espuña, and Puigjaner (2007) consider a SC agent-oriented simulation system to solve the retrofit and design problem of a production/ distribution network under uncertainty. The starting point is a set of possible network structure options. The performance of each SC configuration is assessed through a multi-agent model that is coupled with a genetic algorithm in order to optimize the operation variables associated to each design candidate.

Enterprise-wide networks have been designed using P-graphs in the work of Fan, Kim, Yun, Park, Park, Bertok, and Friedler (2009). P-graph is a graph-theoretic method that has proved to be efficient for process-network synthesis. The method simultaneously yields not only the optimal but also the near-optimal networks in a ranked order in terms of the objective function. This approach has as advantage that the computation time does not exponentially increase with the network complexity; however, further improvements may be done to deal with inventory and mass balance constraints.

Most of the strategic SC models discussed here inherently considered a given SC superstructure. For instance, they do not considered materials flows among entities belonging to the same echelon type (i.e., distribution centers, manufacturing plants). Even more, the possibility of direct flows from upper to not immediate subsequent echelons is scarcely addressed. Additionally, production decisions used to be confined to final products. To date, intermediates and its relation to final products are virtually disregarded in SC models. Hence, further research should be devoted to overcome these current drawbacks in strategic SC modeling.

Tactical level

Planning a SC is a very complex task. Among other things, SC managers are responsible for planning manufacturing processes, selecting appropriate technology within available equipment, determining material flows between echelons, allocating products, and monitoring control systems. Time horizons are up to several months in length. SC planning considers a fixed infrastructure over a short- to medium-term, and seeks to identify how best to use the production, distribution and storage resources to respond to demand (Shah, 2005). Here, a rough capacity planning is carried out, as processing times are typically smaller that the time period unit used at this level.

Wilkinson, Cortier, Shah, and Pantelides (1996) describe a continent-wide industrial case study. This involved optimally planning the production and distribution of a system with 3 factories and 14 market warehouses and over 100 products. It is found that the ability of the model to capture effects such as multipurpose operation, intermediate storage and changeovers give rise to counter-intuitive results, such as producing materials further away from demand points than expected. This shows that the complexity associated with producing many products in each factory may be balanced with the extra distribution costs incurred by concentrating the manufacture of specific products at specific sites.

McDonald and Karimi (1997) deal with a multi-period midterm sourcing and production planning model for semicontinuous multiproduct single-stage processes. The outputs of the model are the assets allocation over the planning horizon. They explore the implications of the incorporation of minimum run length constraints.

Swaminathan, Smith, and Zadeh (1998) present a modeling and simulation framework for developing customized decision support tools for SC planning. They use agents to represent SC entities (e.g., customers, manufacturers, transportation). These agents use different interaction protocols and help in simulation of material, information, and cash flows. The agents use various control policies to manage inventory, procure components, and determine optimal transportation routes. The simulation model is then used to analyze different re-engineering options, such as changing inventory control policies, for a company. Wan *et al.* (2005) propose a simulation-based optimization framework for analyzing SCs planning under uncertainty. It is presented a case of study with a stochastic model with random transportation time and customer demands in which total cost is minimized. The framework employs a surrogate model together with domain reduction and incremental sampling to extract structure information from noisy simulation results; the SC decisions are then optimized using the surrogate model.

Jackson and Grossmann (2003) develop a Mixed Integer Non-Linear Program (MINLP) model for the production planning and product distribution of several continuous multiproduct plants. The authors apply spatial and temporal decomposition schemes based on Lagrangian decomposition in order to solve large-scale instances of the problem.

Ryu and Pistikopoulos (2007a) employ a two-level optimization framework for the planning of SCs. At first, they allocate aggregated demand into the SC entities by using one of the policies presented in their previous work (Ryu & Pistikopoulos, 2005). Secondly, on the basis of the assigned demand, single-site planning problems are then constructed for individual entities.

Neiro and Pinto (2004) present a work that propose an MINLP for modeling petroleum SCs. Processing units are modeled based on the framework developed by Pinto, Joly, and Moro (2000) and particular frameworks are proposed to storage tanks and pipelines. Shulz, Diaz, and Bandoni (2005) also formulate a SC model for a petrochemical complex as a multiperiod MINLP. The model includes production, product delivery, inventory management and decisions such as individual production levels for each product, as well as operating conditions for each plant in the complex. The objective function is the maximization of total profit for the entire site. Kuo and Chang (2008) report an integrated MILP for the coordination of various planning and scheduling decisions in a petroleum SC. The MILP model yields the proper procurement scheme for crude oils, the production schedules, and the corresponding logistics decisions.

Recently, some works are modeling the SC physical distribution in more detail. A SC problem consisting of production planning and distribution scheduling in two tiers is presented by Mokashi and Kokossis (2003). A decomposition of the overall problem into aggregate production planning and 2-echelon distribution scheduling is proposed. The two individual problems are solved by applying customized dispersion algorithms on graphs that represent their constraints and objectives in the form of connections between vertices and its weights. Results are presented for an industrial case study making comparisons with ad-hoc methods for these individual problems. Al-Ameri, Shah, and Papageorgiou (2008) formulate a MILP for a Vendor Managed Inventory (VMI) problem using a modified version of the Resource-Task-Network (RTN) representation (Pantelides, 1994). They propose an aggregated and a detailed model which encompass together production, transportation and inventory decisions. The models are integrated by means of a rolling horizon approach. Verderame and Floudas (2009) extend their previous single-site planning formulation (Verderame & Floudas, 2008) to explicitly take into account transportation tasks and multiple sites. The authors develop an multi-site operational *planning with production disaggregation model* that generates daily production and shipment profiles so that capacity, along with the demand requirements, are concurrently considered. The proposed model is a MILP discrete-time formulation, however duration constraints are included to capture the continuous-time nature of SC tasks.

Berning, Brandenburg, Gürsoy, Kussi, Mehta, and Tölle (2002) shows a manner of approaching the planning- scheduling problem in the chemical process industry involving batch production. Their work addresses three distinct aspects: a scheduling solution obtained from a genetic algorithm based optimizer, a mechanism for collaborative planning among the involved plants, and a tool for manual updates and schedule changes. The implementation of a collaborative planning model allows a distributed decision making and access to the production schedule at the various involved plants . A "chain planner" who is authorized to look at production schedules of multiple plants simultaneously is introduced so as to be a system support for conflict management. Even though, the works of Sung and Maravelias (2007) and Erdirik-Dogan and Grossmann (2007) are dealing with single-site planning and scheduling integration it is important to mention that their approaches may be further exploited in a SC environment. Sung and Maravelias (2007) develop off-line approximating functions for the production feasible targets and production cost. These approximate functions merely involved production planning variables and are created using convex hull approximations for the STN formulation. Erdirik-Dogan and Grossmann (2007) develop a planning model that considers minimum changeover time sequencing constraints. More accurate production plans are obtained by using this model. To reduce the computational expense of large scale problems, they introduce a relaxed version of the model and the utilization of a rolling horizon approach.

Finally, Raj and Lakshminarayanan (2008b) develop a performance assessment and improvement framework for decentralized distribution networks. The proposed methodology aims at identifying the problematic nodes in order to revise and optimize their inventory policies and parameters. Later on, Raj and Lakshminarayanan (2008a) expand their model to account for different objectives by using a multi-objective genetic algorithm approach.

Again, similarly to the strategic level, models discussed here inherently considered a given SC superstructure for the material flows, thus preventing from exploring new potential value-effective planning alternatives. Also, a better representation of production process is required at the SC level for activities planning. Another topic that deserves more research is the not centralized SC planning. There are works addressing such a problem, though how to achieve optimal or near optimal solutions for this kind of problems where not all SC entities related data is available is still an open research subject.

Operational level

On this short-term level, decisions are associated to programming-scheduling issues. The scheduling of production facilities can be generally defined as a decision-making process that answers the questions how, where, and when to produce a set of products in order to satisfy customer demand. How refers to the plant resources required (processing units, steam, electricity, raw materials, manpower, etc.); the question where is answered by allocating every operation to a specific unit; finally, when consists of predicting the start and end times for each operation (Pekny & Reklaitis, 1998). Usually, resources and demand are fixed or known at this level. It is important to notice that the time period unit utilized at this level is typically smaller than task processing times. Therefore, sequencing and assignment decisions are addressed here instead of a rough capacity problem which is considered at higher decision levels (i.e., strategic and tactical levels).

Single-site detailed scheduling has been an active area in the process engineering in the last decade (Shah, 1998). However, few works can be found in the literature considering the multi-site scheduling problem due to the high complexity when attaining this sort of problems. A recent review of single-site short-term scheduling can be found in Méndez, Cerdá, Grossmann, Harjunkoski, and Fahl (2006).

A multi-period optimization model for addressing the SC optimization in continuous process networks is proposed by Bok *et al.* (2000). The main feature of this study is that detailed operational decisions are considered over a short time horizon ranging from 1 week to 1 month. A bi-level decomposition algorithm has been proposed that reduces a large original problem into a smaller *relaxed problem* and a smaller *sub-problem*. Decisions for purchasing raw materials are made in the relaxed problem in which the changeover constraints are relaxed. In the sub-problem, fixing the decisions predicted in the relaxed problem, the SC optimization is performed with non-relaxed job changeovers constraints.

Jetlund and Karimi (2004) consider the maximum-profit scheduling of a fleet of multi-parcel tankers engaged in shipping bulk liquid chemicals. For this, they present a MILP formulation using variable-length slots and propose a heuristic decomposition algorithm that obtains the fleet schedule by repeatedly solving the base formulation for a single ship.

Guillén-Gosálbez, Espuña, and Puigjaner (2006b) use the State- Task- Network (STN) representation to tackle a SC scheduling problem under uncertainty. The resulting MILP formulation is solved using an approximation strategy based on the rolling horizon approach and the deterministic solution of the model. Recently, Amaro and Barbosa-Póvoa (2008b) address the optimal scheduling of SCs considering transportation operations and policies. A discrete MILP formulation is used to solve the problem which includes compatibility and capacity constraints to model transportation tasks.

Additionally, it is important to point out a graphical approach, S-graph, to tackle chemical processes scheduling which has been used in single sites problems so far. S-graph is a scheduling approach that has proven to significantly reduce the computational effort compared to mathematical programming techniques. It allows for the formulation of scheduling problems using similar graph representations as those used to solve the job-shop problem but contemplating the higher complexity of the chemical multipurpose batch scheduling (Sanmartí, Puigjaner, Holczinger, & Friedler, 2002). Eventually, such an approach may be extended to cope with scheduling problems in a SC scenario.

Finally, efficient distribution systems is another important open challenge at the operational level. Usually, transport operations are oversimplified assuming simple distribution processes (e.g., unlimited number of available vehicles, no time-windows limitations). This problem has been of intensive research activity in the operations research arena (Savelsbergh & Sol, 1995). However, there is scarcity of research addressing the transportation problem from a multi-site fashion. In the PSE community, Dondo, Méndez, and Cerdá (2008) develop an exact MILP for the multiple vehicle time-window-constrained pickup and delivery problem for multi-site environments. The proposed optimization approach is capable of handling transport requests with multiple origins and/or destinations, heterogeneous vehicles and multiple depots. For large instances of the problem, a model-based neighborhood search framework that iteratively improves a starting solution is developed. The coordination of production and distribution activities is an open field in SCM as well. An example of a work addressing this problem is the one of Bonfill, Espuña, and Puigjaner (2008). The authors present a methodology to sequentially coordinate production and distribution tasks. Such framework is coupled with a procedure to identify transport schedules based on different combinations of transport rules.

The scheduling/distribution problems are cumbersome in a single site context, needless to discuss about the complexity of scheduling/distribution problems which attain multiple sites in tandem as it is the SC case. Therefore, one of the main research issues at operational level, it is to develop strategies to reduce the high computational effort required to find optimal solutions for the overall problem. Additionally, notice that works addressing the integration of strategic and tactical decisions or tactical and operational decisions can be found in the literature, however the implications of considering scheduling details while designing a SC have not been yet comprehensively analyzed. Research devoted to this issue should be fostered.

2.3.2 Integration of decisions from different business functional areas

Integrated SCM involve making trade-offs between more than one business function within the firm. A close cooperation between the different functional units is a prerequisite being no matter of course in today's firms (Stadtler, 2002). Recent advances in PSE have focused on devising enterprise wide modeling and optimization strategies that integrate decisions of distinct functions of a business into a global model. Nevertheless, despite the effort made in the area, almost all of the models developed to date focus on the process operations side and neglect decisions involving marketing campaigns, investment planning, corporate financial decisions, and many others aspects of enterprise planning related to SCM (Shapiro, 2004).

Following, it is a brief revision of the approaches that endeavor to support the decision making process of different business functionalities, whether the addressed problem belongs to the single site or SC context.

Corporate finances and international issues

The effective control of cash is one of the most important requirements of financial management and its steady and healthy circulation throughout the entire business operation has repeatedly been shown to be the basis of business solvency (Howard & Upton, 1953). In fact, the availability of cash governs the production decisions taken in a company. For this reason, operative models should not consider cash as an infinite resource. A production plan cannot be implemented if it violates the minimum cash flow imposed by the firm (i.e., if the amount of raw materials and/or utilities required cannot be purchased due to a temporary lack of cash). Recently, there is an increasing awareness of the impact that chemical process production systems have on the financial area of the firms.

Badell, Romero, and Puigjaner (2004) build a framework that combines a deterministic cash flow management model with a scheduling algorithm using a MILP formulation. The modeling framework created can support the budgeting activity of firms. The model's objective function represents the value of net revenues obtained from cash transactions over the entire planning horizon. The model allows satisfaction of customer due dates while evaluating transaction costs; incorporating prompt payment discounts if possible; using the line of credit; delaying selling of marketable securities as long as possible, but selling them if it is necessary to secure a discount. As a result, a cash budget is determined that encompasses all aspects of plant cash flow management. Financial decisions such as the best timing of payments, investments and sales of marketable securities are included. This work is extended by Guillén-Gosálbez *et al.* (2006a). Here, it is addressed the integrated planning/scheduling of chemical SCs with multi-product, multi-echelon distribution networks taking into account financial management issues. This work presents a new measure of the effectiveness of a production plan and schedule, based on an economic performance indicator (change in equity) as an alternative to the commonly used makespan, profit, or cost.

Gjerdrum, Shah, and Papageorgiou (2001) have developed an approach to sustainable profit sharing in a n-enterprise SC. A separable programming approach, which utilizes the game theoretical fair bargaining concepts developed by Nash (1950) and Harsanyi (1977) is presented. Semicontinuous transfer prices have been used in order to distribute profits between SC partners. The proposed model is a MINLP problem aiming to determine production resource utilization, production levels, inventory levels, flows, and transfer prices of the products in the SC network so as to maximize the profit levels of the separate enterprises fairly. Vidal and Goetschalckx (2001) formulate a bilinear model to maximize the after tax profits for multinational companies considering transfer prices in the SC. They developed a heuristic procedure that applies successive linear programming based on the reformulation and the relaxation of the original problem. On a later work, Chen *et al.* (2003) build a multiproduct, multistage, and multiperiod production and distribution planning model to maximize the profit of each participant enterprise, to maximize the customer service level, to minimize the safe inventory level, and to ensure a fair profit distribution. A two-phase fuzzy decision-making method is proposed to attain a compromise solution among all participant companies of the SC. Methods for finding a Pareto-optimal solution are thus filled with subjective and fuzzy properties. The model is then formulated as a multi-objective MINLP problem.

Oh and Karimi (2004) introduce and classify the major regulatory factors that can influence strategic decisions in the design and operation of chemical SCs. They model and highlight the effects of two important regulatory factors, corporate tax and import duty, in the capacity-planning decisions. The proposed model treats the sizes of capacity expansions and new facility capacities as decision variables and incorporates SC operation decisions, such as sourcing of raw materials and facility production rates, that can eventually affect the strategic capacity-planning decisions. Finally, the authors extend the deterministic model to solve the problem in which demand and import duty are uncertain. In order to deal with uncertainty, a scenario-based two stage stochastic technique is utilized. In a later work, Oh and Karimi (2006) extend their model to include duty-drawbacks which is a refund of import duty, when the material is destroyed, exported, or consumed as a raw material to produce an exported material.

Yi and Reklaitis (2004) present an integrated analysis of production and financing decisions. A model is constructed in which a cash storage unit is installed to manage the cash flows associated with production activities, such as raw material procurement, process operating setup, inventory holding costs and finished product sales. The SC is modeled as a batch-storage network with recycling streams. The expressions for the Kuhn-Tucker conditions of the optimization problem are reduced to a subproblem and analytical lot-sizing equations. The objective function is to minimize the opportunity costs of annualized capital investment and cash/material inventory minus the benefit to stockholders. In their more recent work, Yi and Reklaitis (2007) develop a model in which multiple currency storage units are installed to manage the currency flows associated with multinational SC activities. Temporary financial investments, bank loans, and currency transfer between multiple nations are allowed to increase the marginal profit. The contribution of this study is its quantitative investigation of the influence of exchange rates and taxes on operational decisions.

Most of SC models in general still considered cash as an unlimited resource, only very few of them incorporate cash flows into the modeling approach (e.g., Badell *et al.*, 2004; Guillén-Gosálbez *et al.*, 2006a; Yi & Reklaitis, 2004, 2007). Notice that international issues have been already incorporated, but most of such models still use profit and cost as SC performance indicators. As it has been stated in Chapter 1, integrated SCM is expected to be a key area to propel value generation and sustainability. However, corporate finances decisions, international issues, and SC models integration impact on value generation has not been fully studied. Indeed, there has not been presented how to explicitly measure firm's value as a function of financial and SC operations decisions.

Product development

The product Research and Development (R&D) functionality include activities such as R&D portfolio management, project management and resource management. In the context of R&D pipeline management, strategic planning deals with the selection of an attractive portfolio of research projects considering capital budgeting limitations, while tactical planning refers to the temporal assignment(i.e., prioritization and allocation) of limited resources to the tasks that are required for the actual execution of a portfolio (Subramanian, Pekny, & Reklaitis, 2001). Ideally, all these decisions need to be coordinated. However, this is often not the case, leading to sub-optimal portfolios and ineffective utilization of capital and R&D resources (Varma *et al.*, 2007). What is more, these decisions impact the current and ordinary activities of SC members. Thus, such operational impact should be assessed and considered when making R&D decisions.

In a pioneering work, Schmidt and Grossmann (1996) address the optimal scheduling of testing tasks in the new product development process. They do not take into account the interaction with production capacity in their model. In a later work, Maravelias and Grossmann (2001) address the problem of simultaneous optimization of resource-constrained scheduling of testing tasks in new product development and design/planning of batch manufacturing facilities. The proposed MILP model integrates a continuous scheduling model for testing with a discrete model for design/planning. A two-stage stochastic optimization approach is adopted to account for the uncertainty in the outcome of the tests. The model predicts which products should be tested, the detailed test schedules that satisfy resource constraints, design decisions for the process network, and production profiles for the different scenarios defined by the various testing outcomes. To solve larger instances of this problem with reasonable computational effort, a heuristic algorithm based on Lagrangian decomposition is proposed.

Papageorgiou *et al.* (2001) describe an optimization-based approach to choose both a product development and introduction strategy and a capacity planning and investment strategy for cases especially related to pharmaceutical sector. The overall problem has been formulated as an MILP model adopting the maximization of the NPV over the horizon of interest. This takes account of both the particular features of pharmaceutical active ingredient manufacturing and the global trading structures. In this work, trading structures are concerned with decisions related to the financial flows between different components of the company. In particular, transfer pricing issues among the various manufacturing and commercialization business centers are modeled. Later on, Levis and Papageorgiou (2004) develop a two-stage stochastic MILP that considers clinical trials outcomes and the customer demand as uncertain parameters. The trading structure of pharmaceutical SC is taken into account as well. A hierarchical algorithm is proposed in order to reduce the computational effort needed for the solution of the resulting MILP problem.

Fandel and Stammen (2004) extend the SC network of procurement, production, distribution and sales to a product life cycle by introducing the business processes of development and recycling. A general MILP model is designed considering the business processes of a product life cycle. Essential modeled elements of this business process are the development projects from which the new marketable products are created and the development centers at which the development projects are carried out. The goal of this approach is to optimize after-tax profit of a company and to fix the product program for the extended SC network.

Sundaramoorthy and Karimi (2004) present a multiperiod, continuous-time, MILP model that addresses product pipeline problem for pharmaceutical plants using multiple parallel production lines in campaign mode and producing products with multiple intermediates. It is addressed a SC planning problem to assess the feasibility or profitability of introducing new active ingredients or intermediates in a pharmaceutical plant. Given a set of due dates, demands for products at these due dates, and several operating and cleaning requirements, the aim is to determine the optimal production levels of various intermediates (new and old) or the optimal outsourcing policy to maximize the overall gross profit for the plant, while considering in detail the sequencing and timing of campaigns and material inventories.

Subramanian *et al.* (2001) develop a computing architecture called Sim-

Opt to deal with the R&D pipeline management problem. Sim-Opt generalizes traditional discrete event simulation to embed a more sophisticated decision capability. Instead of using local rules for decision making, the Sim-Opt approach uses an optimization formulation which depends on the specific state of the simulated system. This work is extended to integrate information from the simulation to improve the optimization problem solution (Subramanian, Pekny, Reklaitis, & Blau, 2003). The authors develop a three step heuristic that improves solutions in terms of expected NPV and the probability of delivering a positive NPV. Finally, Zapata, Varma, and Reklaitis (2008) present a multi-phase version of this simulation optimization architecture. The first, learning phase follows an optimization strategy; whereas the second, execution phase uses resource allocation and scheduling policies. These policies are generated at the end of the learning strategy by using a learning strategy such as statistical inference, path analysis or neural networks.

Recently, Colvin and Maravelias (2008) treat the uncertainty associated with the outcome of clinical trials as endogenous. A multi-stage stochastic programming formulation for the planning of clinical trials in the pharmaceutical R&D pipeline is developed. One of the contributions of this work is the reduction of the number of non-anticipativity constraints necessary to model indistinguishable scenarios.

Most of the models developed so far do not consider the uncertainty associated to the outcomes of clinical trials as endogenous. The consideration of this aspect may considerably vary the solution to this kind of problems. Again, given the capital-intensive and strategic nature of product development, its associated decisions should be assessed taking into account their impact on value generation. What is more, product development decisions imply to eventually introduce new products into the firm's portfolio. So, product development impact on decisions associated to equipment capacity expansion and utilization should be assessed as well. Models covering these aspects are still to be constructed.

Environmental management

Nowadays, a proper handling of SCM should be concerned with the sharing of responsibility from various aspects of performance. It has been realized that significant improvements in terms of environmental performance and market competitiveness may be achieved by concentrating efforts from all SC partners. Actually, managerial practice related to environmental issues has expanded from a narrow focus on pollution control within a single site to include a larger set of inter-organizational management decisions, programs, tools, and technologies that prevent pollution before its generation (Klassen & Johnson, 2004). Consequently, these issues are being considered in recent works and call for further research in the integration of environmental management with ongoing SC operations.

The aforementioned integration may be achieved through the emerging concept regarded as "Green Supply Chain Management" (GrSCM), defined as the integration of environmental thinking into SCM, including product design, material sourcing and selection, manufacturing/processing equipment selection, delivery of final product to the consumers as well as end of life management of the product after its useful life (Srivastava, 2007). Traditionally, the optimization models devised to assist operation and design in the chemical processing industry have concentrated on finding the solution that maximizes a given economic performance indicator while satisfying a set of operational constraints imposed by the topology of the plant. In recent years, however, there has been a growing awareness of the importance of including environmental and financial aspects in the optimization procedure (Puigjaner & Guillén-Gosálbez, 2007). A recent review of GrSCM can be found in Srivastava (2007).

Zhou, Cheng, and Hua (2000) propose an approach for sustainable SC optimization of continuous process industry. Goal Programming (GP) model is utilized to address this multi-objective problem with the integration of non-relaxable constraints and relaxable constraints. The analytic hierarchy process (AHP), a multi-objective decision making method, is used to evaluate the priorities of goals and weights of deviation variables. The objectives included are: economic sustainability, social sustainability (i.e., satisfaction of market demands), resource sustainability (i.e., material and energy consumption, facilities utilization) and environmental sustainability (i.e., amount of hazardous waste generated, amount of recovered materials and energy usage).

Türkay, Oruç, Fujita, and Asakura (2004) report a systematic approach to address the exchange of steam and electricity of companies in the same industrial zone. The proposed approach consists of modeling process units using fundamentals of thermodynamics, conservation of mass and energy and process data so as to develop a MILP model for the SC integration of different process systems. Environmental issues are not included as objective function, but limits on the SO_x emission are taken into account. This work is later extended to include investment cost, and green house gases emission constraints (Soylu, Oruç, Türkay, Fujita, & Asakura, 2006).

Hugo and Pistikopoulos (2005) address the environmentally conscious process selection problem for the long-range planning and design of chemical SC networks. They present a mathematical programming-based methodology for the explicit inclusion of Life Cycle Assessment (LCA) criteria as part of the strategic investment decisions related to the design and planning of SC networks. By considering the multiple environmental concerns together with the traditional economic criteria, the planning task is formulated as a multi-objective MILP problem. At the strategic level, the methodology addresses strategic decisions involving the selection, allocation and capacity expansion of processing technologies and assignment of transportation links required to satisfy the demands at the markets. At the operational level, it determines optimal production profiles and flows of material between various components within the SC.

A discrete event-driven model approach is proposed by Puigjaner and coworkers (Mele, Espuña, & Puigjaner, 2005a; Mele *et al.*, 2006a,b; Puigjaner & Espuña, 2006) to address the sequential decision-making problem under uncertainty at the tactical level. The model contemplates each SC entity as an agent whose activity is described by a collection of states and transitions. Financial and environmental aspects are incorporated into the objective function (Puigjaner & Guillén-Gosálbez, 2007). Environmental criteria is incorporated by using an LCA approach.

Recently, Guillén-Gosálbez and Grossmann (2009) address the SC design explicitly accounting for the uncertainty of released emissions and feedstock requirements associated with the SC operation. The problem is formulated as a stochastic MINLP that includes NPV and the Eco-indicator 99 as objective functions. The stochastic model is converted into its deterministic equivalent by reformulating the probabilistic constraint required to calculate the environmental impacts. The resulting deterministic MINLP is further reformulated as a parametric MINLP.

Obviously, nowadays the environmental impact associated to SC decisions at all levels is of high significance. However, approaches that address the environmental impact evaluation at the operational level (scheduling and distribution) are scarce. On the other hand, as stated by Papageorgiou (2008), there is an increasing interest in reverse logistics and closed loop SCs mainly because they are expected to diminish firms environmental burden. Notwithstanding, most of the approaches developed so far do not assess the environmental reward or impact of such kind of operations (Fleischmann *et al.*, 2001; Schultmann *et al.*, 2003; Amaro & Barbosa-Póvoa, 2008a).

Sales and Marketing

To be successful, the enterprise does not only need to focus on the SC, but also on the demand chain. Understanding the market and customer conditions is extremely crucial for making a good business policy. Sales and marketing function is responsible for direct customer interface and pricing. Sales and marketing makes decisions on sales force deployment based upon the existing market shares, product offerings, marketing costs and budgets. Marketing is a boundary-spanning function, linking the selling organization with buyers and channel intermediaries. Thereby, to operate most effectively, its activities must be coordinated with other functional areas of the firm. Nevertheless, in most companies pricing and promotional decisions are typically made by the marketing and sales functional units, usually without regard to the impact of these decisions on the SC performance. For these reasons, an appealing area that has recently begun to call for research is the marketing-production interface.

A very early work that addresses the coordination of replenishment strategies and pricing policies is presented by Whitin (1955). A model is proposed to analyze the well-known newsvendor problem with price dependent demand. In a more recent piece of work, Chen and Simchi-Levi (2002) analyze a general inventory-pricing model. Specifically, they consider a finite horizon, periodic review, single product model with stochastic demand. Demands in different periods are independent of each other and their distributions depend on product price. Pricing and ordering decisions are made at the beginning of each period, and all shortages are backlogged. The objective is to find an inventory policy and pricing strategy that maximizes expected profit over the planning horizon.

Guillén-Gosálbez, Bagajewicz, Sequeira, Espuña, and Puigjaner (2005a) introduce a strategy for integrating pricing with scheduling decisions for batch plants. The starting point is the modeling and forecasting of the relationship between product prices and demand. A two-stage stochastic mathematical model is developed in order to address the uncertainty associated to the market demand. Also, Guillén-Gosálbez *et al.* (2005c) describe a novel strategy for evaluating offer proposals in production and distribution networks with embedded multi-product batch plants. The proposed approach represents a preliminary step that should be applied before the negotiation process starts, and suggests a set of values for delivery time and price that the supplier can offer when negotiating with a customer. For each of these offer parameters, the SC schedule that optimizes the expected profit of the SC is provided. The solutions provided by this strategy weigh the expected profit and the quality of the offer (e.g., the customer satisfaction that the offer will provide the client). The problem is formulated as a stochastic MILP optimization in which future demand and prices are represented by a set of scenarios.

As it can be noticed, the integration of SC and marketing decisions calls for more attention. It is widely recognized the relevance of such integration, but evidently more research efforts are require to take advantage of the relationship among pricing, promotion and production capacity utilization. The synchronization of these decisions may turn out in a more value-effective planning. Furthermore, both sets of decisions (i.e., marketing and SC operation decisions) must be driven by the common objective of enhancing firm's value.

2.3.3 Decision making under uncertainty

The approaches devised so far to address the problems under uncertainty can be generally classified into two groups: reactive and preventive procedures. The work done following both approaches is discussed in detail in the following sections.

Reactive approaches

Reactive approaches attempt to modify a nominal plan obtained by a deterministic formulation so as to adjust it to changes. In general, reacting to unexpected events is a complex task as various inter-related resources and materials may required to be re-planned/re-scheduled when such a event occurs. Moreover, a new modified plan or scheduled usually should be obtained in a short time. Rule based methodologies, heuristics and intelligent agents, are commonly used to perform the required modifications due to their typical reduced computational times in comparison with mathematical programming techniques. However, rule based methods are problem-specific and consequently difficult to extend.

For instance, Adhitya, Srinivasan, and Karimi (2007a) report a heuristic based re-scheduling for refinery operations. They broke a schedule into operation blocks. Rescheduling is performed by modifying these blocks in the original schedule using simple heuristics to generate a new schedule that is feasible for the new problem data. In another work, Adhitya, Srinivasan, and Karimi (2007b) develop a model-based approach for rescheduling SC operations in response to disruptions. In this approach, the cause-and-effect relationship between all possible SC operations is modeled using a composite-operations graph which represents all possible material-flows among SC entities. The subset of operations that are originally scheduled during a time-horizon is represented in the Scope graph. The consequences of any disruption are manifested as violations in the Scope-graph. Different options to overcome these violations are generated and captured in the rectifications graph by using a greedy approach. The best one that optimizes total profit is proposed as the new schedule. While seeking rectifications, modifications of variables are propagated and new violations are detected. A new schedule is proposed only when all violations have been rectified. Otherwise, a number of researchers (Duffie & Piper, 1987; Lin & Solberg, 1992) have proposed agent based re-scheduling systems, where a bidding mechanism is used to resolve conflicts between different agents (e.g., machines). While the analogy to free-market economics is interesting, this approach still requires that the objectives of the individual agents be set in a manner that will ensure good overall system performance, which is still not clear how to do (Aytug, Lawley, Mckay, Mohan, & Uzsoy, 2005).

Additionally, Model Predictive Control (MPC) has been also applied to SC problems as a reactive approach. MPC is a control strategy based on the explicit use of a process model to predict the process output (performance) over a long period of time (Camacho & Bordons, 1995). The model attempts to predict the control variables for a set of time periods. Predicted control variables depend on disturbance forecasts (i.e. demand, prices, and interest rates) and also on a set of given parameters that are known in the control literature as control inputs. The MPC algorithm attempts to optimize a performance criterion that is a function of the future control variables. By solving the optimizing problem all elements of the control signal are defined. However, only a portion of the control signal, the portion corresponding to the following time period, is applied to the system. Next, as new control input information and disturbance forecasts are collected, the whole procedure is repeated, which produces a feed-forward effect and enables the system to counteract the environment dynamics. The procedure is illustrated in Figure 2.2.

Bose and Pekny (2000) present a model predictive approach for solving planning and scheduling problems under uncertainty. The proposed framework utilizes three components: a forecasting, an optimization, and a simulation model. The forecasting and the optimization (scheduling) models work in tandem in a

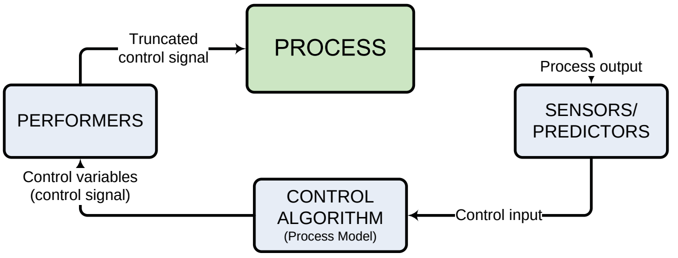


Figure 2.2: Simplified schematic of MPC

simulation environment that incorporates uncertainty. The similarity with the model predictive approach is that in each period, the forecasting model calculates the target inventory (controlled variable) for the future periods. These inventory levels ensure desired customer service level while minimizing average inventory. The scheduling model then tries to achieve these target inventory levels in the future periods by scheduling tasks. They study the interaction among the parts of SC by analyzing different coordination structures (i.e., centralized, decentralized SCs).

Perea-López, Ydstie, and Grossmann (2003) suggest a dynamic analysis model for SCs with multiproduct, multiechelon distribution networks, multiproduct batch plants and a global SC coordinator. The proposed multiperiod MILP model was implemented with an MPC. It takes advantage of a rolling horizon approach to quickly update the decisions whenever changes in the forecasts of the demand arise. The rolling horizon allows them to solve problems of considerable size and in a short time because of the finite horizon it uses. This work uses the same dynamic characterization as in Perea-López *et al.* (2001), which defines inputs, outputs, states and disturbances for the SC dynamic system.

A two-layered optimization-based control approach for multi-product, multiechelon SC networks is presented by Seferlis and Giannelos (2004). The control strategy applies multivariable model-predictive control principles to the entire network while maintaining the safety inventory levels through the use of dedicated feedback controllers for each product and storage node. The optimization-based controller aims at maximizing customer satisfaction with the least operating costs. The inventory controllers are embedded within the optimization framework as additional equality constraints. The performance of the suggested two-layered control strategy is compared to a single layered control scheme that does not use inventory feedback controllers at the inventory nodes.

Braun, Rivera, Flores, Carlyle, and Kempf (2003) examine the efficacy of different information sharing structures using a MPC framework, the benefits of placing penalties on the rate of change in variables (i.e. move suppression term) under conditions of uncertainty is explored as well. A three-echelon network developed by Intel Corporation which mimics the back end configuration of a semiconductor chain is used as example. Later on, a more extensive application of MPC to the semiconductor SC is presented by Wang, Rivera, and Kempf (2007). The effectiveness of this approach is demonstrated using three benchmark problems developed by Intel scientists.

Recently, Mestan, Türkay, and Arkun (2006) address the optimal operation of multiproduct SC systems using model predictive control. The SC considered is a hybrid system governed by continuous/discrete dynamics and logic rules. For optimization purposes, it is modeled within the framework of the mixed logical dynamical system and the overall profit is optimized through an MPC. Dynamic responses of the different nodes of the SC are analyzed when the SC is subjected to unknown changes in customer demand. The performances of a centralized decision-making scheme and two types of decentralized decision making schemes are compared. Centralized MPC configuration results in better inventory management and production scheduling. The effects of including move suppression control strategy and information sharing, on the performance of decentralized SC configurations are investigated.

Another reactive approach is multi-parametric optimization whose origins can be traced in Fiacco (1983). In an optimization framework, where the objective is to optimize a performance criterion subject to a given set of constraints and where some of the parameters in the optimization problem are uncertain, parametric programming is a technique for obtaining (i) the objective function and the optimization variables as a function of the uncertain parameters, and (ii) the regions in the space of the parameters where these functions are valid. With such a complete map of optimal solutions, as the operating conditions fluctuate, one does not have to re-optimize for the new set of conditions since the optimal solution as a function of parameters (i.e., the new set of conditions) is already available (Pistikopoulos *et al.*, 2002). A very recent review of multi-parametric programming and its futures challenges can be found in Pistikopoulos (2009).

Multi-parametric programming has been applied to PSE problems such process synthesis (Acevedo & Pistikopoulos, 1996; Banerjee & Ierapetritou, 2003), scheduling (Li & Ierapetritou, 2007; Ryu, Dua, & Pistikopoulos, 2007; Ryu & Pistikopoulos, 2007b), and predictive control (Pistikopoulos *et al.*, 2002; Dua, Kouramas, Dua, & Pistikopoulos, 2008). The only work that shows the application of multi-parametric programming to SC problems is the one of Ryu, Dua, and Pistikopoulos (2004). This work presents a bilevel programming framework to capture conflicting interests of multiple elements in the context of SC planning problems. The proposed bilevel framework is comprised of a upper level problem corresponding to distribution network planning and a lower level to production planning problem. Operation strategies under varying demand are obtained by using parametric optimization techniques. Once demand is realized, the corresponding optimal production policy can be determined.

Under a reactive approach, each time a unexpected event occurs or uncertainty unveils, they are accommodated and a new planning emerges that remains in force until the next unexpected event. A central theme of this research is that of planning repair, namely, the need to have a plan in existence that is feasible at all times. Clearly, this requires the constant monitoring of the SC status against the actual plans, and possibly the interruption of operations while the new plans are generated. As a result, strategies that timely generate new feasible plans are required, that is why (i) heuristics are preferred over optimization strategies and (ii) Multi-parametric programming is a promising tool in this area. However, the use of heuristics has the disadvantage that they cannot usually guarantee convergence and good quality solutions. Here, it is also important to point out that integrating low level supervisory modules with SC models is a need in order to efficiently monitor the SC state. As more reliable information of the SC state is timely gathered, more efficient plans are obtained to face uncertain events.

Preventive approaches

Preventive approaches explicitly take into account uncertainties into the problem formulation. In order to include the description of uncertain parameters within the models, several methods can be used:

- Bounded form. In many cases, there is not enough information to develop an accurate description of the probability distribution that characterize the uncertain parameters, but only error bounds can be obtained. In this case interval mathematics can be used for uncertainty estimation.

- Probability description. This is a common approach for the treatment of uncertainties when information about the behavior of uncertainty is available since it requires the use of probabilistic models to describe the uncertain parameters.

- Fuzzy description. Fuzzy sets allow modeling of uncertainty in cases where historical (i.e., probabilistic) data are not readily available. Fuzzy sets have to be defined for each uncertain variable based generally on subjective judgment and managerial experience. Each element of the set has associated a degree of membership between 0, not at all in the set; and 1, completely in the set.

The most commonly adopted approach in the literature as preventive procedure is the stochastic programming with recourse. In this approach, a solution with the maximum expected performance is obtained by including estimated scenarios in the model; these estimated scenarios are generated by representing uncertain parameters as random variables. The goal is to find a solution that is feasible for all the possible data scenarios and which maximizes the expectation of a performance indicator. The most widely applied stochastic programming models are two-stage programs. In models of this type, the decision maker takes some actions in the first stage, after which a random event occurs and affects the outcome of those first-stage decisions. A recourse decision can then be made in the second stage that compensates for any negative effects that might have been experienced as a result of the first-stage decisions. However, most problems entail a sequence of decisions that must not anticipate future outcomes of the uncertain factors that evolve over more than one time event. A multistage stochastic program is required to rigorously tackle this type of practical problems.

Other preventive approaches are chance constraint programming, fuzzy programming and simulation based optimization (see section 2.2.2). Chance constraint or probabilistic programming focuses on the reliability of the system. Reliability is expressed as a minimum probability requirement on satisfying those constraints which include random parameters. While in fuzzy programming, random parameters are considered as fuzzy numbers and constraints are treated as fuzzy sets. A comprehensive review of optimization under uncertainty can be found in the contribution of Sahinidis (2004).

One important factor influencing business decisions is risk. It should be borne in mind that optimizing the expectation of a performance metric (e.g., NPV, profit and cost) proved to be incompatible with lowering risk measures. The maximization of expected metrics by itself is not an appropriate objective since solutions with higher risk exposure are obtained (Barbaro & Bagajewicz, 2004). Consequently, a quantitative evaluation of risk is desirable in stochastic models in order to manage such a trade-off. An extensive discussion of risk concepts and measures is presented in Bagajewicz (2005). Some of the most relevant risk measures that have been proposed so far are:

- Variability. It is the standard deviation of the expected performance distribution, which is also known as *Robustness* (Mulvey *et al.*, 1995).
- Downside risk. This concept is first introduced by Eppen *et al.* (1989). It is defined as the expected value of the positive deviation from a certain target performance level.
- Financial risk. It is defined as the probability of not attaining a certain target performance level. This concept is considered one of the best ways of defining risk (Barbaro & Bagajewicz, 2004).

Next, some preventive approaches developed to cope with SC problems under uncertainty are examined. Gupta and Maranas (2000, 2003) utilize the framework of mid-term SC planning under demand uncertainty to safeguard against inventory depletion at the production sites and excessive shortage at the customer. A chance constraint programming approach in conjunction with a two-stage stochastic programming methodology is utilized. The second stage recourse function (i.e., inner optimization) is resolved by first obtaining a solution of the problem using linear programming duality followed by expectation evaluation by analytical integration. Analytical expressions for the mean and standard deviation of the inventory are derived and used for setting the appropriate customer demand satisfaction levels in the SC. The key feature of their model is the identification of optimal supply policies under low, intermediate and high demand regimes.

Tsiakis, Shah, and Pantelides (2001) propose a MILP model for the SC design problem under uncertainty. The authors consider demand uncertainties by generating a representative number of scenarios. The decisions to be determined include the number, location, and capacity of warehouses and distribution centers, the transportation links, and the materials flows and production rates. The stochastic system is modeled using a two stage stochastic programming approach. The objective is the minimization of the total annualized cost. Santoso, Ahmed, Goetschalckx, and Shapiro (2005) integrate the sample average approximation (SAA) scheme with an accelerated Benders decomposition algorithm to solve SC design problems with continuous distributions for the uncertain parameters. The viability of the proposed methodology is proved using two real supply chain problems. Later on, Guillén-Gosálbez, Mele, Espuña, and Puigjaner (2006c) address the design of chemical SCs under demand uncertainty by using a multistage stochastic formulation. A decomposition technique is introduced aiming at the objective of overcoming the numerical difficulties associated with the underlying large-scale stochastic MILP. The proposed strategy combines genetic algorithms and mathematical programming tools.

For tactical decisions, Lababidi, Ashmed, Alatiqi, and Al-Enzi (2004) develop an optimization model for the SC of a petrochemical company operating under uncertain demand and market prices. A stochastic formulation is developed, which is based on the scenario based two-stage problem method. First-stage decisions are the production volumes of different products for every planning period, while second-stage decisions are the volumes shipped to demand sources.

In the operational level, Guillén-Gosálbez *et al.* (2006b) present a multistage stochastic optimization model to address the scheduling of SCs with embedded multipurpose batch chemical plants under demand uncertainty. An approximation strategy comprising two steps and based on the resolution of a set of deterministic and two-stage stochastic models is presented in order to overcome the computational effort required to solve this kind of problems. The performance of the proposed strategy is studied through comparison with other traditional approaches (e.g., stand-alone two-stage stochastic programming and two-stage shrinking-horizon algorithms).

Chen and Lee (2004) investigate the simultaneous optimization of multiple conflict objectives and the uncertain product prices problem in a typical SC network with market demand uncertainties. The demand uncertainty is modeled as discrete scenarios with given probabilities for different expected outcomes, and the uncertain product prices are described as fuzzy variables. The problem is formulated as a MINLP model which include objective functions such as fair profit distribution among SC members and maximum customer service levels. A two-level coordination which uses hierarchical inventories control is developed by Xie, Petrovic, and Burnham (2006) for decentralized SCs. The SC system is decomposed into independent subsystems that are individually optimized under fuzzy customer demand. The coordination function is designed to determine the facility whose inventory policy has to be changed in order to improve the SC performance as a whole and to induce changes in subsystems by increasing the shortage cost.

Barbaro and Bagajewicz (2004) apply a risk management tool to the capacity expansion problem with the use of inventory and option contracts. The work shows that the usual assumption that the introduction of inventory reduces risk at low profit expectations is not always true, and that appropriate risk management techniques are needed to accomplish such objectives. The article also shows that the usual assumption that option contracts will by itself reduce the risk exposure at small profits is not always true, and that proper risk management tools are needed for this purpose as well. Later on, a stochastic programming approach based on a recourse model with two stages is proposed by Guillén-Gosálbez, Mele, Bagajewicz, Espuña, and Puigjaner (2005b) to incorporate the uncertainty associated to the demand within the SC design process. The problem objective is assessed by taking into account the profit over the time horizon as well as the resulting demand satisfaction. Their approach enables to consider and manage the financial risk associated to the different design options, resulting in a set of Pareto optimal solutions that can be used for decision-making.

Al-Qahtani, Elkamel, and Ponnambalam (2008) considers uncertainty in process yield, raw material cost, product prices, and product market demand for a Petrochemical SC design problem. Risk is accounted for in terms of variability of benefits and forecasted demand and is included as a cost in the objective function. The problem is formulated as a two-stage stochastic MINLP with nonlinearity arising from modeling the variability. Lakkhanawat and Bagajewicz (2008) introduce an optimization model for refinery planning which integrates pricing decisions. The relationship between product prices and demand are modeled using the microeconomic concept of "utility function". The two-stage stochastic program with fixed recourse consider the demand and client budget uncertainties. Risk management is introduced by using the opportunity value and the value at risk metrics.

A SC planning problem under demand uncertainty is analyzed by Mitra, Gudi, Patwardhan, and Sardar (2008) using chance constrained programming. The planning model of McDonald and Karimi (1997) is adopted. Costs and reliability are considered as objective functions. The multi-objective problem is tackled by using the ϵ-constrained method. You and Grossmann (2008) address the SC optimization under demand uncertainty considering responsiveness and NPV as the objectives to be maximized. They used a chance constraint approach where safety stocks are regarded as model variables which depend on stock out probability. The authors have succeeded in quantitatively analyzing how network configurations may have an effect on the flexibility to respond to market changes. They proposed the expected total lead time as an indicator of responsiveness.

Acevedo and Pistikopoulos (1997) present a very interesting piece of work that could be exploited to address SC problems. In order to reduce the computation burden of solving stochastic MILP problems, decomposition techniques (e.g., Benders decomposition, Lagrangian relaxation, Gaussian quadratures) have been widely applied. These techniques usually decompose the original problem into (i) one master problem and (ii) many subproblems. Each subproblem is associated with one uncertain scenario. The main difficulty of these techniques is the explosion of the number of subproblems as more scenarios are considered. To avoid the repetitive optimization of subproblems at different values of the uncertain parameters, the authors propose to use multi-parametric programming. Thus, the subproblem optimal solution is obtained by just evaluating the functions provided by the multi-parametric solution. Two approaches are examined: in the first approach parametric programming is applied to each master problem solution; whereas in the second approach the first-stage variables are also treated as uncertain parameters so that parametric programming is only applied once in the algorithm. Hené, Dua, and Pistikopoulos (2002) extend this idea to stochastic MINLP problems.

Jung *et al.* (2004) deal with the problem of determining the safety stock level to use to meet a desired level of customer satisfaction using a Sim-Opt approach similar to the one proposed by Subramanian *et al.* (2001). To address this problem they propose an approximate strategy which relies on the use of deterministic SC planning and scheduling models employed in a rolling horizon mode. The deterministic model is built using expected values of future demands and incorporates safety stock levels for each product and site within the inventory balance constraints. In order to determine the customer satisfaction level function, a discrete event simulation of the SC is executed implementing the scheduling plans obtained via the deterministic model for different scenarios. The safety stock level parameters are then adjusted as an outer loop optimization in which the weighted sum of the deviations from the target customer satisfaction levels are minimized. This work is focused on the SC production plants. An extension to multi-stage SCs which considers warehouses operations is reported in Jung *et al.* (2008).

A discrete event-driven model approach is proposed by Puigjaner and coworkers (Mele *et al.*, 2005a, 2006a,b; Puigjaner & Espuña, 2006) to address the sequential decision-making problem under uncertainty at the strategic and tactical levels. The approach considers two important components: an agent-based model used to represent the SC network and a meta-heuristic optimization algorithm that is designed to improve the operation of SC networks. The SC activity is characterized by a set of parameters whose values can be optimized to achieve a better system performance. Genetic algorithms are incorporated as a tool to find parameters values that improve the expected profit over a finite time horizon. After a given number of generations, a meta-model of the SC system is constructed on the basis of the simulator outputs by using neural network technology. Once the neural network is trained, it is used for filtering purposes, so as to reduce computational load associated with number of model simulations.

Here, it is important to point out that two of the main drawbacks of stochastic optimization are the computational effort required to obtain optimal solutions and the assumption that probability distributions governing the uncertain factors are known or can be estimated. Also, it is relevant to emphasize that while significant progress has been made towards the solution of two-stage stochastic programs, the multi-stage case represents a significant challenge. In the case of stochastic integer programming with integer variables in stages other than the first, this represents a conceptual in addition to computational challenge. Deeper understanding of problem structure and properties is required in order to devise applicable algorithms (Sahinidis, 2004). Special strategies to solve problems under endogenous uncertainty are also desirable as well.

2.4 Trends and challenges

In section 2.3, a survey has been conducted of that literature related to integrated solutions for SCM. Based on that literature review, it is foreseen the need to devote further research efforts in order to meet the following trend and challenges:

- All the reviewed SC design models consider a given superstructure which restricts how potential SC members may interchange materials. Models that do not contemplate a superstructure a priori are needed so that the whole set of possible connections is explored. Accordingly, new alternatives to enhance value creation may appear.

- SC design used to be confined to final products and their relation to the production or supply of intermediates is usually disregarded (Melo *et al.*, 2009). The inclusion of this aspect may have a strong impact in the design of SCs. It still remains the issue of what an appropriate description of production processes at the SC level is.

- Trends in PSE, which is moving towards an enterprise wide optimization framework, aims to integrate different functional decisions into a global model. This model should optimize an overall key performance measure. Therefore, a posed challenge is to find a suitable measure which is able to account relevant functional trade-offs.

- A large proportion of the SC models proposed in the literature minimize costs. This is not sufficient to help a business create and sustain a competitive advantage. To this end, the objective should be sustainable value creation (Klibi *et al.*, 2009). Indeed, the treatment of financial factors is restricted to primary operating and fixed capital costs and, typically, some form of NPV with interest rate fixed over the time horizon is used as performance metric. Metrics which are able to quantify the shareholder's value are worth to explore.

- There is a need to model financial planning decisions (e.g., allocation of capital), R&D resource allocation and scheduling as well as downstream capacity expansion decisions within an integrated model (Varma *et al.*, 2007). Consequently, capital and capacity allocation decision making can be performed simultaneously with R&D projects selection and prioritization so as to enhance value generation.

- Analysis of relationship among partial environmental impacts for each of SC echelons is needed with the aim of discovering improvement opportunities. This sort of analysis will also provide information regarding where to focus emission control activities. Moreover, models considering the whole SC environmental impact could be helpful (i) to the assessment of current environmental regulatory policies and (ii) to the definition of more adequate environmental policies, so that effective industrial changes are induced.

- Reverse logistics and closed-loop SCs require further study. Additionally, the explicit environmental impact change caused by such kind of operations has not been sufficiently examined yet.

- Research is called for into the coordination of pricing, production and distribution decisions to cut across traditional organizational barriers. In recent years, firms are employing methods such as dynamically adjustment of prices over time based on inventory levels or production schedules as well as segmenting customers based on their sensitivity to prices, lead time and invoicing. These methods do impact SC operation and the associated trade-off should be examined.

- Further advances in optimality of distributed decision making is a need. In this direction, duality and separability principles may provide the background that could permit to optimize the whole system performance without knowledge of production cost functions and operation constraints of every SC member.

- Strategies which could handle uncertainty and incidences by combining reactive and preventive approaches capabilities are a promising direction of research. This will render a framework with (i) anticipating capabilities from a preventive approach which also and (ii) a review and a updating procedure from a reactive approach.

- One of the key components in integrated SCM is the decision making coordination and integration at all decision levels. As shown by the literature review, current approaches offer models to separately tackle problems arising in the three standard SC hierarchical decision levels. These models, because of their nature and purpose, have very different timescales. It becomes evident the challenge of considering the integration of decision levels in order to take advantage of potential benefits of integrated solutions.

- A virtually unexplored research topic is the integration of supervisory control modules with the SCM to timely provide and update the SC state information needed by the different decision-making hierarchical levels. Such a integration has the potential of reducing the risk of unexpected events and improving the efficiency of SC planning. Analysis to determine which process supervisory modules should be integrated is also required.
- On the one hand, nowadays, great amounts of data are acquired, stored, and managed through transactional information systems such as ERPs. On the other, SC analytical models depend on data quality in order to suggest adequate alternatives for management. Notwithstanding, there is still a lack of information technology capable of integrating analytical tools with the data stored in transactional databases. Future research efforts should be focused on devising information technologies to accomplish this integration. This aspect is even more sensitive if supervisory control information is eventually incorporated for SCM. In this direction, knowledge management systems such as ontologies seem to be a suitable choice to bridge this gap.
- A single monolithic model that can be used to jointly and efficiently optimize each and every enterprise decision is unlikely to exist for the foreseeable future. Even though, the previous challenges require developing and solving complex large size multi-scale optimization problems which turns out to high computational burden. With the purpose of reducing the computational effort, it is envisaged that:
  - Further research efforts are needed to identify and develop appropriate decomposition strategies which are capable of handling information and feedback from the different model structures (i.e., decision levels and functionalities) is needed. This kind of strategies decomposes the overall problem into blocks which are solved iteratively while achieving the optimal solution of the overall problem.
  - As parametric programming techniques mature, the exploitation of hybrid approaches that combine them with stochastic programming and mathematical decomposition seem to be a research avenue worthy to be further investigated.
  - Appropriate algorithm architectures based on knowledge of the specific problematic (e.g., S-graph, P-graph) are a good choice so as to reduce the solutions feasible space.
  - As Min and Zhou (2002) argue, theory of constraints is a well-suited methodology to simplify the complexity of SC models. It may be a useful tool to discover those SC processes that heavily influences the SC performance. Subsequently, modeling should be focused on those critical processes and non-critical processes may be disregarded when possible or treated in less detail. This point

clearly applies to the selection of supervisory modules that should be integrated with SC models as well.

Given this, it may be inferred that trends in SCM are oriented to four issues: better representation of production-distribution processes at the SC level, integrated approaches, uncertainty considerations, and decomposition strategies.

Chapter 3

Methods and Tools

3.1 Introduction

In this chapter, the background of those methods and tools that are utilized in the development and implementation of the different models presented throughout this thesis are described. Some general principles of mathematical programming are discussed since it is the optimization technique used in this thesis. First, deterministic programs are briefly introduced. Then, some basic aspects of stochastic programming are commented. Later, the basic ideas behind multi-objective optimization and decomposition techniques are presented. Finally, a short introduction to the computer platform used to solve the posed problems is given.

3.2 Generalities of mathematical programming

Mathematical programming is an important tool in decisions science and is that branch of mathematics dealing with techniques for optimizing the performance of a system. Its name is due to its military origins. The military refer to their various plans or proposed schedules of training, logistical supply and deployment of combat units as a *program*. George B. Dantzig, who was a mathematical advisor to the US Air Force controller in the Pentagon and the inventor of the Simplex method in 1947, was the first using the term linear *programming* (Gill *et al.*, 2008). Later on, in the early 1950's many optimization subfields were collected in the term mathematical programming.

A general representation of a mathematical program can be written as:

$$\left.\begin{array}{ll} \underset{\boldsymbol{x}}{\text{minimize}} & f(\boldsymbol{x}) \\ \text{subject to} & \\ & \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0} \\ & \boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0} \\ \text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}, & \\ \boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^l, \boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m & \end{array}\right\} \tag{3.1}$$

Its main components are:

- *Objective function* It is a quantitative measure of the performance of the system under study (i.e., f).
- *Variables* These are the unknowns which values are to be determined such that the objective function is optimized (i.e., $\boldsymbol{x}$).
- *Constraints* These are any restriction the decision variables must satisfy (i.e., $\boldsymbol{h} \wedge \boldsymbol{g}$).

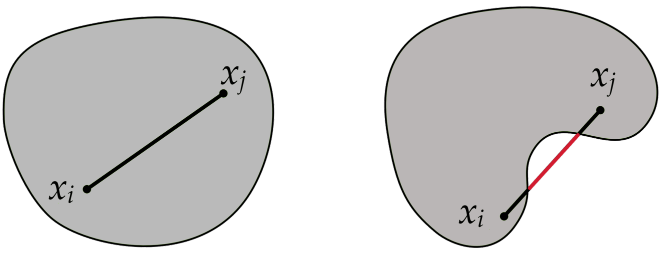
The process of identifying these components is known as modeling. Depending on the properties of the functions f, $\boldsymbol{h}$, $\boldsymbol{g}$, and the set $\mathcal{X}$, program (3.1) is called:

- *Linear* If the set $\mathcal{X}$ is continuous and the functions f, $\boldsymbol{h}$, and $\boldsymbol{g}$ are linear. The appearance of a single nonlinear function, either on the objective or in the constraints, suffices to reject the problem as a linear program.
- *Nonlinear* If the set $\mathcal{X}$ is continuous and at least one of the functions f, $\boldsymbol{h}$, and $\boldsymbol{g}$ is nonlinear.
- *Mixed integer linear* If the set $\mathcal{X}$ requires at least some of the variables $\boldsymbol{x}$ to take integer values only; and the functions f, $\boldsymbol{h}$, and $\boldsymbol{g}$ are linear.
- *Mixed integer nonlinear* If the set $\mathcal{X}$ requires at least some of the variables $\boldsymbol{x}$ to take integer values only; and at least one of the functions f, $\boldsymbol{h}$, and $\boldsymbol{g}$ is nonlinear.

3.2.1 Convexity

A set $\mathcal{X}$ is convex if for every pair of points (x_i, x_j) within the set, every point on the straight line segment that connects them is also within the set $\mathcal{X}$ as shown in Fig. 3.1. This definition is mathematically expressed as:

$$\mathcal{X} \text{ is convex} \quad \Longleftrightarrow \quad \forall (x_i, x_j) \in \mathcal{X} \wedge \theta \in [1, 0] : ((1-\theta)x_i + \theta x_j) \in \mathcal{X}$$



(a) A convex set (b) A noncovex set

Figure 3.1: Convexity graphical representation

Then, a function is convex if and only if the set of points lying above it is a convex set. Convexity plays an important role in mathematical programming due to the following theorem.

Theorem 3.1 *If a mathematical program is convex then any local (i.e., relative) minimum is a global minimum.*

The subfield that deals with nonconvex programs is referred to as global optimization. The global optimization aims finding the globally best solution of models in the potential presence of multiple local optima.

3.2.2 Karush-Kuhn-Tucker first order conditions

One of the most important theoretical results in optimization are the Karush, Kuhn and Tucker conditions. They must be satisfied at any optimum, local or global, of any linear and most nonlinear programs. The vector $\boldsymbol{x} \in \mathbb{R}^n$ satisfies these conditions for the program (3.1) if there exists vectors $\boldsymbol{\mu} \in \mathbb{R}^m$ and $\boldsymbol{\lambda} \in \mathbb{R}^l$ such that

$$\begin{aligned}
\nabla f(\boldsymbol{x}) + \sum_{i=1}^{l} \lambda_i \nabla h_i(\boldsymbol{x}) + \sum_{j=1}^{m} \mu_j \nabla g_j(\boldsymbol{x}) &= \mathbf{0} && (3.2)\\
h_i(\boldsymbol{x}) &= 0 \quad \forall i = 1, \dots, l && (3.3)\\
g_j(\boldsymbol{x}) &\leq 0 \quad \forall j = 1, \dots, m && (3.4)\\
\mu_j g_j(\boldsymbol{x}) &= 0 \quad \forall j = 1, \dots, m && (3.5)\\
\mu_j &\geq 0 \quad \forall j = 1, \dots, m && (3.6)
\end{aligned}$$

The vectors $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ are called Lagrangian multipliers. If the Lagrangian function is defined by:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T \boldsymbol{h}(\boldsymbol{x}) + \boldsymbol{\mu}^T \boldsymbol{g}(\boldsymbol{x})$$

the Karush-Kuhn-Tucker (KKT) conditions can be written as:

$$\begin{array}{rcl} \nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) & = & \mathbf{0} \\ \nabla_{\boldsymbol{\lambda}}\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) & = & \mathbf{0} \\ \nabla_{\boldsymbol{\mu}}\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) & \leq & \mathbf{0} \\ \boldsymbol{\mu}^T\nabla_{\boldsymbol{\mu}}\mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu}) & = & \mathbf{0} \\ \boldsymbol{\mu} & \geq & \mathbf{0} \end{array}$$

3.2.3 Duality

The term "duality" is often used to invoke a contrast between two related concepts. Duality is one of the most fundamental concepts in mathematical programming and establishes a connection between two "symmetric" programs, namely, the primal and dual problem.

First of all, the dual function is introduced as:

$$\phi(\boldsymbol{\lambda},\boldsymbol{\mu}) = \underset{\boldsymbol{x}}{\text{Infimum}} \quad \{f(\boldsymbol{x}) + \boldsymbol{\lambda}^T\boldsymbol{h}(\boldsymbol{x}) + \boldsymbol{\mu}^T\boldsymbol{g}(\boldsymbol{x})\} \tag{3.7}$$

Then, the dual problem of the primal problem (3.1) is defined as follows:

$$\begin{array}{ll} \underset{\boldsymbol{\lambda},\boldsymbol{\mu}}{\text{maximize}} & \phi(\boldsymbol{\lambda},\boldsymbol{\mu}) \\ \text{subject to} & \\ & \boldsymbol{\mu} \geq \mathbf{0} \end{array} \tag{3.8}$$

Using the Lagrangian function, the dual problem can also be rewritten as:

$$\underset{\boldsymbol{\lambda},\boldsymbol{\mu};\boldsymbol{\mu}\geq\mathbf{0}}{\text{maximize}} \quad \left\{\underset{\boldsymbol{x}}{\text{Infimum}} \quad \mathcal{L}(\boldsymbol{x},\boldsymbol{\lambda},\boldsymbol{\mu})\right\} \tag{3.9}$$

The theorem 3.2 establishes an important relationship between the dual and primal problems.

Theorem 3.2 ***Weak duality*** *For any feasible solution $\boldsymbol{x}$ of the primal problem (3.1) and for any feasible solution $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$, of the dual problem (3.8), the following holds*

$$f(\boldsymbol{x}) \geq \phi(\boldsymbol{\lambda},\boldsymbol{\mu}) \tag{3.10}$$

Additionally, the theorem 3.3 is of relevant importance in mathematical programming. It shows that for convex programs the primal problem solution can be obtained by solving the dual problem.

Theorem 3.3 *If the primal problem is convex, then $f(\boldsymbol{x}^*) = \phi(\boldsymbol{\lambda}^*,\boldsymbol{\mu}^*)$. Otherwise, one or both of the two sets of feasible solutions is empty.*

Here, $\boldsymbol{x}^*$ represents the optimal solution of the primal problem; and $\boldsymbol{\lambda}^*,\boldsymbol{\mu}^*$ are the optimal solutions of the dual problem.

For nonconvex programs, the difference between the optimal objective function values of the dual and primal problems ($\phi(\boldsymbol{\lambda}^*,\boldsymbol{\mu}^*) - f(\boldsymbol{x}^*)$) is called *duality gap*. For nonconvex programs of engineering applications, the duality gap is usually relatively small (Conejo, Nogales, & Prieto, 2002).

3.3 Linear programming

The main feature of a LP problem is that all functions involved, the objective function and those expressing the constraints, must be linear. The solution space or feasible region of an n-variables LP is geometrically defined by the intersection of the hyperplanes and halfspaces representing each of the constraints. Such a set is characterized as a convex polytope.

Theorem 3.4 *If an LP has an optimal solution, there is a vertex (i.e., extreme point) of the feasible polytope that is optimal.*

Theorem 3.4 is the fundamental theorem of linear programming and is the basis of algorithms for solving linear programs: the Simplex and interior point methods.

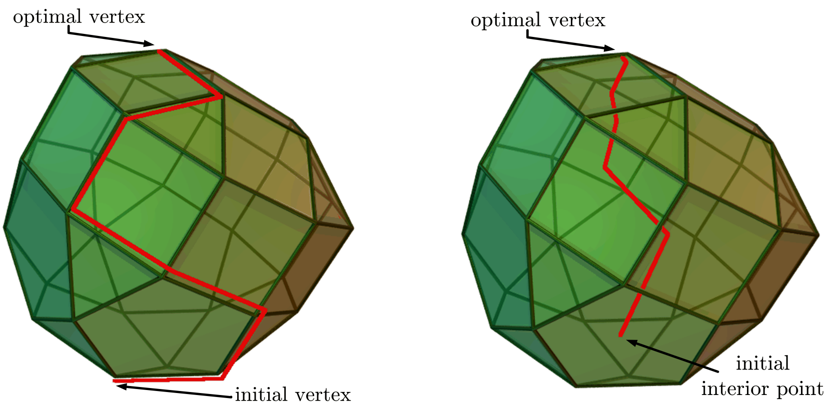
3.3.1 The Simplex method

The algorithm starts with an initial vertex feasible solution and tests its optimality. If some optimality condition is verified, then the algorithm terminates. Otherwise, the algorithm identifies an adjacent vertex, with a better objective value. The optimality of this new solution is tested again, and the entire scheme is repeated, until an optimal vertex is found. Since every time a new vertex is identified the objective value is improved (except from a certain pathological case), and the set of vertices is finite, it follows that the algorithm will terminate in a finite number of iterations. Given the above description of the algorithm, it is inferred that the Simplex essentially starts from some initial extreme point, and follows a path along the edges of the feasible region towards an optimal extreme point, such that all the intermediate extreme points visited are not worsening the objective function (see Fig. 3.2a).

3.3.2 Interior point methods

An interior-point algorithm is one that improves a feasible interior solution point of the linear program by steps through the interior, rather than one that improves by steps around the boundary of the feasible region, as the Simplex does (see Fig. 3.2b). A theoretical breakthrough for interior point methods came in 1979; the Russian mathematician L.G. Khachian discovered an ellipsoid algorithm whose running time in its worst case was significantly lower than that of the Simplex Algorithm. Other theoretical results quickly followed, notably that of N. Karmarkar who discovered an interior-point algorithm whose running time performance in its worst case was significantly lower than that of Kachiyan's (Dantzig & Thapa, 1997a). Assuming an initial feasible interior point is available and that all moves satisfy the whole set of constraints, the key ideas behind interior-point methods are as follows:

- Move through the interior in directions that show promise of moving quickly to the optimal solution (i.e., the steepest descent direction).



(a) Simplex method (b) Interior point methods

Figure 3.2: Graphical interpretation of linear programming methods

- Recognize that a movement in a direction that sets the new point too “close” to the boundary will be an obstacle; it will impede moving quickly to an optimal solution. One way around this is to transform the feasible region so that the current feasible interior point is at the center of the transformed feasible region. Once a movement has been made, the new interior point is transformed back to the original space, and the whole process is repeated with the new point as the center.

- The stopping rule typically followed is to finish with an approximate optimal solution when the difference between iterates is sufficiently small in the original space.

There is still no valid way to characterize the classes of practical problems from which one could expect a superior performance of a specific algorithm. Because of this, commercial software usually tend to be some sort of a hybrid. For detail explanation about linear programming algorithms the reader is referred to Dantzig and Thapa (1997a,b).

3.4 Nonlinear programming

As previously stated, if the objective function f or any constraint $\boldsymbol{h}$, $\boldsymbol{g}$ is nonlinear and all variables $\boldsymbol{x}$ are continuous, program (3.1) is denominated a nonlinear program. The algorithms to solve this kind of programs can be classified as unconstrained and constrained optimization methods. A brief discussion of both classes is giving next.

3.4.1 Unconstrained optimization

To begin with, programs which do not comprised any constraint ($\boldsymbol{h}$, and $\boldsymbol{g}$) are discussed. For unconstrained optimization, the algorithms can be classified in two groups: line search methods and trust region methods. Both of them require a initial feasible solution ($\boldsymbol{x}_0$) for the problem. They basically determine a *direction* ($\hat{\mathbf{p}_k}$), and a *distance* or *step length* (α_k) to move towards an improved solution.

Line search methods This kind of algorithms firstly chooses a direction and then searches along this direction for an adequate step length, so that one moves from the current iterate ($\boldsymbol{x}_k$) for a new iterate ($\boldsymbol{x}_{k+1}$) with a better objective function value. The most important methods to obtain a search direction are briefly described next.

- The *steepest-descent direction* ($-\nabla f(\boldsymbol{x})$) is the most obvious choice for search direction, however it may converge very slow in case of complex functions.

- Another important search direction method is the *Newton direction*. This direction is derived from the second-order Taylor series. Methods that use the Newton direction have a fast rate of local convergence. Nevertheless, the main drawback is that it requires the explicit computation of the Hessian matrix ($\nabla^2 f(\boldsymbol{x})$).

- *Quasi-Newton search directions* provide an attractive alternative in that they do not require computation of the Hessian and yet still attain a good rate of convergence. Instead of the Hessian, these methods use an approximation $\mathbf{B}_k$, which is updated after each iteration to incorporate the additional knowledge gained during the iteration. Two of the most popular formulæ for updating the approximation $\mathbf{B}_k$ are the *symmetric-rank-one (SR1) formula*, and the *BFGS formula*.

The step length should be chosen such that a sufficient improvement is assured and the length is not too short. For this purpose, a good step length must satisfy the so-called *Wolfe conditions*. There are several methods to determine the step length; among them the interpolation method, the golden section method, and the Fibonacci's method.

Another very important algorithm in this optimization subfield is the *conjugate gradient method*. The idea of this method is to improve convergence through the construction of search directions by using the conjugate (A–orthogonal) of the steepest-decent direction. This method was firstly devised for convex quadratic functions, but it has been extended to approach general nonlinear functions. Extensions of this kind are the Fletcher-Reeves method and the Polak-Ribière method.

Trust region methods This kind of algorithms firstly constructs a model function (trust region) m_k whose behavior near the current solution $\boldsymbol{x}_k$ is similar to that of the actual objective function f. Then, these methods choose the step and the direction to find the approximate optimizer of the model in this trust region.

The trust region is usually assumed to be the first two terms of the Taylor-series expansion of f around $\boldsymbol{x}_k$. Each step $\mathbf{p}$ (i.e., direction and step length) of iteration $k+1$ is obtained from the solution of the next subproblem:

$$\underset{\mathbf{p}\in\mathbb{R}^n}{\text{minimize}}\, m_k(\mathbf{p}) = f_k + \nabla f_k^T \mathbf{p} + \frac{1}{2}\mathbf{p}^T \mathbf{B}_k \mathbf{p} \qquad \text{s.t. } \|\mathbf{p}\| \leq \Delta_k \tag{3.11}$$

where Δ_k and $\mathbf{B}_k$ are the trust region radius and an approximation of the Hessian of f, respectively. These methods require a strategy to determine the trust region radius. This strategy is formulated based on a measure of how well the previous trust-region m_k mimics the actual function f. Besides, a second strategy to find an approximate solution to subproblem (3.11) is needed. Some approaches for this are the dogleg method, the two-dimensional subspace minimization, the Moré and Sorensen method and the Steihaug method. It is important to notice that the trust-region subproblem (3.11) can be approximately solved by means of the conjugate gradient method.

3.4.2 Constrained optimization

Here, methods to solve constrained programs are addressed. This type of methods seek an approximate solution by replacing the original constrained problem by a sequence of unconstrained subproblems. So, the underlying idea is to construct a closely related, unconstrained optimization problem and apply to it some of the algorithms discussed in the previous section. There are mainly two categories of these methods: (i) those ones which do not attain Lagrange multipliers information, and (ii) those methods based on the KKT conditions. The former category includes the techniques of penalization and barriers, and in the latter category are the dual method and the augmented Lagrangian algorithm.

Penalization and barriers methods Both of them consider a problem as follows:

$$\underset{\boldsymbol{x}}{\text{minimize}}\, f(\boldsymbol{x}) + \hat{f}(\boldsymbol{x}) \tag{3.12}$$

where $\hat{f}(\boldsymbol{x})$ is a function penalizing infeasible solutions or mimicking the barrier between feasible and infeasible solutions.

Penalization methods These methods use $\hat{f}(\boldsymbol{x})$ as a penalization term when constraints are not met so as to discourage infeasible solutions. One of the most popular families of penalizations is the following:

$$\hat{f}(\boldsymbol{x}) = r\left(\sum_i \max\{0, g_i(\boldsymbol{x})\}^p + \sum_j |h_j(\boldsymbol{x})|^q\right)$$

where $p, q > 1$ are exponents and r is a penalization parameter. One typical case that is used often is the quadratic penalization corresponding to $p = q = 2$. After replacing the constraints by means of the incorporation of the penalization term in the objective function, the program becomes a unconstrained optimization problem. Only when r becomes big enough, the corresponding approximations to the unconstrained program (3.12) are close to the solution of the constrained program (3.1).

Barriers methods As previously mentioned, another choice is to use $\hat{f}(\boldsymbol{x})$ as a barrier function. One interesting possibility is the next one.

$$\hat{f}(\boldsymbol{x}) = r\left(-\frac{1}{r}\sum_i \log(-g_i(\boldsymbol{x})) + r^3 \sum_j \frac{h_j(\boldsymbol{x})^2}{1 - r^2 h_j(\boldsymbol{x})^2}\right)$$

Notice that again only when parameter r is large, good approximations can be obtained by applying an unconstrained algorithm to program (3.12).

Dual method The idea behind this method is to utilized the dual problem (3.8) to find an approximate solution of the primal problem (3.1). The advantage of the dual is that the definition of the dual function is an unconstrained problem, and, at the same time, the constraint itself for the dual problem is much simpler, in particular linear ($\boldsymbol{\mu} \geq \mathbf{0}$). The dual function ϕ (program (3.7)) is found for given values of vectors $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ using a unconstrained optimization method. Notice that these two vectors can be updated using a line search method at each iteration bearing in mind that

$$\nabla_\mu \phi(\boldsymbol{\lambda}, \boldsymbol{\mu}) = \boldsymbol{g}(\boldsymbol{x}) \wedge \nabla_\lambda \phi(\boldsymbol{\lambda}, \boldsymbol{\mu}) = \boldsymbol{h}(\boldsymbol{x}).$$

The KKT conditions are used as stopping criterion in this method.

Augmented Lagrangian method This method follows a procedure similar to the dual method. However, a quadratic penalization of the type that was discussed earlier is used in order to include the constraints in the dual function ϕ. Consequently, the augmented Lagrangian $\mathcal{L}_{\mathcal{A}}$ is defined as follows.

$$\begin{aligned}\mathcal{L}_{\mathcal{A}}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}, r) = \nabla f(\boldsymbol{x}) + \sum_{i=1}^{l} \lambda_i \nabla h_i(\boldsymbol{x}) + \sum_{j=1}^{m} \mu_j \nabla g_j(\boldsymbol{x})& \\ +r\left(\sum_i \max\{0, g_i(\boldsymbol{x})\}^2 + \sum_j h_j(\boldsymbol{x})^2\right)&\end{aligned}$$

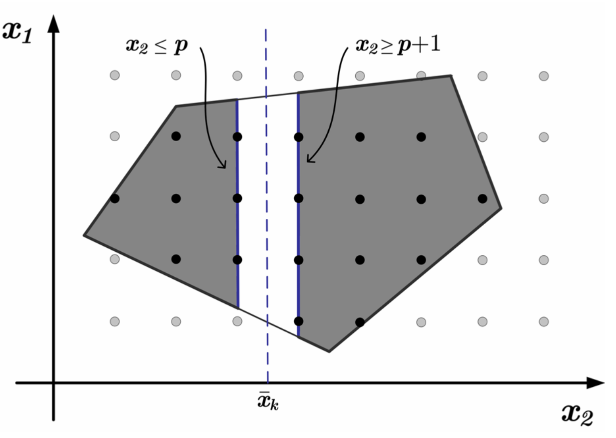


Figure 3.3: Branching procedure

The key feature of this method is that it can be proved that good explicit Lagrange multiplier estimates at each iteration $k+1$ can be obtained using the following expressions, where $c > 1$.

$$\begin{aligned} \boldsymbol{\lambda}_{k+1} &= \boldsymbol{\lambda}_k + r_k \boldsymbol{h}(\boldsymbol{x}_k) \\ \boldsymbol{\mu}_{k+1} &= \boldsymbol{\mu}_k + r_k \max\{0, \boldsymbol{g}(\boldsymbol{x}_k)\} \\ r_{k+1} &= c r_k \end{aligned}$$

The reader is referred to Nocedal and Wright (1999) and Pedregal (2004) for a complete revision of nonlinear programming algorithms.

3.5 Mixed integer programming

The need for using binary variables turns out from a variety of purposes such as modeling yes/no decisions, enforcing logical conditions, modeling fixed costs or piecewise linear functions. Additionally, integer variables appear when modeling indivisible entities. Mathematical programs which some of its variables are integer are called *mixed integer programs*. Basically, there are two algorithms for solving this class of programs, the Branch and Bound (B&B) and the cutting planes methods.

3.5.1 Branch & bound methods

An B&B algorithm consists in generating a sequence of continuous subproblems, solving them, and analyzing and comparing the different solutions until an optimal solution is reached for the original problem. The algorithm searches the complete space of solutions. The use of bounds for the function to be optimized combined with the value of the current best solution (i.e., the *incumbent*) enables the algorithm to implicitly search parts of the solution space.

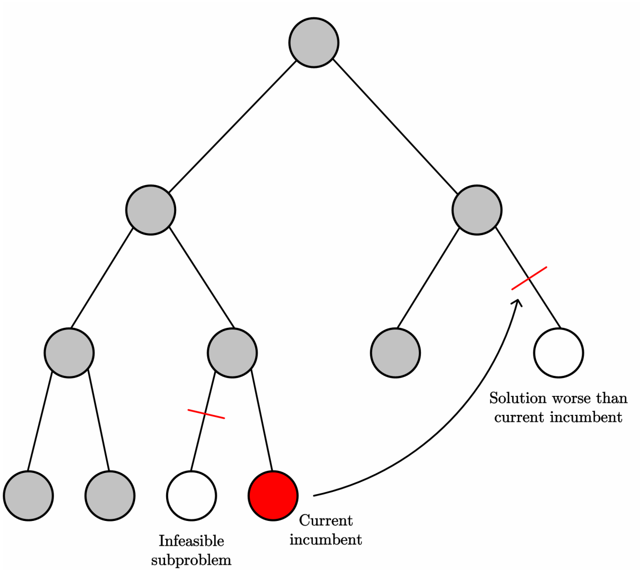


Figure 3.4: Bounding procedure

The solution of a problem with an B&B algorithm is traditionally described as a search through a tree, in which the root node corresponds to the relaxed original problem, and each other node corresponds to a subproblem of the original problem. So, given a node (problem) Q of the tree, assume that x_k is a variable whose solution is $\bar{x}_k \in \mathbb{R}^n$ that is not satisfying the integrality constraint in the node Q solution. Then, the *branching* procedure consist in creating two children nodes of Q. The two children nodes of Q are disjoint subproblems derived from adding to the Q problem the further constraint $x_k \leq p$ in one case, and $x_k \geq p+1$ in the other as shown in Fig. 3.3. Here, p is an integer value ($p \in \mathbb{Z}$) and must satisfy the next condition:

$$\bar{x}_k - 1 < p \leq \bar{x}_k \leq p + 1 < \bar{x}_k + 1.$$

On the other hand, the *bounding* procedure consists in discarding a node when is infeasible or when its objective function is not better than the incumbent as depicted in Fig. 3.4. The initial incumbent may be the objective function of a known feasible solution or it may be set to $+\infty$. The incumbent value is updated when a solution satisfying integrality is found during the B&B search and its corresponding objective function value is better than the current incumbent.

As it can be seen, there are two questions to be answered during the branching procedure so as to select the next subproblem, namely, What node Q should be selected for branching? and What variable not satisfying integrality in Q should be chosen for branching? Several strategies have been proposed for these purposes, but they are out of the scope of this chapter.

3.5.2 Cutting plane methods

There is an alternative to B&B algorithm called cutting planes which can also be used to solve mixed integer programs. The core idea behind cutting planes is to add constraints to a program until the optimal solution satisfies integrality constraints. Of course, a cut (i.e., constraints) to be added to a current fractional (i.e. not satisfying integrality) solution must assure that:

- Every feasible integer solution of the actual program is feasible for the cut.
- The current fractional solution is not feasible for the cut.

Some of the most known techniques to generate these cuts are the Gomory's cuts methods, the Kelley's method, and the Kelley-Cheney-Goldstein method.

Both, B&B and cutting plane techniques, can be applied to linear and nonlinear programs. An special methodology for mixed integer nonlinar programs is the outer-approximation algorithm developed by Duran and Grossmann (1986). Also, it is noteworthy to mention an special set of integer programs called disjunctive programs. The theory of disjunctive programming can be found in the work of Raman and Grossmann (1994) and Lee and Grossmann (2000). In a nutshell, disjunctive programs comprised a logical system of conjunctive and disjunctive statements, where each statement is defined by a constraint.

For details about mixed integer programming algorithms the reader is referred to Nemhauser and Wolsey (1999).

3.6 Multi-objective optimization

Multi-objective optimization (MO) plays an important role in engineering design, management, and decision making in general. Usually, a decision maker needs to make tradeoffs between disparate and conflicting objectives. The field of multi-objective optimization defines the art and science of making such decisions.

The mathematical representation of an MO problem is as follows:

$$\left.\begin{array}{l} \underset{\boldsymbol{x}}{\text{minimize}} \quad \{f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_P(\boldsymbol{x})\} \quad (P \geq 2) \\[1em] \text{subject to} \\ \qquad\qquad \boldsymbol{h}(\boldsymbol{x}) = \mathbf{0} \\ \qquad\qquad \boldsymbol{g}(\boldsymbol{x}) \leq \mathbf{0} \\[1em] \text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}, \\ \boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^l, \boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m \end{array}\right\} \tag{3.13}$$

The solution of an MO problem is said to be a set of *Pareto* solutions, or a Pareto frontier. A Pareto solution is one for which any improvement in one objective can only take place if at least one other objective worsens (Messac, Ismail-Yahaya, & Mattson, 2003).

Dominance In order to formally define a Pareto solution, the concept of *dominance* is introduced next. A solution $\boldsymbol{x}_a$, associated to the objective function values $\{z_{1_a}, z_{2_a}, \ldots, z_{P_a}\}$ *dominates* other solution $\boldsymbol{x}_b$, with its corresponding point $\{z_{1_b}, z_{2_b}, \ldots, z_{P_b}\}$, if and only if:

$$[\ z_{p_a} \leq z_{p_b}\ \forall\ p \in \{1 \ldots P\}\ ] \wedge [\ \exists\ p \in \{1 \ldots P\}\ /\ z_{p_a} < z_{p_b}\ ]$$

where $z_{p_a} = f_p(\boldsymbol{x}_a) \quad \forall p \in \{1 \ldots P\}$ and $z_{p_b} = f_p(\boldsymbol{x}_b) \quad \forall p \in \{1 \ldots P\}$. From here forth, z_p is a scalar that shall be associated to the objective function value $f_p(\boldsymbol{x})$.

Thereby, if a solution $\boldsymbol{x}^*$ is Pareto solution then it does not exist a different solution $\boldsymbol{x} \in \mathcal{X}$ that dominates it.

There are several approaches to obtaining such solutions (see section 2.2.1). Basically, they are based on the conversion of the MO problem into one single objective function problem. The next section is focused on the ϵ-constrained method which is the one used in this thesis.

3.6.1 The ϵ-constraint method

The ϵ-constrained method was proposed by Haimes, Lasdon, and Wismer (1971). The method approximates the Pareto frontier by finding a set of Pareto solutions that belong to it. Each single Pareto solution is found by solving a single objective optimization problem. Such an optimization problem incorporates bounds for the remaining objective functions which are not being directly optimized. The method is described following a procedure similar to the one presented by Messac *et al.* (2003). Here, the normalization step for the objectives values is not considered. To better describe this method it will be useful to define the *utopia point* and the *p-anchor points*.

The utopia point The utopia point $\{z_1^u, z_2^u, \ldots, z_P^u\}$ is defined as comprised by every single optimized objective function z_p value. Obviously, this ideal point is an imaginary solution for conflicting objectives, in the sense that does not corresponds to any feasible solution. The utopia point can be found by solving P times the program (3.14). Here, it would be useful to define $\boldsymbol{x}_p^u$ as the solution associated to z_p^u.

$$\left.\begin{array}{ll} \underset{\boldsymbol{x}}{\text{minimize}} & f_p(\boldsymbol{x}) \\[1em] \text{subject to} & \\ & \boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{0} \\ & \boldsymbol{g}(\boldsymbol{x}) \leq \boldsymbol{0} \\[1em] \multicolumn{2}{l}{\text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n, f : \mathbb{R}^n \rightarrow \mathbb{R},} \\ \multicolumn{2}{l}{\boldsymbol{h} : \mathbb{R}^n \rightarrow \mathbb{R}^l, \boldsymbol{g} : \mathbb{R}^n \rightarrow \mathbb{R}^m} \end{array}\right\} \forall\ p \in \{1 \ldots P\} \tag{3.14}$$

Algorithm 3.1: The p-anchor point

```
Data: p, z_p^u
Result: {z_{1p}^a, z_{2p}^a, ..., z_{Pp}^a}
begin
    z_{pp}^a ⟵ z_p^u
    for p' ∈ {1...P} ∧ p' ≠ p do
        z_{p'p}^a ⟵ +∞
    for p'' ∈ {1...P} ∧ p'' ≠ p do
        solve program (3.15)
        z_{p''p}^a ⟵ f_p(x*)
        if p = P and p'' = P − 1 then
            x_p^a ⟵ x*
        else
            if p'' = P then
                x_p^a ⟵ x*
end
```

The p-anchor points The p-anchor point $\{z_{1p}^a, z_{2p}^a, \ldots, z_{Pp}^a\}$ is a nondominated point, an extreme Pareto solution, whose z_{pp}^a value is equal to z_p^u. The algorithm 3.1 must be followed so as to find the p-anchor point. In some cases it may happen the solution of an anchor point $\boldsymbol{x}_p^a$ to be equal to $\boldsymbol{x}_p^u$.

The algorithm 3.1 must be executed P times to find every p-anchor point. Recall that P refers to the number of objective functions comprising the MO problem. In algorithm 3.1 the program 3.15 is as follows:

$$\left.\begin{array}{llll} \underset{\boldsymbol{x}}{\text{minimize}} & f_{p''}(\boldsymbol{x}) & & \\ & & & \\ \text{subject to} & & & \\ \quad \boldsymbol{h}(\boldsymbol{x}) & = & \boldsymbol{0} & \\ \quad \boldsymbol{g}(\boldsymbol{x}) & \leq & \boldsymbol{0} & \\ \quad f_{p'''}(\boldsymbol{x}) & \leq & z_{p'''p}^a & \forall\, p''' \in \{1\ldots P\} \wedge\ p''' \neq p'' \\ & & & \\ \multicolumn{4}{l}{\text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}, \boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^l, \boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m} \end{array}\right\} \tag{3.15}$$

Now, the procedure to find the non-extreme Pareto solutions so as to approximate the Pareto frontier is presented. Such a procedure is shown in Fig. 3.5. Firstly, one needs to define the number N of Pareto solutions that are to be found along directions parallel to the axis representing z_p. The total number of non-extreme Pareto solutions to be generated is equal to N^{P-1}. The space between consecutive Pareto solutions (ϵ_p) along directions parallel to the axis z_p is determined using the next expression.

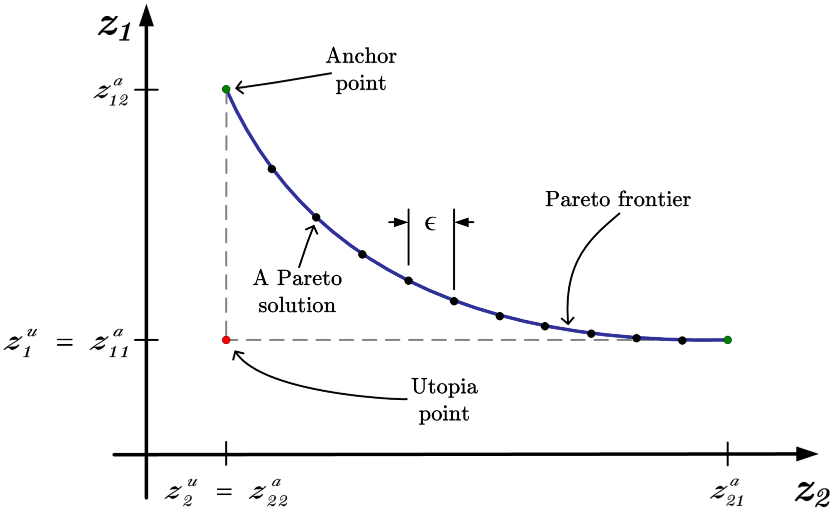


Figure 3.5: The ϵ-constrained method for a bi-objective optimization problem

$$\epsilon_p = \frac{\left(\max\limits_{p' \in \{1\ldots P\}} \{z^a_{pp'}\}\right) - z^u_p}{N+1} \quad \forall\, p \in \{1 \ldots P\}$$

Then, each non-extreme Pareto solution is obtained by solving the program (3.16) for every combination of $\{n_1, n_2, \ldots, n_P\}$ where each $n_p \in \{1, 2, \ldots, N\}$.

$$\left.\begin{array}{lll} \underset{\boldsymbol{x}}{\text{minimize}} & f_{p'}(\boldsymbol{x}) & \\ & & \\ \text{subject to} & & \\ \quad \boldsymbol{h}(\boldsymbol{x}) & = & \boldsymbol{0} \\ \quad \boldsymbol{g}(\boldsymbol{x}) & \leq & \boldsymbol{0} \\ \quad f_p(\boldsymbol{x}) & \leq & z^u_p + n_p \epsilon_p \\ & & \quad \forall\, p \in \{1 \ldots P\} \wedge\ p \neq p' \\ & & \\ \multicolumn{3}{l}{\text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}, \boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^l,} \\ \multicolumn{3}{l}{\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m} \end{array}\right\} \forall\, n_1, n_2, \ldots, n_P \tag{3.16}$$

The ϵ-constraint method is applied in Chapters 4 and 8 for tackling multi-objective optimization problems. An extensive review of multi-objective optimization methods can be found in Ehrgott and Gandibleux (2002).

3.7 Stochastic programming with recourse

All previously discussed optimization problems are deterministic, that is, all the data required in those models is assumed to be perfectly known. In this section, stochastic programs in which some data may be considered uncertain are addressed. In this kind of problems, it is relevant to distinguish between two set of decisions (i.e., variables): the first stage decisions, and the recourse decisions.

First stage decisions This set of decisions are taken before any uncertain parameter is unveiled. They are also known as "here and now" decisions. The interval of time associated with them is known as the *first stage* of the stochastic program.

Recourse decisions They are determined after some or all the random data is disclosed. This kind of decisions are also known as the second and so forth stage or "wait and see" decisions.

Two stage programs The most widely used and simplest stochastic program is the two-stage program. Here, the first stage decisions are represented by the vector $\boldsymbol{x}$, while second stage decisions are represented by the vector $\boldsymbol{y}$. The uncertain parameter is represented by ξ. Notice that the second stage decisions $\boldsymbol{y}$ are a function of both, the first stage decisions $\boldsymbol{x}$ and the uncertain event ξ. In order to simplify the problem representation, the recourse function Q is introduced next.

$$Q(\boldsymbol{x}, \xi) = \left[\begin{array}{ll} \min\limits_{\boldsymbol{x}} & f_2(\boldsymbol{y}, \xi) \\ \text{s.t.} & \\ & \boldsymbol{h}_2(\boldsymbol{x},\ \boldsymbol{y}, \xi) = \boldsymbol{0} \\ & \boldsymbol{g}_2(\boldsymbol{x},\ \boldsymbol{y}, \xi) \leq \boldsymbol{0} \\ & \\ \multicolumn{2}{l}{\text{where } \boldsymbol{y} \in \mathcal{Y} \subset \mathbb{R}^{n_2}, f_2 : \mathbb{R}^{n_2} \to \mathbb{R},} \\ \multicolumn{2}{l}{\boldsymbol{h}_2 : \mathbb{R}^{n_2} \to \mathbb{R}^{l_2}, \boldsymbol{g}_2 : \mathbb{R}^{n_2} \to \mathbb{R}^{m_2}} \end{array} \right] \tag{3.17}$$

All those equations involving recourse decisions $\boldsymbol{y}$ are taken into account in Q. As it can be seen, Q is a mathematical program that minimizes the second-stage "cost" for a given value of the uncertain parameter ξ. Then, the expected recourse function $\mathcal{Q}$, the mathematical expectation of Q, is defined by the expression (3.18).

$$\mathcal{Q}(\boldsymbol{x}) = E_\xi \left[Q(\boldsymbol{x}, \xi) \right] \tag{3.18}$$

Finally, a two-stage program can be mathematically represented as follows:

$$\left.\begin{array}{ll}\min\limits_{\boldsymbol{x}} & f_1(\boldsymbol{x}) + \mathcal{Q}(\boldsymbol{x}) \\ \text{s.t.} & \\ & \boldsymbol{h}_1(\boldsymbol{x}) = \mathbf{0} \\ & \boldsymbol{g}_1(\boldsymbol{x}) \leq \mathbf{0} \\ & \\ \multicolumn{2}{l}{\text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^{n_1}, f : \mathbb{R}^{n_1} \to \mathbb{R},} \\ \multicolumn{2}{l}{\boldsymbol{h}_1 : \mathbb{R}^{n_1} \to \mathbb{R}^{l_1}, \boldsymbol{g}_1 : \mathbb{R}^{n_1} \to \mathbb{R}^{m_1}}\end{array}\right\} \tag{3.19}$$

Multistage programs Most of engineering problems entail a sequence of decisions that must not anticipate future outcomes of the uncertain factors that evolve over more than one time event. For these cases, a multistage stochastic program is required. The above two-stage problem can be easily extended to a multistage (K-stage) recourse program bearing in mind that instead of the two set of decisions $\boldsymbol{x}$ and $\boldsymbol{y}$, to be taken at first and second stages, now one is dealing with K sequential set of decisions $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_K\}$. Notice that in a K-stage stochastic problem, one is facing $K-1$ uncertain events $\{\xi^1, \xi^2, \ldots, \xi^{K-1}\}$ and the uncertain events $\xi^1, \xi^2, \ldots, \xi^{\tau-1}$ are already known when the set of decisions $\boldsymbol{x}_\tau$ is made at stage τ. Consequently, the expected recourse function of stage τ can be defined by:

$$\mathcal{Q}_\tau(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\tau-1}) = E_{\xi^\tau}\left[Q(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\tau-1}, \xi^1, \ldots, \xi^{\tau-1})\right] \quad \tau \geq 2 \tag{3.20}$$

Then, a K-stage program can be mathematically represented as follows:

$$\left.\begin{array}{ll}\min\limits_{\boldsymbol{x}_1} & f_1(\boldsymbol{x}_1) + \sum\limits_{\tau=2}^{K} \mathcal{Q}_\tau(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\tau-1}) \\ \text{s.t.} & \\ & \boldsymbol{h}_1(\boldsymbol{x}_1) = \mathbf{0} \\ & \boldsymbol{g}_1(\boldsymbol{x}_1) \leq \mathbf{0} \\ & \\ \multicolumn{2}{l}{\text{where } \boldsymbol{x}_1 \in \mathcal{X} \subset \mathbb{R}^{n_1}, f : \mathbb{R}^{n_1} \to \mathbb{R},} \\ \multicolumn{2}{l}{\boldsymbol{h}_1 : \mathbb{R}^{n_1} \to \mathbb{R}^{l_1}, \boldsymbol{g}_1 : \mathbb{R}^{n_1} \to \mathbb{R}^{m_1}}\end{array}\right\} \tag{3.21}$$

In the case that a continuous probability function is utilized to represent the uncertain parameter ξ, programs (3.19) and (3.21) can be analytically solved just for few simple problems. However, approximations can be obtained by constructing a discrete number of scenarios which mimics the continuous distribution behavior.

3.7.1 The scenario based approach

In case that ξ has a discrete number of possible scenarios (i.e., a finite discrete distribution) $\{(\xi_s, \mathcal{P}_s)\ \forall\, s \in \{1, \ldots, S\}\ /\mathcal{P}_s > 0 \wedge \sum_s \mathcal{P}_s = 1\}$; a *deterministic equivalent program* can be formulated for a stochastic program. For instance, the equivalent deterministic program for the two stage program (3.19) can be posed as:

$$\left.\begin{array}{ll}\min\limits_{\boldsymbol{x}} & f_1(\boldsymbol{x}) + \sum\limits_{s=1}^{S} \mathcal{P}_s f_2(\boldsymbol{y}_s, \xi_s) \\ \text{s.t.} & \\ & \begin{array}{rl} \boldsymbol{h}_1(\boldsymbol{x}) = \boldsymbol{0} & \\ \boldsymbol{g}_1(\boldsymbol{x}) \leq \boldsymbol{0} & \\ \boldsymbol{h}_2(\boldsymbol{x},\ \boldsymbol{y}_s, \xi_s) = \boldsymbol{0} & \forall\ s \in \{1, \ldots, S\} \\ \boldsymbol{g}_2(\boldsymbol{x},\ \boldsymbol{y}_s, \xi_s) \leq \boldsymbol{0} & \forall\ s \in \{1, \ldots, S\} \end{array} \\ & \\ \multicolumn{2}{l}{\text{where } \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^{n_1}, f : \mathbb{R}^{n_1} \rightarrow \mathbb{R}, \boldsymbol{h}_1 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{l_1},} \\ \multicolumn{2}{l}{\boldsymbol{g}_1 : \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{m_1}, \boldsymbol{y}_s \in \mathcal{Y} \subset \mathbb{R}^{n_2}, f_2 : \mathbb{R}^{n_2} \rightarrow \mathbb{R},} \\ \multicolumn{2}{l}{\boldsymbol{h}_2 : \mathbb{R}^{n_2} \rightarrow \mathbb{R}^{l_2}, \boldsymbol{g}_2 : \mathbb{R}^{n_2} \rightarrow \mathbb{R}^{m_2}} \end{array}\right\} \tag{3.22}$$

where $\boldsymbol{y}_s$ is the set of recourse decisions related to the uncertain scenario ξ_s.

It is noteworthy that sampling techniques can be used to approximate to discrete functions the continuous probability functions included in a stochastic program. By doing so, an approximate deterministic equivalent program can be obtained for most stochastic programs.

The deterministic equivalent program of a multistage stochastic optimization can be formulated in a similar manner to program (3.22). However, special care should be taken to preserve the so called *non-anticipativity principle* in such cases.

The non-anticipativity principle

Non-anticipativity of the decision process is an inherent component of stochastic optimization. The non-anticipativity principle ensures that the solution for stage τ does not depend on unavailable information. If two scenarios s and s' are indistinguishable at time t on the basis of information available about them at time t, then the decisions associated to scenarios s and s' until time t must be the same. Namely, a set of decisions related to two different scenarios, if it is to make sense, cannot require different courses of action at time t if there is no way to distinguish between those two scenarios at time t (Rockafellar & Wets, 1991). This principle is shown in Fig. 3.6 by using a scenario tree representation for the different scenarios in which uncertain parameter ξ may disclose throughout the time horizon. Such a principle can be mathematically posed as expressed in Eq. (3.23).

$$\boldsymbol{y}_{t,s} = \boldsymbol{y}_{t,s'} \quad \forall\ t < t^{s,s'} \tag{3.23}$$

In Eq. (3.23), $t^{s,s'}$ is the time when scenarios s and s' become distinguishable; and $\boldsymbol{y}_{t,s}$ represents those decisions associated to scenario s and taken at time t. Note that in order to be consistent with previous notation $\boldsymbol{y}_s = [\boldsymbol{y}_{1,s}^T|\boldsymbol{y}_{2,s}^T|\cdots|\boldsymbol{y}_{t,s}^T|\cdots|\boldsymbol{y}_{t_l,s}^T]^T$, where t_l is the last time period in the

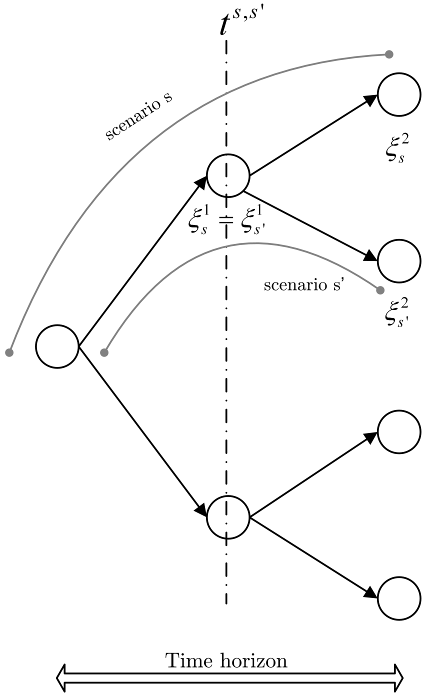


Figure 3.6: The non-anticipativity principle

problem time horizon. The uncertainty encompassed in stochastic problems can be classified in two types according to the nature of $t^{s,s'}$. Hence, one is dealing with *exogenous uncertainty* if $t^{s,s'}$ is fixed, otherwise *endogenous uncertainty* appears when $t^{s,s'}$ is variable and depends upon the decisions to be taken during the optimization.

A multistage stochastic program is presented to deal with the endogenous uncertainty associated to clinical trials during new pharmaceutical products development in Chapter 5. In Chapters 9 and 11, multistage stochastic programs are developed to address the exogenous uncertainty associated to product prices and demand. Good references for stochastic optimization are the books of Kall and Wallace (1994) and Birge and Louveaux (1997).

3.8 Decomposition techniques

There are some mathematical programs that have structural properties that can be computationally exploited. In order to apply a decomposition technique, the problem under study should have an appropriate structure or it may be possible to manipulate the problem to make it have such a structure. Figures 3.7 and 3.8 show the two main decomposable structures that are suitable for decomposition techniques: one involving *complicating constraints* and one involving *complicating variables*.

$$
\begin{array}{llllll}
\text{minimize} & \boxed{f_1(\boldsymbol{x}_1)} + & \boxed{f_2(\boldsymbol{x}_2)} + & \dots + & \boxed{f_N(\boldsymbol{x}_N)} \\
\text{subject to} & & & & \\
& \boxed{\begin{array}{c} \boldsymbol{g}_1(\boldsymbol{x}_1) \le \mathbf{0} \\ \boldsymbol{h}_1(\boldsymbol{x}_1) = \mathbf{0} \end{array}} & & & \\
& & \boxed{\begin{array}{c} \boldsymbol{g}_2(\boldsymbol{x}_2) \le \mathbf{0} \\ \boldsymbol{h}_2(\boldsymbol{x}_2) = \mathbf{0} \end{array}} & & \\
& & & \ddots & \\
& & & & \boxed{\begin{array}{c} \boldsymbol{g}_N(\boldsymbol{x}_N) \le \mathbf{0} \\ \boldsymbol{h}_N(\boldsymbol{x}_N) = \mathbf{0} \end{array}} \\
& \multicolumn{4}{c}{\boxed{\begin{array}{c} \boldsymbol{G}(\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N) \le \mathbf{0} \\ \boldsymbol{H}(\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N) = \mathbf{0} \end{array}}}
\end{array}
$$

Figure 3.7: A decomposable structure with complicating constraints

The idea behind decomposition techniques is to decentralize the solution of the problem; instead of solving the entire problem in a monolithic manner, many blocks or "independent" *subproblems* are solved iteratively while achieving the optimal solution of the whole problem. Note that the set of common equations $\boldsymbol{H}$ and $\boldsymbol{G}$ prevent the problem shown in Fig. 3.7 to be solved in a decentralized manner. If $\boldsymbol{H}$ and $\boldsymbol{G}$ could be disregarded, the problem could be directly optimized by solving each of the n-subproblems. For that reason, the set of constraints $\boldsymbol{H}$ and $\boldsymbol{G}$ are known as complicating constraints. On the other hand, the variable vector $\boldsymbol{y}$ is preventing a decentralized solution for the problem shown in Fig. 3.8. This vector represents the complicating variables of this problem.

In this section a methodology to tackle problems which have a structure with complicating constraints is presented. However, it is important to point out that a structure with complicating variables can be transformed to one with complicating constraints by duplicating the complicating variables.

3.8.1 Lagrangian relaxation

This technique is suitable for problems with complicating constraints. The idea is to apply the duality function (see section 3.2.3) to this kind of problems in order to reduce their complexity. At this point, it is noteworthy that no all the problem constraint must be included in the Lagrangian function in order to construct the dual function (Bazaraa, Sherali, & Shetty, 1993). The Lagrangian function for the problem shown in Fig. 3.7 can then be written as:

$$\mathcal{L}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\scriptscriptstyle N}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \sum_{n=1}^{N} f_n(\boldsymbol{x}_n) + \boldsymbol{\lambda}^T \boldsymbol{H}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\scriptscriptstyle N}) + \boldsymbol{\mu}^T \boldsymbol{G}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\scriptscriptstyle N})$$

Consequently, the dual function can be expressed as the mathematical program (3.24).

$$\left.\begin{array}{lrcl} \phi(\boldsymbol{\lambda}, \boldsymbol{\mu}) = & \underset{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\scriptscriptstyle N}}{\text{Infimum}} & & \mathcal{L}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\scriptscriptstyle N}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \\ \text{subject to} & & & \\ & \boldsymbol{g}_1(\boldsymbol{x}_1) & \leq & \mathbf{0} \\ & & \vdots & \\ & \boldsymbol{g}_{\scriptscriptstyle N}(\boldsymbol{x}_1) & \leq & \mathbf{0} \\ & \boldsymbol{h}_1(\boldsymbol{x}_1) & = & \mathbf{0} \\ & & \vdots & \\ & \boldsymbol{h}_{\scriptscriptstyle N}(\boldsymbol{x}_{\scriptscriptstyle N}) & = & \mathbf{0} \end{array}\right\} \qquad (3.24)$$

Then, the dual problem can be defined by using the program (3.8). The Lagrangian relaxation appears when the dual function is evaluated for given values $\bar{\boldsymbol{\lambda}}$ and $\bar{\boldsymbol{\mu}}$ of the multipliers $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$. Given a structure with complicating constrains, program (3.24) can be decomposed in N subproblems as follows:

$$\left.\begin{array}{lcl} \underset{\boldsymbol{x}_n}{\text{minimize}} & & \mathcal{L}(\boldsymbol{x}_n, \bar{\boldsymbol{\lambda}}, \bar{\boldsymbol{\mu}}) \\ \text{subject to} & & \\ \boldsymbol{g}_n(\boldsymbol{x}_n) & \leq & \mathbf{0} \\ \boldsymbol{h}_n(\boldsymbol{x}_n) & = & \mathbf{0} \end{array}\right\} \qquad (3.25)$$

where $n \in \{1, 2, \ldots, N\}$. Then, the resulting subproblems can be solved independently. This is the main feature of Lagrangian relaxation. The main issue now is to develop a method that is able to determine the optimal values of $\bar{\boldsymbol{\lambda}}$ and $\bar{\boldsymbol{\mu}}$ in an iteratively manner. Many methods have been proposed for this purpose; among them the sub-gradient method, the cutting plane method, the

$$\begin{array}{llcccccll} \text{minimize} & \boxed{f_1(\boldsymbol{x}_1)} & + & \ldots & + & \boxed{f_{\scriptscriptstyle N}(\boldsymbol{x}_{\scriptscriptstyle N})} & + & \boxed{f_y(\boldsymbol{y})} & \\ \text{subject to} & & & & & & & & \\ & \boxed{\begin{array}{c}\boldsymbol{g}_1(\boldsymbol{x}_1)\\ \boldsymbol{h}_1(\boldsymbol{x}_1)\end{array}} & + & & & & & \boxed{\begin{array}{c}\boldsymbol{G}_1(\boldsymbol{x}_1, \boldsymbol{y})\\ \boldsymbol{H}_1(\boldsymbol{x}_1, \boldsymbol{y})\end{array}} & \begin{array}{cc}\leq & \mathbf{0}\\ = & \mathbf{0}\end{array} \\ & & & \ddots & & & & & \\ & & & & & \boxed{\begin{array}{c}\boldsymbol{g}_n(\boldsymbol{x}_{\scriptscriptstyle N})\\ \boldsymbol{h}_{\scriptscriptstyle N}(\boldsymbol{x}_{\scriptscriptstyle N})\end{array}} & + & \boxed{\begin{array}{c}\boldsymbol{G}_{\scriptscriptstyle N}(\boldsymbol{x}_{\scriptscriptstyle N}, \boldsymbol{y})\\ \boldsymbol{H}_{\scriptscriptstyle N}(\boldsymbol{x}_{\scriptscriptstyle N}, \boldsymbol{y})\end{array}} & \begin{array}{cc}\leq & \mathbf{0}\\ = & \mathbf{0}\end{array} \end{array}$$

Figure 3.8: A decomposable structure with complicating variables

bundle method, the augmented Lagrangian method. The next section is dedicated to the Optimal Condition Method.

Optimal condition decomposition

The Optimal Condition Decomposition (OCD) is a particular case of the Lagrangian relaxation procedure. One of OCD advantages is that it provides information to update multiplier estimates ($\bar{\boldsymbol{\lambda}}$ and $\bar{\boldsymbol{\mu}}$) in each subproblem iteration, therefore no master problem exists for this purpose and the algorithm converges in fewer iterations.

The main difference between the OCD and the other classical Lagrangian decomposition methods is that the OCD does not dualize all the complicating constraints. Instead, a subproblem is obtained by dualizing all the complicating constraints of other subproblems, but maintaining its own complicating variables. Following this idea, the Lagrangian function of the n-subproblem would be as follows:

$$
\begin{aligned}
\underset{\boldsymbol{x}_n}{\text{minimize}} \quad & f_n(\boldsymbol{x}_n) + \sum_{n'=1, n' \neq n}^{N} \Big(\boldsymbol{\lambda}_{n'}^T \boldsymbol{H}_{n'}(\bar{\boldsymbol{x}}_1, \ldots, \boldsymbol{x}_n, \ldots, \bar{\boldsymbol{x}}_N) \\
& \qquad + \boldsymbol{\mu}_{n'}^T \boldsymbol{G}_{n'}(\bar{\boldsymbol{x}}_1, \ldots, \boldsymbol{x}_n, \ldots, \bar{\boldsymbol{x}}_N) \Big) \\
\text{subject to} \quad & \\
& \boldsymbol{g}_n(\boldsymbol{x}_n) \leq \mathbf{0} \\
& \boldsymbol{h}_n(\boldsymbol{x}_n) = \mathbf{0} \\
& \boldsymbol{G}_n(\bar{\boldsymbol{x}}_1, \ldots, \boldsymbol{x}_n, \ldots, \bar{\boldsymbol{x}}_N) \leq \mathbf{0} : \boldsymbol{\mu}_n \\
& \boldsymbol{H}_n(\bar{\boldsymbol{x}}_1, \ldots, \boldsymbol{x}_n, \ldots, \bar{\boldsymbol{x}}_N) = \mathbf{0} : \boldsymbol{\lambda}_n
\end{aligned}
\tag{3.26}
$$

Therefore, the OCD does not need any procedure to update the multipliers since this updating process is automatic and results from keeping some complicating constraints in every subproblem. The decomposition methodology is described in Algorithm 3.2. Details about the convergence properties and the procedure of this decomposition technique can be found in Conejo *et al.* (2002). Notice that the application of this technique requires knowledge about the overall problem being addressed and the relationships among the potential subproblems. Ad hoc applications of this decomposition strategy can be found in Chapters 5 and 11.

For further explanations about decomposition techniques in mathematical programming the reader is referred to the book of Conejo, Castillo, Mínguez, and Bertrand (2006).

3.9 Software

Here, it is given a brief description of the software used to solve the optimization models presented throughout this thesis. There are some commercial tools for

Algorithm 3.2: Optimal Condition Decomposition algorithm

Data: Initial values for initialize variables and multipliers $(\hat{\boldsymbol{x}}_n^0, \hat{\boldsymbol{\lambda}}_n^0, \hat{\boldsymbol{\mu}}_n^0)$, gap tolerance (*tolerance*).
Result: The optimal solution $\boldsymbol{x}_n^*, f_n(\boldsymbol{x}_n^*)$.
begin
  $gap \longleftarrow \infty$;
  $k \longleftarrow 0$;
  while $gap > tolerance$ **do**
    forall $n \in 1, \ldots, N$ **do**
      forall $n' \neq n$ **do**
        $\bar{\boldsymbol{x}}_n \longleftarrow \hat{\boldsymbol{x}}_n^k$;
        $\bar{\boldsymbol{\lambda}}_n \longleftarrow \hat{\boldsymbol{\lambda}}_n^k$;
        $\bar{\boldsymbol{\mu}}_n \longleftarrow \hat{\boldsymbol{\mu}}_n^k$;
      Solve sub-problem (3.26);
      $\hat{\boldsymbol{x}}_n^{k+1} \longleftarrow \boldsymbol{x}_n^*$;
      $\hat{\boldsymbol{\lambda}}_n^{k+1} \longleftarrow \boldsymbol{\lambda}_n^*$;
      $\hat{\boldsymbol{\mu}}_n^{k+1} \longleftarrow \boldsymbol{\mu}_n^*$;
    $gap \longleftarrow \|[\hat{\boldsymbol{x}}_1^{k+1} - \hat{\boldsymbol{x}}_1^k]^T| \ldots |[\hat{\boldsymbol{x}}_n^{k+1} - \hat{\boldsymbol{x}}_n^k]^T| \ldots |[\hat{\boldsymbol{x}}_N^{k+1} - \hat{\boldsymbol{x}}_N^k]^T\|$;
    $k \longleftarrow k + 1$;
end

general optimization purposes such as GAMS, AIMMS and AMPL. All of them render very similar characteristics. Nonetheless, GAMS has been selected given that the research group where this thesis is carried out, CEPIMA, is familiar with this tool. Additionally, GAMS is the most widely used modeling and optimization software in the PSE field.

3.9.1 GAMS – Generic Algebraic Modeling System

GAMS is a programming language that allows modeling and solving optimization problems. Castillo, Conejo, Pedregal, García, and Alguaci (2001) point out that the more important characteristics of GAMS are:

- The ability to model small size problems and afterwards transform them into large scale problems without significantly varying the code.
- The modeling task is completely apart from the solving procedure. Once the model of the system under study has been built, one can choose among the diverse solvers available to optimize the problem.
- In GAMS the model representation is analogous to the mathematical description of the problem. Then, learning GAMS language is almost natural for those working in the optimization field.

- GAMS provides various programming features that allow coding decomposition algorithms without requiring additional software.
- GAMS can be easily linked with MATLAB (The Mathworks, 1998) using the matgams (Ferris, 1999) library if some special data manipulation is needed.

Finally, it should be mentioned that optimization algorithms outlined in sections 3.3 to 3.5 are embedded in some of the different GAMS solvers. Each solver is usually developed to tackle a specific type of program (i.e., LP, NLP, MILP, MINLP).

3.10 Final remarks

In this chapter, the different optimization techniques used throughout this thesis have been outlined. The main ideas behind each technique have been briefly introduced with the purpose of providing the reader a general understanding of the theory behind the solution techniques applied in this thesis. For the interested reader, specialized references where in-depth explanations and discussions can be found are quoted at the end of each section.

In order to implement Multi-objective optimization, stochastic programming and decomposition techniques in GAMS, one requires to have a good understanding of their principles. For that reason, special emphasis has been made to these topics. That is not the case of "basic" linear, nonlinear and mixed integer programming since the algorithms to solve this kind of problems are already embedded in the solvers. However, it is necessary to know their fundamentals in order to interpret results and improve modeling and debugging skills.

Part II

Functional Business Integration for Strategic Decision Making

Chapter 4

Enhancing Corporate Value in the Design of SCs

4.1 Introduction

The tight profit margins under which Process Industries operate are forcing companies to pay more and more attention to the design and operation of their SCs. Traditional approaches available in the PSE literature to address the design and operation of SCs usually focus on the process operations side and neglect the financial part of the problem. This chapter deals with the design and retrofit of SCs.

In simple terms, the SC design problem involves the identification of the combination of suppliers, producers, and distributors able to provide the right mix and quantity of products and services to customers in an efficient way (Talluri & Baker, 2002). Here, a novel framework to address this problem is proposed. Its main novelty lies in the inclusion of financial considerations at this strategic decision making level. Within this framework, the decisions that have a long-lasting effect on the firm are assessed through integrated models that are capable of holistically optimizing the combined effects of process operations and finances. The proposed approach adopts the corporate value of the firm as the objective to be maximized. The integrated solution guarantees the feasibility of the strategic decisions from the financial point of view by ensuring liquidity control. Furthermore, it also leads to a superior economic performance as it exhibits a greater capacity of improving the value of the firm.

4.2 Integrating process operations and finances

The design and operation of an SC can both be posed as large-scale dynamic decision problems (Applequist, Pekny, & Reklaitis, 2000). These problems are receiving increasing attention in both the Operations Research and the PSE communities and, as a result of this effort, significant progress has been made in problem formulations and decomposition strategies aiming at their solution.

One of the major challenges in the chemical industry for the new millennium is the optimization of the SC operation to achieve value preservation and growth (Grossmann, 2004). Unfortunately, the SC models that currently exist usually assist practitioners in determining the location of the facilities embedded in the network, as well as the tasks that should be accomplished at each moment in order to maximize a given criteria. This kind of models are no longer enough. If companies want to achieve a competitive advantage in the marketplace, they must implement tools that play a more inter-functional role and are able to provide integrated plans for the whole SC. These plans should include optimal financial as well as operative planning decisions in terms of value preservation.

Recent advances in PSE have focused on devising enterprise wide modeling and optimization strategies that integrate decisions of distinct business functions into a global model. Nevertheless, despite the effort made in the area, almost all of the models developed to date focus on the process operations side and neglect decisions involving marketing campaigns, investment planning, corporate financial decisions, and many others aspects of enterprise planning related to SCM (Shapiro, 2004). Current approaches still address the overall problem in a sequential fashion through the optimization of partial KPIs. The use of these traditional sequential procedures is mainly motivated by the functional organizational structures of firms. Nowadays, companies still have separate departments for production, supply, logistics, service to customers, etc. In an environment of this type, each functional area's plan is sequentially considered as input to the others according to a hierarchy. Thus, the models supporting the decision-making operate in an isolated way. They optimize partial sets of decision variables but they do not lead to real integration of relationships despite promoting the sharing of information between different business entities (Romero, Badell, Bagajewicz, & Puigjaner, 2003). This partitioning of decision-making in companies has been reflected in the goals of the studies and the optimization models developed to support them.

Today's turbulent business environment has caused a greater awareness among managers of the financial dimension of decision making, with business managers progressively becoming more driven by the goal of enhancing shareholder value. Owing to this, planning and scheduling models for SCM should proposed solutions that improve an overall business performance measure; however, they usually disregard the financial side of the problem and pursue a biased key performance indicator as the objective to be optimized. In fact, most of the available SC approaches account for the maximization of objectives that are based on the classical transactional analysis of costs and benefits, or in key operative parameters that act as intermediate cost-related performance measures. Table 4.1 shows the results of a review made to analyze the KPIs applied so far in SC modeling in the PSE field. The objective functions of these approaches have been classified into four categories: (i) economic basis, (ii) cus-

Table 4.1: Supply Chain Models for the CPI

	Performance Measures																		
	Economic basis							Customer service basis		Efficiency basis					Environmental basis				
Authors	Dividend	Net Revenue	Profit	Cost	NPV	Risk	Equity	CSL	Earliness	Tardiness	Inventory Level	Makespan	Setup	Cleanup	Facilities utilization	Material Consumption	Energy Consumption	Waste Generation	Eco-indicator 99
Ahmed and Sahinidis (1998)					✓														
Applequist *et al.* (2000)					✓	✓													
Berning *et al.* (2002)[a]									✓	✓	✓	✓	✓	✓					
Badell *et al.* (2004)	✓	✓	✓				✓												
Bok *et al.* (2000)			✓																
Cakravastia *et al.* (2002)				✓						✓									
Chen and Lee (2004)			✓					✓			✓								
Fandel and Stammen (2004)			✓																
Gjerdrum *et al.* (2001)			✓																
Guillén-Gosálbez *et al.* (2006a, 2005a, 2006b)					✓	✓	✓	✓											
Gupta and Maranas (2003)				✓															
Gupta, Maranas, and McDonald (2000)				✓															
Hugo and Pistikopoulos (2005)					✓														✓
Iyer and Grossmann (1998)					✓														
Ryu *et al.* (2004)				✓															
Jung *et al.* (2004)				✓															
Kallrath (2002)		✓	✓	✓															

Continued on next page

[a]The objective function is a weighted sum of performance measures indicated in the Table

Table 4.1 – continued from previous page

	Performance Measures																		
	Economic basis							Customer service basis			Efficiency basis					Environmental basis			
Authors	Dividen	Net Revenue	Profit	Cost	NPV	Risk	Equity	CSL	Earliness	Tardiness	Inventory Level	Makespan	Setup	Cleanup	Facilities utilization	Material Consumption	Energy Consumption	Waste Generation	Eco-indicator 99
Lababidi *et al.* (2004)				✓															
Lasschuit and Thijssen (2004)				✓															
Lee, Lee, and Reklaitis (2000)			✓																
Liu and Sahinidis (1996)					✓														
Mokashi and Kokossis (2003)				✓															
Neiro and Pinto (2004)			✓																
Oh and Karimi (2004)					✓														
Papageorgiou *et al.* (2001)					✓														
Perea-López *et al.* (2003)			✓																
Romero *et al.* (2003)	✓																		
Sabri and Beamon (2000)				✓				✓											
Seferlis and Giannelos (2004)				✓															
Shulz *et al.* (2005)			✓																
Sundaramoorthy and Karimi (2004)			✓																
Tsiakis *et al.* (2001)				✓															
Türkay *et al.* (2004)				✓															
Wan *et al.* (2005)				✓															
Zhou *et al.* (2000)			✓					✓							✓	✓	✓	✓	

tomer service basis, (iii) efficiency basis and (iv) environmental basis. As one can see from Table 4.1, profit and cost have been the most exploited indicators while financial matters have been systematically neglected in the models devised to date in the literature.

Nevertheless, the effective control of cash is one of the most important requirements of financial management and its steady and healthy circulation throughout the entire business operation has repeatedly been shown to be the basis of business solvency (Howard & Upton, 1953). Indeed, the availability of cash governs the production decisions taken in a company. For this reason, SC operations models should not consider cash as an infinite resource. A production plan cannot be implemented if it violates the minimum cash flow imposed by the firm (i.e., if the amount of raw materials and/or utilities required cannot be purchased due to a temporary lack of cash). Moreover, assessing the feasibility of the scheduling/planning decisions from a financial point of view may not be enough for companies that want to achieve a competitive advantage in the marketplace. Fierce competition in today's global markets is forcing companies to perform further financial analysis in order to find the best production-distribution decisions to be carried out in their SCs. If they wish to remain competitive, it is essential that they properly assess the different process operations alternatives in terms of their ability to markedly enhance the firm's value. What is more, maximum-profit or minimum-cost decisions may lead to poor financial results if their financial impact is not properly assessed prior to being implemented.

Consequently, managers should extend their analysis to include the more general objective of maximizing the firm's value as opposed to the common optimization of traditional biased key performance indicators (KPIs) such as cost or profit. Calculating the firm's value involves a number of complex issues, although there is consensus as to Buffet's view that the valuation of a business is determined by the discounted free cash flows occurring from its operations over its lifetime (Buffet, 1994). Therefore, the challenge faced by SC managers who are seeking to enhance corporate value is to identify strategies that improve free cash flow generation.

In order to create value, companies need to devise integrated approaches for SCM. Such enterprise-wide management strategies are envisaged to be capable of holistically optimizing the combined effects of process operations and finances so as to exploit the synergy between different management disciplines. In fact, the need to extend the studies and analysis of process operations to incorporate financial considerations has been widely recognized in the literature (Applequist *et al.*, 2000; Shapiro, 2006, 2004; Grossmann, 2004; Shah, 2005). Notwithstanding, relatively few integrated corporate financial models have been implemented so far (Yi & Reklaitis, 2003, 2004; Guillén-Gosálbez *et al.*, 2006a).

Fact-based strategic planning is increasingly desired and pursued by firms, but many issues remain about how to do it (Shapiro, 2004). Optimization models seem to offer an appealing framework for analyzing corporate financial decisions and constraints, as well as for integrating them with process operation decisions and constraints (Shapiro, 2006). Currently, with the recent advances in optimization theory and software applications there is no apparent reason why models for SCM that merge concepts from diverse areas of the firm cannot be constructed.

This chapter proposes a general framework for the design of SCs based on the development of holistic models which cover two areas of the company, the process operations and the finances. To achieve this goal (i.e., the integration of the decision-making at different business levels) a mathematical formulation which utilizes mixed integer modeling techniques and merges variables and constrains belonging to each of the above mentioned disciplines is derived and applied to a case study. The presented strategy considers the financial performance as a design objective and not merely as a constraint on operations. Furthermore, the corporate value (CV) of the firm is adopted as the objective to be maximized as an alternative to the commonly used profit or cost. The resulting model can be used as a decision-support tool for strategic planning. The main advantages of this approach are highlighted through a case study in which the integrated strategy is compared with the traditional approach that computes the maximum-profit or net present value (NPV) design without financial considerations. Numerical results show that significant benefits can be obtained if an integrated formulation accounting for the optimization of a suitable financial performance indicator is applied.

4.3 Problem statement

The intent of the SC network design problem is typically to determine the optimal manufacturing and distribution network for the entire product line of a company. The most common approach is to formulate a large-scale mixed-integer linear program that captures the relevant fixed and variable operating costs for each facility and each major product family. The fixed costs are usually associated with the investment and/or overhead costs for opening and operating a facility, or with placing a product family in a facility. The variable costs include not only the manufacturing, procurement and distributions costs, but also the tariffs and taxes that depend on the network design. The network design problem focuses on the design of two or three major echelons in the SC for multiple products. Due to the nature of the problem being solved, network design is typically solved every two to five years (Graves & Willems, 2003).

With regard to the financial area, it is widely recognized that financial assets bear a strong and direct relation to core aspects of SCs, such as inventories, capacity expansion and allocation and purchases of raw material and services. Most SC modeling approaches also account for fixed assets when the economic performance of the available alternatives is assessed in the design phase. However, in the planning formulation, they usually ignore the net working capital (NWC), which represents the variable assets associated with the

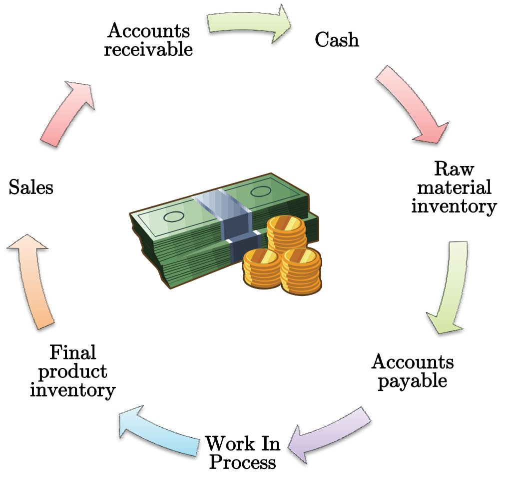


Figure 4.1: Cash conversion cycle

daily SC operations. NWC is constituted by material inventories, accounts receivable (physical distribution), accounts payable (procurement), and cash. All of these components are directly affected by decisions regarding SC operations. NWC can be understood as the capital tied up within the cash conversion cycle, which measures how efficiently an enterprise converts its inputs into cash through final product sales (Figure 4.1). The less capital that is tied up by SC operations, the better the performance will be in terms of the business's bottom line. The NWC is not a static figure; indeed, it may change from period to period throughout the planning horizon, in accordance with tactical SC decisions.

The mathematical program endeavors to model the CV components that are specified in Figure 4.2. Among these components, the NWC and its change is explicitly considered. The CV of the firm is calculated by means of the discounted-free-cash-flow (DFCF) method and is adopted as the objective to be maximized.

The deterministic design/planning problem of a multi-echelon SC with financial considerations can be stated as follows.

The following information is given:

Process operations data

- A fixed time horizon.
- A set of products.
- A set of markets where products are available to customers and their demands.
- A set of potential geographical sites for locating manufacturing plants and distribution centers.

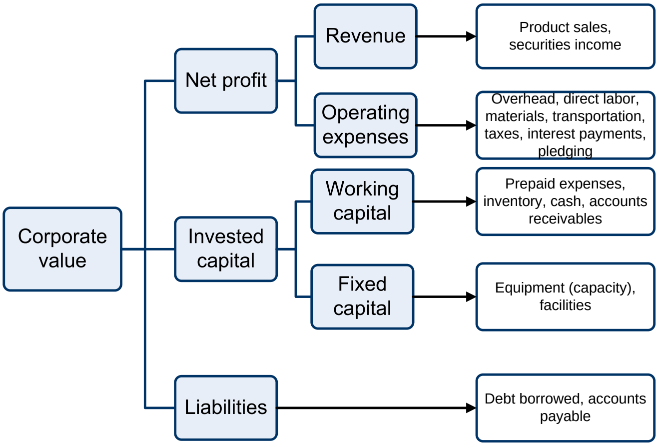


Figure 4.2: Corporate value components

- A set of potential equipment for manufacturing the different products at the set of plants.
- Lower and upper bounds for capacity increment of equipment and distribution centers .
- Product recipes (mass balance coefficients and consumption of capacity).
- Suppliers capacity.
- Minimum utilization rate of capacity.

Financial data

- Direct cost parameters such as production, handling, transportation and raw material costs.
- Product prices at each market during the time horizon.
- Coefficients for investment and sales of marketable securities.
- Discount factors for prompt payment and amount purchased to suppliers.
- Relationship between capital investment and capacity of plants and distribution centers.
- Relationship between indirect expenses and equipment capacity of plants and distribution centers.
- Pledging costs.
- Tax rate and number of depreciation time periods.
- Interest rate for the long and short term debt.
- Salvage value.
- Shareholders risk premium data.

The goal is to determine:

- The facilities to be opened.
- The increment of equipment capacity at each potential plant and distribution center.

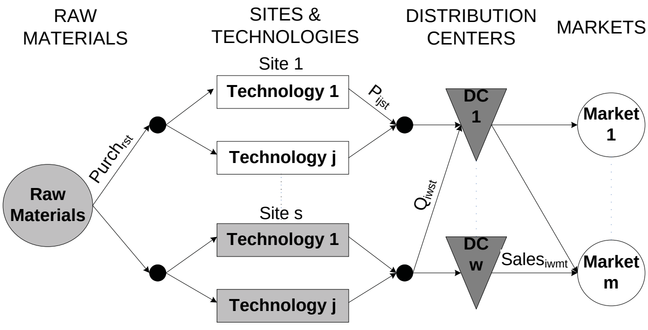


Figure 4.3: Supply chain model structure.

- The assignment of manufacturing and distribution tasks to the network nodes.
- The amount of final products to be sold.
- The investments and sales of marketable securities.
- The amount of accounts receivable pledged at each period.
- The schedule of payments to suppliers at each time period.
- The long and short term debt acquired and repaid at each time period.

such that corporate value evaluated at the end of the planning horizon is maximized.

4.4 Mathematical formulation: a holistic model

The mathematical formulation derived to address the problem described above is next presented. The model variables and constraints can be classified into four groups. The first one concerns the process operations constraints given by the SC topology. The equations that allows integrating the operations and financial models are included in the second group. The third one deals with the financial area. Finally, the equations and variables required to compute the corporate value are presented. These sets of equations are next described in detail.

4.4.1 Design–planning formulation

The structure of the SC taken as reference to develop the mathematical model is illustrated in Fig. 4.3. The design/planning mathematical formulation is based on the work of Hugo and Pistikopoulos (2005) in which the authors presented a mathematical methodology that included life cycle assessment criteria as an additional objective to be optimized at the strategic level of SCM. The model has been enhanced to allow the storage of products and to include distribution center nodes in the SC network. The model equations are described in detail in the next sections.

Mass balance constraints

The mass balance must be satisfied in each of the nodes that integrate the SC network.

Manufacturing sites Eq. (4.1) represents the mass balance for each raw material r consumed at each manufacturing site s in every time period t. Thus, this equation states that the purchases of raw material r provided by suppliers e (E_r) plus the initial inventory kept at the site must equal the inventory at the end of period t plus the quantity consumed by the manufacturing tasks. Note that this equation should be only applied to those products consuming raw material r ($i \in (I_j \cap I_r)$) and manufactured in equipment j of plant s.

$$\sum_{e \in E_r} Purch_{erst} + SI_{rst-1} = SI_{rst} + \sum_{j} \sum_{i \in (I_j \cap I_r)} \alpha_{rij} P_{ijst} \qquad \forall\ r, s, t \quad (4.1)$$

The mass balance for final products i in each manufacturing site s is enforced via Eq. (4.2). This expression states that the amount of final product manufactured at each site during a given time period t plus the initial stock of the product must equal the final inventory of the product plus the amount transported from the site to the distribution centers w.

$$\sum_{j \in J_i} P_{ijst} + SO_{ist-1} = SO_{ist} + \sum_{w} Q_{iwst} \qquad \forall\ i, s, t \quad (4.2)$$

Distribution centers Eq. (4.3) expresses the mass balance for distribution centers w. Thus, this equation states that the total amount of final product i coming from all sites s plus the initial inventory of the product kept at the distribution center must equal the final inventory plus the sales in final markets m.

$$\sum_{s} Q_{iwst} + SW_{iwt-1} = SW_{iwt} + \sum_{m} Sales_{iwmt} \qquad \forall\ i, w, t \quad (4.3)$$

Marketplaces Unlike other models in the literature, this model assumes that part of the demand can actually be left unsatisfied due to limited production capacity. Thus, Eq. (4.4) forces the sales of product i carried out in market m during time period t to be less than or equal to the demand.

$$\sum_{w} Sales_{iwmt} \leq Dem_{imt} \qquad \forall\ i, m, t \quad (4.4)$$

The ability of responding to customer requirements turns out to be one of the most basic functions of SCM (Guillén-Gosálbez *et al.*, 2005b). Thus, customer service level (CSL) should also be taken into consideration when formulating a SC model (Chen *et al.*, 2003). As proposed by Guillén-Gosálbez *et al.*

(2005b), constraint (4.5) can be considered to explicitly take into account the demand satisfaction strategy of the enterprise. This equation imposes a minimum target for the demand satisfaction ($MinCLS$), which must be attained in all time periods t.

$$\frac{\sum_i \sum_w \sum_m Sales_{iwmt}}{\sum_i \sum_m Dem_{imt}} \geq MinCLS \qquad \forall\ t \tag{4.5}$$

Capacity and facilities location constraints

These constraints are also inspired in the work of Hugo and Pistikopoulos (2005). Two different variables are defined, FS_{jst} and FW_{wt}, which represent the total capacity of equipment j in manufacturing sites s and distribution centers w respectively during time period t.

Furthermore, variables FSE_{jst} and FWE_{wt} denote the capacity expansion of the different facilities of the network during time period t. Thus, the establishment of a facility takes place in the first time period in which these variables take a non-zero value. Note that the model is general enough to address not only the design of a new SC, but also the retrofitting of an existing network. In the latter case, the problem should be formulated by fixing at time period $t = 0$ the value of the variables representing the facilities capacity according to the initial network topology.

Capacity expansion Eqns. (4.6) and (4.7) are added to control the changes in facilities capacities over time. These constraints include the binary variables V_{jst} and X_{wt}, which take a value of 1 if the facility being represented (either the equipment j at manufacturing site s or the distribution center w) is expanded in capacity and zero otherwise. Notice that the capacity increments are bounded in the range $[FSE^L_{jst}, FSE^U_{jst}]$, which represents the realistic physical interval in which they must fall.

$$V_{jst} FSE^L_{jst} \leq FSE_{jst} \leq V_{jst} FSE^U_{jst} \qquad \forall\ j, s, t \tag{4.6}$$

$$X_{wt} FWE^L_{wt} \leq FWE_{wt} \leq X_{wt} FWE^U_{wt} \qquad \forall\ w, t \tag{4.7}$$

Eqns. (4.8) and (4.9) are added to update the total capacity (FS_{jst} and FW_{wt}) by the amount increased during planning period t (FSE_{jst} and FWE_{wt}).

$$FS_{jst} = FS_{jst-1} + FSE_{jst} \qquad \forall\ j, s, t \tag{4.8}$$

$$FW_{wt} = FW_{wt-1} + FWE_{wt} \qquad \forall\ w, t \tag{4.9}$$

Establishing of new facilities Eqns. (4.10) to (4.12) are included to determine the planning period t when a manufacturing site s initiates its operations. SB_{st} is a binary variable that takes the value of 1 if the facility is opened at period t and 0 otherwise. Equation (4.10) enforces the necessary conditions to define the new binary variable. Thus, if the binary variable that represents the capacity increment of any equipment j at site s in period t (V_{jst}) equals one, the summation of the new binary variable from the initial period to the current one must also equal one. Equation (4.12) is the reformulation of the previous logic condition and it is obtained by replacing the implication by its equivalent disjunction (see Equation 4.11). Equation (4.13), which is similar to constraint (4.12), is applied to enforce the definition of the binary variable SW_{wt}, which must equal 1 if the warehouse w is opened in period time t and 0 otherwise.

$$V_{jst} = 1 \Rightarrow \sum_{t'=1}^{t} SB_{st'} = 1 \qquad \forall\ j, s, t \tag{4.10}$$

$$[\neg V_{jst}] \vee [\sum_{t'=1}^{t} SB_{st'} = 1] \qquad \forall\ j, s, t \tag{4.11}$$

$$1 - V_{jst} + \sum_{t'=1}^{t} SB_{st'} \geq 1 \qquad \forall\ j, s, t \tag{4.12}$$

$$1 - X_{wt} + \sum_{t'=1}^{t} SW_{wt'} \geq 1 \qquad \forall\ w, t \tag{4.13}$$

Capacity utilization Eq. (4.14) forces the total production rate in each plant to be greater than a minimum desired production rate ($\beta_{sj} FS_{jst-1}$) and lower than the available capacity (FS_{jst-1}). In this equation, θ_{ij} represents the capacity utilization rate of equipment j by product i and β_{sj} is the minimum percentage of utilization of equipment j at site s.

$$\beta_{sj} FS_{jst-1} \leq \sum_{i \in I_j} \theta_{ij} P_{ijst} \leq FS_{jst-1} \qquad \forall\ j, s, t \tag{4.14}$$

Eq. (4.15) is analogous to constraint (4.14). Here, υ_i and γ_w constitute the specific volume of product i and the minimum percentage of capacity utilization of distribution center w, respectively.

$$\gamma_w FW_{wt-1} \leq \sum_{i} \upsilon_i SW_{iwt} \leq FW_{wt-1} \qquad \forall\ w, t \tag{4.15}$$

Suppliers limitations The model assumes a maximum availability of raw materials. Thus, Eq. (4.16) forces the amount of raw material r purchased from supplier e at each time period t to be lower than an upper bound given by physical limitations (A_{ert}). In this expression, R_e denotes the set of raw materials provided by supplier e.

$$\sum_{s} Purch_{erst} \leq A_{ert} \qquad \forall\ e, r \in R_e, t \tag{4.16}$$

4.4.2 Integration between models

The integration between both formulations is carried out through the sales of products, the purchases of raw materials, transport services and utilities to final providers, the fixed cost associated with the operation of the network and the total investment in capital.

Revenue

Revenue is calculated by means of net sales which are the income source related to the normal SC activities. Thus, the total revenue incurred in any period t can be easily computed from the sales of products executed in period t as it is stated in Eq. (4.17).

$$ESales_t = \sum_{i}\sum_{w}\sum_{m} Sales_{iwmt} Price_{imt} \qquad \forall\ t \tag{4.17}$$

Additionally, the cash collected from sales executed in any period t and maturing in period t' ($ASales_{tt'}$) can be easily computed from the sales of products executed in period t, the fraction of these sales that will be collected in period t' and the prices of the products sold, as it is stated in equation (4.18). Here, $\delta_{mtt'}$ denotes the fraction of sales carried out in market m in period t that will be paid in period t'.

$$ASales_{tt'} = \sum_{i}\sum_{w}\sum_{m} Sales_{iwmt}\delta_{mtt'} Price_{imt} \qquad \forall\ t, t' > t \tag{4.18}$$

Direct cost

The external purchases from supplier e at every period t ($EPurch_{et}$), which are computed through equation (4.19), include the purchases of raw materials and transport services and production utilities.

$$EPurch_{et} = Purch_{et}^{rm} + Purch_{et}^{tr} + Purch_{et}^{prod} \qquad \forall\ e, t \tag{4.19}$$

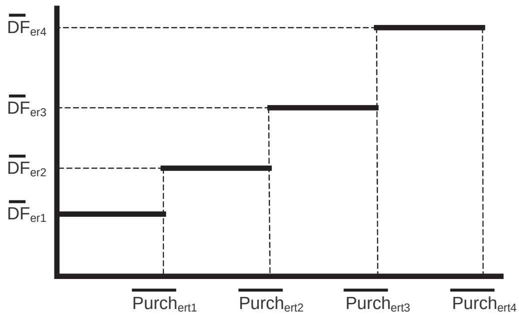


Figure 4.4: Piecewise linear function of the discount factors.

Raw materials The external raw material purchases to supplier e at every period t ($EPurch_{et}$) can be then computed through equation (4.20).

$$Purch_{et}^{rm} = \sum_{r}\sum_{s} Purch_{erst}\psi_{ert} \qquad \forall\ e,t \tag{4.20}$$

Quantity discount Furthermore, Eqns. (4.21) to (4.23) can be added to model quantity discounts, i.e., price reductions offered by the suppliers to induce large orders. Certainly, the relationship between the discount factor offered by external supplier e for raw material r (DF_{erd}) and the amount of raw material purchased can be modeled as a piecewise linear function (see Figure 4.4). The inclusion of these constraints allows the potential benefits of reduced purchase prices and fewer orders to be traded-off against the increase in inventory costs. Specifically, one defines a set of discounts intervals D_{er} for each raw material r for which supplier e offers quantity discounts ($r \in DR_e$). Each interval corresponds to a different discount factor DF_{erd}. The limits of interval $d \in D_{er}$ are denoted as $\overline{Purch}_{ertd-1}^{rm}$ and $\overline{Purch}_{ertd}$. We introduce a new set of binary variables F_{ertd} that take the value of 1 if the amount of raw material r purchased from supplier e in period t by all the sites falls into discount interval d, and 0 otherwise:

$$F_{ertd} = \begin{cases} 1 & \text{if } Purch_{ert}^{rm} \in [\overline{Purch}_{ertd-1}^{rm}, \overline{Purch}_{ertd}^{rm}] \\ 0 & \text{otherwise} \end{cases}$$

To enforce the above definition, the following linear constraints are applied (Tsiakis *et al.*, 2001):

$$\sum_{d \in D_{er}} F_{ertd} = 1 \qquad \forall\ e \in DR_e, r, t \tag{4.21}$$

$$\begin{aligned} F_{ertd-1}\overline{Purch}_{ertd-1}^{rm} \leq Purch_{ertd}^{rm} \leq F_{ertd}\overline{Purch}_{ertd}^{rm} \\ \forall\ e \in DR_e, r, t, d \in D_{er} \end{aligned} \tag{4.22}$$

$$Purch_{ert}^{rm} = \sum_{d \in D_{er}} Purch_{ertd}^{rm} \qquad \forall\ e \in DR_e, r, t \tag{4.23}$$

Constraint (4.21) forces each order to fall into a single interval, i.e., only one of the variables X_{ertd} (say, for $d = d^*$) takes a value of 1, with all others being zero. Constraint (4.22) allocates each of the orders to its corresponding interval using the defined binary variable F_{ertd}. Such equation forces the auxiliary continuous variable $Purch_{ertd}^{rm}$ to equal 0 for all $d \neq d^*$, while also bounding $Purch_{ertd^*}$ in the range $[\overline{Purch}_{ertd^*-1}^{rm}, \overline{Purch}_{ertd^*}^{rm}]$. Finally, constraint 4.23 expresses the condition for which the summation of the auxiliary variable $Purch_{ertd}^{rm}$ over d must equal the variable $Purch_{ert}$. This implies that $Purch_{ert}^{rm} = Purch_{ertd^*}^{rm}$ and, therefore, $Purch_{ert}^{rm} \in [\overline{Purch}_{ertd^*-1}^{rm}, \overline{Purch}_{ertd^*}^{rm}]$, as desired. Note that similar constraints could be easily derive to account for other types of quantity discounts, i.e., in utilities, transportation services and so forth.

Taking into account the discounts offered by the suppliers e for raw material r for a set of discount intervals d, which are denoted by DF_{erd}, the total amount of money to be invested in raw materials is the following:

$$Purch_{et}^{rm} = \sum_{r} \sum_{d \in D_{er}} Purch_{ertd}^{rm} \psi_{ert} F_{ertd} (1 - DF_{erd}) \qquad \forall\ e \in DR_e, t \tag{4.24}$$

Distribution and production costs On the other hand, external "purchases" of transport services and production utilities are determined through equations (4.25) and (4.26). Here, ρ_{eiws}^{tr1} and ρ_{eiwm}^{tr2} denote the unitary transport cost associated with sending products from plants to warehouses and from warehouses to markets, respectively. Furthermore, τ_{ijse}^{ut1} represents the unitary production cost associated to the plants, whereas τ_{rse}^{ut2}, τ_{ise}^{ut3}, and τ_{iwe}^{ut4} represent the inventory costs.

$$Purch_{et}^{tr} = \sum_{i} \sum_{j} \sum_{s} Q_{iwst} \rho_{eiws}^{tr1} + \sum_{i} \sum_{w} \sum_{m} Sales_{iwmt} \rho_{eiwm}^{tr2} \qquad \forall\ e, t \tag{4.25}$$

$$\begin{aligned} Purch_{et}^{prod} = & \sum_{i} \sum_{j} \sum_{ijs} P_{ijst} \tau_{ijse}^{ut1} + \sum_{r} \sum_{s} SI_{rst} \tau_{rse}^{ut2} + \\ & \sum_{i} \sum_{s} SO_{ist} \tau_{ise}^{ut3} + \sum_{i} \sum_{w} SW_{iwt} \tau_{iwe}^{ut4} \qquad \forall\ e, t \end{aligned} \tag{4.26}$$

Indirect cost

The total fixed cost of operating a given SC structure in every time period t can be computed by means of equation (4.27) as the sum of the fixed costs associated with the current plant equipment j already installed in every site s ($FCFS_{jst}FS_{jst-1}$) plus the sum of the fixed costs of each distribution center w ($FCFW_{wt}FW_{wt-1}$).

$$FCost_t = \sum_j \sum_s FCFS_{jst}FS_{jst-1} + \sum_w FCFW_{wt}FW_{wt-1} \qquad \forall\, t \quad (4.27)$$

Investment

Finally, the total investment in capital or fixed assets is computed through equation (4.28). This term includes the investment made to expand the capacity of equipment j in manufacturing site s in period t ($Price^{FS}_{jst}FSE_{jst}$), plus the investment required to open a manufacturing plant, in case it is opened at period t ($I^S_{st}SB_{st}$), plus the investment required to support distribution center w capacity increase ($Price^{FW}_{wt}FWE_{wt}$), plus the investment required to set a distribution center if it is opened at period t ($I^S_{st}SB_{st}$).

$$\begin{aligned} FAsset_t = \sum_s \left(\sum_j Price^{FS}_{jst}FSE_{jst} + I^S_{st}SB_{st} \right) + \\ \sum_w \left(Price^{FW}_{wt}FWE_{wt} + I^W_{wt}SW_{wt} \right) \qquad \forall\, t \end{aligned} \quad (4.28)$$

4.4.3 Financial formulation

In the presented approach, the cash management associated with the SC operation is analyzed by extending the mathematical formulation developed by Guillén-Gosálbez *et al.* (2006a). Such formulation is thus connected to the process operations variables and constraints through the periods and sizes of purchases of raw materials and utilities from suppliers, the final products sales to customers and the investment costs. As a result of the application of this integrated model, optimal SC design and financial decisions can be computed simultaneously. Therefore, payments to providers, short and long term borrowing, pledging decisions and the buying/selling of securities are planned in conjunction with manufacturing and distribution tasks. The financial side of the problem is then tackled through the inclusion of a set of constraints that accommodate the aforementioned economical issues. Such constraints are next described in detail.

Cash management model

The financial variables and constraints of the model should be determined according to the specific applicable rules (e.g., depreciation), legislation (e.g, taxes), etc. This may lead to different formulations depending on the case being analyzed. To overcome this problem, a set of general equations which intend to reflect a general case have been developed. Nevertheless, the mathematical formulation is general enough to be extended to other particular cases.

The financial model considers the same t planning periods applied in the strategic SC formulation that cover the whole time horizon. This assumption allows an easy integration of both sets of constraints into a single holistic model.

The cash balance for each planning period is the following:

$$\begin{aligned} Cash_t = {} & Cash_{t-1} + ECash_t + Net_t^{CLine} - \sum_e \sum_{t'=1}^{t} Pay_{et't} - FCost_t \\ & + Net_t^{MS} - FAsset_t + Capital_t + Net_t^{LDebt} + Other_t \qquad \forall\, t \end{aligned} \tag{4.29}$$

The cash at each period t ($Cash_t$) is a function of the available cash at period $t-1$ ($Cash_{t-1}$), the exogenous cash from sales of products or, in general, from any other cash inflow ($ECash_t$), the amount borrowed or repaid to the short-term credit line (Net_t^{CLine}), the raw materials, production and transport payments on accounts payable incurred in any previous or actual period t ($Pay_{ett'}$), the fixed cost ($FCost_t$), the sales and purchases of marketable securities (Net_t^{MS}), the amount invested on facilities ($FAsset_t$), the capital supported by the shareholders of the company ($Capital_t$), the amount borrowed or repaid to the long-term credit line (Net_t^{LDebt}) and finally other expected cash outflows or inflows ($Other_t$).

Pledging and receivables A certain proportion of accounts receivable may be pledged at the beginning of a period. Pledging is the transfer of a receivable from the previous creditor (i.e., assigner) to a new creditor (i.e., assignee). Therefore, when a firm pledges its future receivables, it receives in the same period only a part, normally 80%, of their face value. Thus, it can be assumed that a certain proportion of the receivables outstanding at the beginning of a period is received during that period through pledge, as stated by Eq. (4.30).

$$\sum_{t''=t-\tilde{d}_M^{max}}^{t'} Pled_{tt''} \leq \sum_{t''=t-\tilde{d}_M^{max}}^{t'} ASales_{t''t} \qquad \forall\, t, \forall\, t-\tilde{d}_M^{max} \leq t'' \leq t \tag{4.30}$$

In this equation the variable $Pled_{tt'}$ represents the amount pledged within period t' on accounts receivable maturing in period t, while $ASales_{t't}$ represents the accounts receivable associated with the sales of products executed in period t' and maturing in t. Here, the parameter d_M^{max} denotes the maximum maturing period at the markets.

$$\tilde{d}_M^{max} = \max_m \left\{ \tilde{d}_m \right\} \tag{4.31}$$

Note that pledging represents a very expensive way of getting cash that will only be used when no more credit can be obtained from the bank.

Finally, the exogenous cash is computed by means of Eq. (4.32) as the difference between the amount of sales maturing in period t and executed in previous periods t' ($ASales_{t't}$) minus the amount of receivables pledged in previous periods on accounts receivable maturing in period t, plus the amount pledged in the actual period on accounts receivable maturing in future periods. In this expression, $\phi_{t't}$ represents the face value of the receivables being pledged.

$$\begin{aligned} ECash_t = & \sum_{t'=t-\tilde{d}_M^{max}}^{t} ASales_{t't} - \sum_{t'=t-\tilde{d}_M^{max}}^{t-1} Pled_{tt'} \\ & + \sum_{t'=t+1}^{t+\tilde{d}_M^{max}} \phi_{t't} Pled_{t't} \qquad \forall\, t \end{aligned} \tag{4.32}$$

Payment to suppliers With regard to payable, which are due to the consumption of raw materials, production and transport services, notice that the formulation assumes that the financial officer, at his/her option, may stretch or delay payments on such accounts. Discounts for prompt payment can be obtained if purchases are paid in short time and cannot be taken if the payments are stretched. Thus, Eq. (4.33) forces the payments executed in period t' on accounts payable to supplier e incurred in period t to equal the total amount due. In this expression, technical coefficients ($Coef_{ett'}$) that multiply the payments executed in periods $t^{'}$ on accounts payable incurred in t, are introduced in the formulation in order to take into account the terms of raw materials, production and transport credits (i.e., 2 percent-one week, net-28 days).

$$\sum_{t'=t}^{t+\hat{d}_e} Pay_{ett'} Coef_{ett'} = EPurch_{et} \qquad \forall\, e, t \leq T - \hat{d}_e \tag{4.33}$$

The payment constraints belonging to the last periods of time are formulated as inequalities (Eq. (4.34)), as it is not reasonable to require that total accounts payable to be zero at the end of the planning period.

$$\sum_{t'=t}^{t+\hat{d}_e} Pay_{ett'} Coef_{ett'} \leq EPurch_{et} \qquad \forall\, e, t > T - \hat{d}_e \tag{4.34}$$

Short term financing A short-term financing source is represented by an open credit line with a maximum limit imposed by the bank (Eq. (4.35)). Under an agreement with the bank, loans can be obtained at the beginning of any period and are due after one year at a given interest rate (ir_t^{SD}) that depends on the specific agreement reached with bank. Eqns. (4.36) and (4.37) make a balance on borrowings, considering for each period the updated debt ($CLine_{t-1}$) from the previous periods, the balance between borrows and repayments (Net_t^{CLine}) and the interest of the credit line ($ir_t^{SD} CLine_{t-1}$). Moreover, the bank regularly requires a repayment greater than or equal to the interests accumulated in previous periods, as it is stated by Eq. (4.38).

$$CLine_t \leq CLine^{max} \qquad \forall\, t \tag{4.35}$$

$$CLine_t = CLine_{t-1}(1 + ir_t^{SD}) + Borrow_t - Repay_t \qquad \forall\, t \tag{4.36}$$

$$Net_t^{CLine} = Borrow_t - Repay_t \qquad \forall\, t \tag{4.37}$$

$$Repay_t \geq ir_t^{SD} CLine_{t-1} \qquad \forall\, t \tag{4.38}$$

Long term financing Eq. (4.39) balances the investment with the capital supported by shareholders ($Capital_t$) and the amount borrowed to banks as long term debt ($LBorrow_t$) at each time period t.

$$FAsset_t = LBorrow_t + Capital_t \qquad \forall\, t \tag{4.39}$$

Eqns. (4.40) to (4.42) reflect the payment conditions associated with the long term debt. Note that these constraints are similar to those associated with the short term credit line, as in practice both types of debts can be treated in a similar way. Nevertheless, in the case of long term debt, the amount repaid in each time period $LRepay_t$ usually remains along the planning horizon.

$$LDebt_t = LDebt_{t-1}(1 + ir_t^{LD}) + LBorrow_t - LRepay_t \qquad \forall\, t \tag{4.40}$$

$$Net_t^{LDebt} = LBorrow_t - LRepay_t \qquad \forall\, t \tag{4.41}$$

$$LRepay_t \geq ir_t^{LD} LDebt_{t-1} \qquad \forall\, t \tag{4.42}$$

Marketable securities Eq. (4.43) makes a balance for marketable securities. The portfolio of marketable securities held by the firm at the beginning of the first period includes several sets of securities with known face values maturing within the time horizon (S_t^{MS}). All marketable securities can be sold prior to maturity at a discount or loss for the firm, as stated by Eq. (4.43). Revenues and costs associated with the transactions in marketable securities are given by technical coefficients ($D_{tt'}^{MS}$ and $E_{tt'}^{MS}$). $Y_{t't}^{MS}$ is the cash invested at period t on securities maturing at period t'. $Z_{t't}^{MS}$ is the cash income obtained through the security sold at period t maturing at period t'.

$$
\begin{aligned}
Net_t^{MS} = S_t^{MS} - \sum_{t'=t+1}^{T} Y_{t't}^{MS} + \sum_{t'=t+1}^{T} Z_{t't}^{MS} + \\
\sum_{t'=1}^{t-1} \left(1 + D_{tt'}^{MS}\right) Y_{tt'}^{MS} - \sum_{t'=1}^{t-1} \left(1 + E_{tt'}^{MS}\right) Z_{tt'}^{MS} \qquad \forall\ t
\end{aligned}
\tag{4.43}
$$

Eq. (4.44) is applied to constraint in each period the total amount of marketable securities sold prior to maturity to be lower than the available ones (i.e., those belonging to the initial portfolio plus the ones purchased in previous periods minus those sold before).

$$
\sum_{t''=1}^{t'} Z_{tt''}^{MS} \left(1 + E_{tt''}^{MS}\right) \leq S_t^{MS} + \sum_{t''=1}^{t'-1} \left(1 + D_{tt''}^{MS}\right) Y_{tt''}^{MS} \qquad \forall\ t, t' < t \tag{4.44}
$$

Liquidity Eq. (4.45) limits the cash in each period ($Cash_t$) to be larger than a minimum value ($MinCash$). A minimum cash is usually required to handle uncertain events, like delays in customer payments, thus ensuring enterprise liquidity. The bank requires a compensating balance, normally higher than the 20% of the amount borrowed. Therefore, the minimum cash ($MinCash$) has to be higher than the compensating balance imposed by the bank.

$$
Cash_t \geq MinCash \qquad \forall\ t \tag{4.45}
$$

4.4.4 Objective function: Using a valuation method

While the more common objectives used by the PSE community are maximum profit, net present value (NPV), maximum revenue, minimum makespan, and minimum cost, the finance community has been making financial business decisions for years by taking into account other indicators such as market to book value, liquidity ratios, leverage, capital structure ratios, return on equity, sales margin, turnover ratios and stock security ratios, among others.

Nevertheless, nowadays the maximization of the shareholder's value (SHV) of the firm seems to be the main priority of the firms and what really drives their decisions. The use of SHV as the objective to be maximized is mainly motivated by the fact that it reflects in a rather accurate way the capacity that the company has to create value. The SHV of the firm can bee indeed improved by maximizing its CV. Specifically, according to Weissenrieder (1998), the market value of a company is a function of four factors: (i) investment, (ii) cash flows, (iii) economic life, and (iv) capital cost. Specifically, this model applies the discounted-free-cash-flow method (DFCF) to compute the CV of a company.

The discounted-free-cash-flow method (DFCF)

The strategy applies the discounted free cash flow method (DFCF) to assess the decisions undertaken by a firm. This method has recently become the most preferred approach for the valuation of companies given its capacity of properly assessing the four main factors that contribute to create the market value of a firm. In fact, the DFCF method is well entrenched in finance theory and its use is gaining wider acceptance in industrial scenarios. The DFCF method values a project or an entire company by determining the present value of its future cash flows and discounting them taking into account the appropriate capital cost during the time horizon for which it is defined (i.e., economic life) (Grant, 2003).

According to financial theory, the enterprise market value of a firm is given by the difference between the discounted stream of future cash flows during the planning horizon and the net total debt at the beginning of its life time ($NetDebt_0$), as it is stated by constraint (4.46). The initial total debt includes both, the short and the long term debt and also the cash (equation (4.47)).

$$CV = DFCF - NetDebt_0 \tag{4.46}$$

$$NetDebt_0 = CLine_0 + LDebt_0 - Cash_0 \tag{4.47}$$

In the calculation of the DFCF, one must discount the free cash flows of each period t and the salvage value (SV) at a rate equivalent to the capital cost (see equation (4.48)). The salvage value could be calculated as a percentage of the total investment or by any other applicable method. The capital cost reflects the time value of the money and also the risk of the investment. In fact, the capital cost can be regarded as the expected return required to attract funds to a particular investment (Pratt, 2002).

$$DFCF = \sum_{t=0}^{T} \frac{FCF_t}{(1 + WACC_t)^t} + \frac{SV}{(1 + WACC_t)^T} \tag{4.48}$$

The weighted average capital cost (WACC) The capital cost can be determined through the weighted average method. This method considers the total capital structure of the company, including the overall equity and the debt, as it is shown in equation (4.49). In this expression, λ_t denotes the proportion of equity over the total capital investment.

$$WACC_t = \lambda_t E(ROE) + ir_t(1 - \lambda_t)(1 - trate) \qquad \forall\ t \tag{4.49}$$

To compute the expected return on equity, which is denoted by $E(ROE)$, equation (4.50) is applied. In this expression, $E(ROE)$ is computed as the sum of a risk free rater^0 and a risk premium (φRe). The former term represents the rate of return of an investment free of default risk available in the market and is usually equal to the yield to maturity offered by a government security. The latter, represents the expected amount of return above the risk-free rate in exchange for a given amount of variance (Pratt, 2002; Applequist *et al.*, 2000). One of the most commonly employed methods to estimate the risk premium is the Capital Asset Pricing Model (CAPM). For more details regarding this topic the reader is referred to Sharpe (1999).

$$E(ROE) = r^0 + \varphi Re \tag{4.50}$$

Free cash flows Free cash flows at every period t (FCF_t) are given by the profit after taxes, net change in investments and change in net working capital. Specifically, the free cash flows are the difference between the net operating profit after taxes (NOPAT) and the increase in capital invested. From this definition it follows that there will be value creation if the incoming value ($Profit_t\,(1 - trate)$) is greater than the consumed value ($\Delta NWC_t - NetInvest_t$) as shown in equation (4.51).

$$FCF_t = Profit_t\,(1 - trate) - NetInvest_t - \Delta NWC_t \qquad \forall\, t \tag{4.51}$$

Net operating profit Equation (4.52) is applied to compute the profit at each period t from the incomes associated with the sales of final products ($ESales_t$), the production costs, the cost of the transport services ($EPurch_{et}$), fixed costs ($FCost_t$) and the change in inventory(ΔInv_t).

$$Profit_t = ESales_t - \left(\sum_e EPurch_{et} + FCost_t - \Delta Inv_t \right) \qquad \forall\, t \tag{4.52}$$

Net investment The net investment at each period t represents the monetary value of the fixed assets acquired in that period minus the depreciation. As mentioned before, the depreciation term should be computed according to the specific applicable rules (e.g, Straight Line, Sum-of-years Digits, Declining Balance)

$$NetInvest_t = FAsset_t - Dep_t \qquad \forall\, t \tag{4.53}$$

Net working capital The change in net working capital associated with period t (NWC_t) is computed from the change in accounts receivable, plus the change in inventory, minus the change in accounts payable, plus any other financial expenses or incomes (FEx_t), as stated by equation (4.54).

$$\Delta NWC_t = (\Delta ARec_t + \Delta Inv_t - \Delta APay_t + FEx_t) \qquad \forall\, t \tag{4.54}$$

Equation (4.55) computes the accounts receivables corresponding to period t from the sales executed in the actual or any earlier period and maturing in periods beyond the present one minus the receivables pledged in previous periods, including those associated with the actual one. Equation (4.56) determines the change in accounts receivable at time period t.

$$ARec_t = \sum_{t'=t-\tilde{d}_M^{\max}+1}^{t} \sum_{t''=t+1}^{t'+\tilde{d}_M^{\max}} ASales_{t't''} - \sum_{t'=t+1}^{t+\tilde{d}_M^{\max}} \sum_{t''=t'-\tilde{d}_M^{\max}}^{t} Pled_{t't''} \qquad \forall\, t \tag{4.55}$$

$$\Delta ARec_t = ARec_t - ARec_{t-1} \qquad \forall\, t \tag{4.56}$$

Eq. (4.57) expresses changes in inventory including raw material stocks in manufacturing sites, as well as final product stocks in distribution centers and manufacturing sites. Iu_{rt}^{RM} and Iu_{it}^{FP} represent the inventory values for each raw material r and product i at each planning period t, respectively.

$$\begin{aligned}\Delta Inv_t = {} & \sum_i Iu_{it}^{FP}\left[\sum_s (SO_{ist} - SO_{ist-1}) + \sum_w (SW_{iwt} - SW_{iwt-1})\right] \\ & + \sum_r \sum_s Iu_{rt}^{RM}(SI_{rst} - SI_{rst-1}) \qquad \forall\, t\end{aligned} \tag{4.57}$$

The accounts payable ($APay_t$) are determined as the difference between all the purchases executed in previous periods ($EPurch_{et'}$) minus all payments done until the actual period ($Pay_{et''t'}$), as stated in equation (4.58). This constraint takes also into account the discounts for prompt payments ($Coef_{ett'}$). The change in accounts payable at time period t is thus represented by constraint (4.59).

$$APay_t = \sum_e \sum_{t'=1}^{t} EPurch_{et'} - \sum_e \sum_{t''=1}^{t} \sum_{t'=t''}^{t} Coef_{ett'} Pay_{et''t'} \qquad \forall\, t \tag{4.58}$$

$$\Delta APay_t = APay_t - APay_{t-1} \qquad \forall\, t \tag{4.59}$$

Finally, equation (4.60) computes other financial expenses and incomes (FEx_t) associated with the SC operation at every time period t. This term includes pledging costs ($(1-\phi_{t't})Pled_{t't}$), discounts for prompt payments to suppliers ($Pay_{et't}(Coef_{et't} - 1)$) and also the earnings ($D_{tt'}^{MS} Y_{tt'}^{MS}$) and expenses ($E_{tt'}^{MS} Z_{tt'}^{MS}$) associated with the transactions of marketable securities.

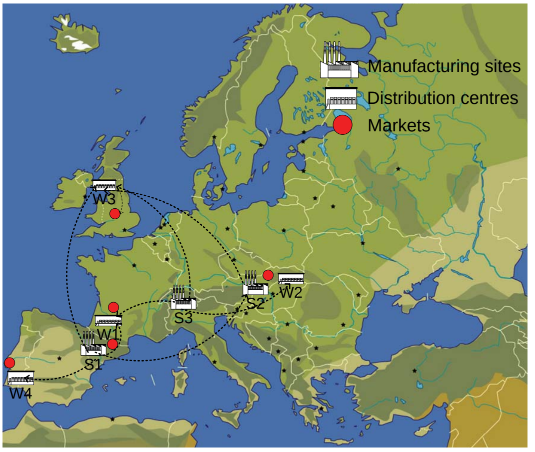


Figure 4.5: Supply chain structure of case study.

$$
\begin{aligned}
FEx_t = \sum_{t'=t+1}^{t+\tilde{d}_M^{\max}} (1-\phi_{t't})Pled_{t't} - \sum_{e}\sum_{t'=1}^{t} Pay_{et't}\,(Coef_{et't}-1) \\
+\sum_{t'} E_{tt'}^{MS} Z_{tt'}^{MS} - \sum_{t'} D_{tt'}^{MS} Y_{tt'}^{MS} \qquad \forall\, t
\end{aligned} \tag{4.60}
$$

The overall problem can be therefore mathematically posed as follows:

$$
\begin{gathered}
\underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\, CV \\
\text{subject to} \\
\text{Eqns. (4.1)–(4.60)} \\
\mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R}
\end{gathered}
$$

Here $\mathscr{X}$ denotes the model binary variables set, while $\mathscr{Y}$ represents the model continuous variable set.

4.5 Motivating example

The capabilities of the proposed integrated approach are illustrated by solving a retrofitting problem of an SC comprising several manufacturing sites, distribution centers and markets located in different European countries. A set of potential technologies are assumed to be available in the manufacturing sites. Furthermore, several potential locations for the manufacturing sites and the distribution centers, from which the products should be transported to the final markets, are also considered, as is depicted in Figure 4.5. The potential locations for the plants embedded in the SC ($S1$, $S2$ and $S3$) are Barcelona

Table 4.2: Maximum profit network design

	Total profit	121,653,714.87 m.u.			
	Net present value (NPV)	47,476,865.35 m.u.			
	Corporate value (CV)	36,392,463.16 m.u.			
		Time period (t)			
		0	1	24	48
Manufacturing sites					
s	j	Capacity increment (c.u.)			
S1	TA	10,000.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	0.0	0.0	0.0
	TD	0.0	0.0	0.0	0.0
S2	TA	0.0	500,000.0	0.0	0.0
	TB	0.0	407,796.6	0.0	0.0
	TC	0.0	500,000.0	0.0	0.0
	TD	0.0	500,000.0	0.0	0.0
S3	TA	50,000.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	496,610.2	0.0	0.0
	TD	0.0	478,813.6	0.0	0.0
Distribution centres					
w		Capacity increment (m^3)			
W1		4,000.0	0.0	0.0	0.0
W2		0.0	2,000.0	0.0	0.0
W3		0.0	0.0	0.0	0.0
W4		0.0	0.0	0.0	0.0

(B), Budapest(Bu) and Milan (Mi). These plants can manufacture three different products ($P1$, $P2$ and $P3$) with four different technologies (TA to TD). These final products must be transported to the distribution centers prior to being sent to the final markets ($M1$ to $M5$), where they become available to customers. It is assumed an existing installed capacity of TA in $S1$ and $S3$ of 10,000 c.u. and 50,000 c.u., respectively. The investment cost associated with the establishment of a manufacturing site is equal to 8,800,000 m.u. The potential locations for the distribution centers ($W1$ to $W4$) are B, Bu, Manchester (M) and Lisbon (Li), whereas for the final markets are B, Bu, London (L), Li and Toulouse (T). It is also assumed that at time zero $W1$ has an installed capacity of 4,000 m^3. The investment needed to open a distribution center is equal to 2,500,000 m.u.

The initial inventories are supposed to be equal to zero for all products and raw materials. The upper bound imposed to the capacity increment of technologies at each manufacturing site is equal to 500,000 c.u. and the lower bound is 50,000 c.u. The upper and lower bounds imposed to the capacity increment of distribution centers are 2,000 and 30,000 m^3. The capacities of the facilities can only be increased every two years. The salvage value is considered negligible at the end of the planning horizon. The availability of utilities is assumed to be unlimited.

With regard to financial matters, it is assumed that the firm has at the beginning of the planning horizon an initial portfolio of marketable securities.

Table 4.3: Maximum net present value network design

	Total profit	121,464,749.10 m.u.			
	Net present value (NPV)	47,623,655.11 m.u.			
	Corporate value (CV)	39,557,152.26 m.u.			
		Time period (t)			
		0	1	24	48
Manufacturing sites					
s	j	Capacity increment (c.u.)			
S1	TA	10,000.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	0.0	0.0	0.0
	TD	0.0	0.0	0.0	0.0
S2	TA	0.0	500,000.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	500,000.0	0.0	0.0
	TD	0.0	500,000.0	0.0	0.0
S3	TA	50,000.0	329,830.5	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	496,610.2	0.0	0.0
	TD	0.0	478,813.6	0.0	0.0
Distribution centres					
w		Capacity increment (m^3)			
W1		4,000.0	0.0	0.0	0.0
W2		0.0	2000.0	0.0	0.0
W3		0.0	0.0	0.0	0.0
W4		0.0	0.0	0.0	0.0

Table 4.4: Maximum corporate value network design

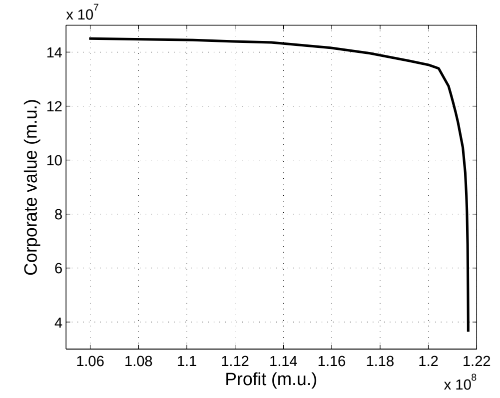
	Total profit	105,955,397.81 m.u.			
	Net present value (NPV)	42,068,183.09 m.u.			
	Corporate value (CV)	145,023,155.58 m.u.			
		Time period (t)			
		0	1	24	48
Manufacturing sites					
s	j	Capacity increment (c.u.)			
S1	TA	10,000.0	500,000.0	0.0	0.0
	TB	0.0	395,796.6	0.0	0.0
	TC	0.0	500,000.0	0.0	0.0
	TD	0.0	500,000.0	0.0	0.0
S2	TA	0.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	0.0	0.0	0.0
	TD	0.0	0.0	0.0	0.0
S3	TA	50,000.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	496,610.2	0.0	0.0
	TD	0.0	478,813.6	0.0	0.0
Distribution centres					
w		Capacity increment (m^3)			
W1		4,000.0	2,000.0	0.0	0.0
W2		0.0	0.0	0.0	0.0
W3		0.0	0.0	0.0	0.0
W4		0.0	0.0	0.0	0.0

Specifically, the firm owns 15,000 m.u. in marketable securities maturing in period 2 and 18,000 m.u. maturing in period 3. The initial cash is assumed to be equal to the minimum allowed cash, which is 125,000 m.u. Under an agreement with a bank, the firm has an open line of short term credit at a 15% annual interest with a maximum allowed debt of 4,000,000 m.u. The initial debt is assumed to be equal to zero and the value of the materials kept as inventories at the end of the time horizon are assumed to be a 85% of their market prices for final products and a 100% for raw materials.

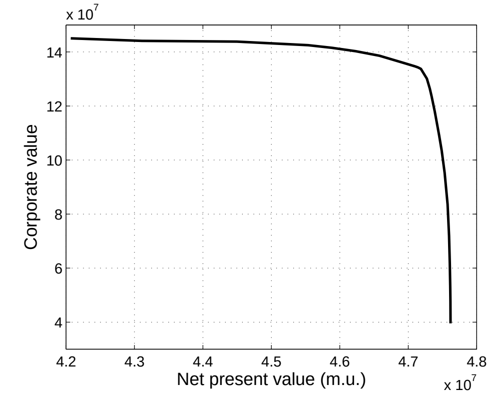
The SC under study has three external suppliers, the first one providing raw materials, the second one transportation services and the third one labour. Liabilities incurred with the raw materials supplier must be repaid within one month according to the terms of the credit (2 percent-same period, net-28 days for the raw materials supplier). The supplier of raw materials offers discounts for large orders. Thus, a 3% discount is applied for orders of raw material $R1$ higher than 45,000 kg, and a 5% for orders above 80,000 kg. The payments associated with the transport services and labor tasks cannot be stretched and must be fulfilled within the same time period in which the purchase incidence takes place. The technical coefficients associated with the set of marketable securities that the firm has agreed to purchase and sale have been computed by considering a 2.8% annual interest for purchases and a 3.5% for sales. It is considered outflows of cash equal to 5.0, 7.5 and 10.0 millions m.u. in periods 13, 15 and 17 due to wages, rents, and dividends. It is also assumed that the ratio between the long term debt and the equity must always be kept equal to 0.41. With regard to the long term debt, note that the firm can access a long term credit at a 10% annual interest. Shareholders expect an annual ROE of 30%. The taxes rate is 30%. Depreciation is calculated by means of the straight line method applied over a time horizon of ten years. The rest of this case study data is found in Appendix B.

Sixty one monthly planning periods are considered. The implementation in GAMS (Brooke, Kendrik, Meeraus, Raman, & Rosenthal, 1998) of the integrated formulation leads to an MILP model with 40,306 equations, 46,916 continuous variables, and 252 discrete variables. It takes 185 CPU seconds to reach a solution with a 0 % integrality gap on a AMD Athlon 3000 computer using the MIP solver of CPLEX (10.0). The integrated model is firstly solved by maximizing the CV of the firm. To explicitly show the trade-off between the CV and the standard KPIs that neglect financial considerations (i.e., NPV and profit) the ϵ-constraint method is applied (see Section 3.6), taking into account in each case the above commented objectives, CV and NPV and CV and profit, respectively, at the same time. The objective of this analysis is to further explore the trade-off between an integrated holistic solution and a sequential one. Thus, the NPV and the profit are computed by applying equations 4.62 and 4.63, respectively.

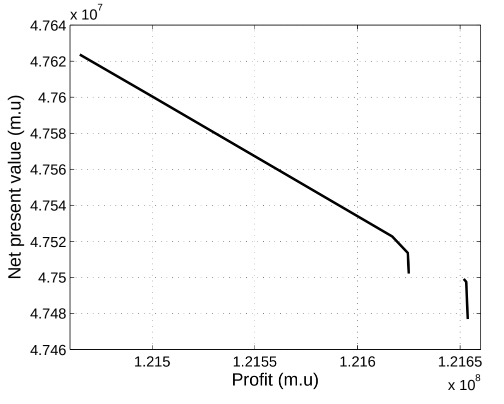
$$FF_t = (Profit_t - FAsset_t) \tag{4.61}$$



(a) Corporate value vs. profit



(b) Corporate value vs. NPV



(c) NPV vs. profit

Figure 4.6: Pareto frontiers

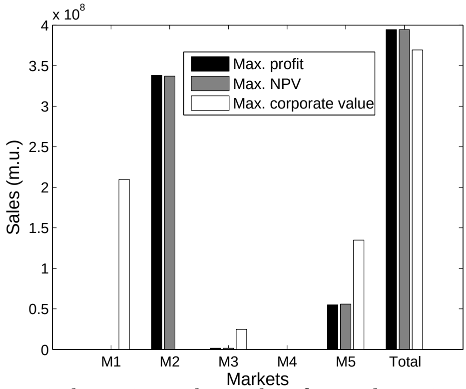


Figure 4.7: Sales carried out in each market for each optimal SC network configuration

$$TProfit = \sum_{t} FF_t \tag{4.62}$$

$$NPV = \sum_{t=1}^{T} \frac{FF_t}{(1+RR)^t} \tag{4.63}$$

The SC network configurations obtained by following this procedure are summarized in Tables 4.2, 4.3 and 4.4. The Pareto curves obtained by applying the aforementioned procedure are shown in Figure 4.6. Numerical results show

Table 4.5: Value accumulation at each quarter for maximum profit SC network structure (1x10^{6}m.u.)

Quarter	Profit after sales	Δ accounts receivable	Δ accounts payable	Net investment	Other expenses	Change in invested capital	Discounted free cash flows
0	0.000	0.000	0.000	-30.351	0.000	-30.351	-30.351
1	4.979	-13.727	3.473	0.759	-1.031	-10.526	-5.400
2	5.252	-7.203	0.010	0.759	-0.575	-7.009	-1.642
3	5.235	-7.177	0.026	0.759	-0.557	-6.950	-1.539
4	5.244	-2.188	0.028	0.759	-0.526	-1.927	2.810
5	5.146	1.081	-0.016	0.759	-0.811	1.013	5.110
6	5.381	5.931	0.046	0.759	-4.053	2.684	6.507
7	5.331	2.857	-0.092	0.759	-10.469	-6.945	-1.231
8	5.379	2.157	-0.019	0.759	-9.875	-6.978	-1.169
9	5.376	1.554	0.017	0.759	-9.267	-6.937	-1.097
10	5.375	-1.939	-0.020	0.759	-5.699	-6.900	-1.029
11	5.334	0.267	0.070	0.759	-7.901	-6.805	-0.953
12	5.401	-0.988	-0.080	0.759	-6.558	-6.867	-0.911
13	5.378	2.972	0.027	0.759	-10.554	-6.797	-0.847
14	5.385	-5.259	0.021	0.759	-2.293	-6.772	-0.795
15	5.354	0.034	-0.003	0.759	-7.484	-6.693	-0.737
16	5.397	-6.640	0.000	0.759	-0.836	-6.717	-0.698
17	5.365	-2.724	0.058	0.759	-4.729	-6.637	-0.645
18	5.417	-6.582	-0.079	0.759	-0.290	-6.193	-0.381
19	5.337	16.801	-3.465	0.759	-0.068	14.027	9.058
20	5.338	20.772	3.462	0.759	0.069	25.062	13.619

Table 4.6: Value accumulation at each quarter for maximum NPV SC network structure ($1x10^6$m.u.)

Quarter	Profit after sales	Δ accounts receivable	Δ accounts payable	Net investment	Other expenses	Change in invested capital	Discounted free cash flows
0	0.000	0.000	0.000	-29.832	0.000	-29.832	-29.832
1	4.954	-13.684	3.473	0.746	-1.035	-10.500	-5.400
2	5.226	-7.171	0.010	0.746	-0.567	-6.983	-1.642
3	5.210	-7.148	0.026	0.746	-0.550	-6.927	-1.540
4	5.214	-2.151	0.028	0.746	-0.520	-1.897	2.809
5	5.107	1.231	-0.016	0.746	-0.769	1.192	5.226
6	5.357	5.393	0.046	0.746	-3.617	2.568	6.395
7	5.307	3.162	-0.092	0.746	-10.742	-6.926	-1.234
8	5.356	-1.238	-0.019	0.746	-6.447	-6.959	-1.173
9	5.352	-3.654	0.017	0.746	-4.027	-6.919	-1.100
10	5.351	5.696	-0.020	0.746	-13.304	-6.882	-1.033
11	5.310	-6.120	0.070	0.746	-1.483	-6.788	-0.957
12	5.378	-6.572	-0.080	0.746	-0.944	-6.851	-0.916
13	5.354	-4.029	0.027	0.746	-0.364	-3.621	1.016
14	5.362	-0.452	-3.469	0.746	-0.019	-3.194	1.230
15	5.331	0.240	0.000	0.746	0.070	1.056	3.515
16	5.373	-0.027	0.000	0.746	0.107	0.825	3.271
17	5.342	-0.850	0.000	0.746	0.145	0.041	2.733
18	5.393	-0.196	0.000	0.746	0.179	0.729	2.979
19	5.313	16.801	0.000	0.746	0.218	17.765	10.781
20	5.314	20.772	3.462	0.746	0.175	25.156	13.650

Table 4.7: Value accumulation at each quarter for maximum corporate value SC network structure ($1x10^6$m.u.)

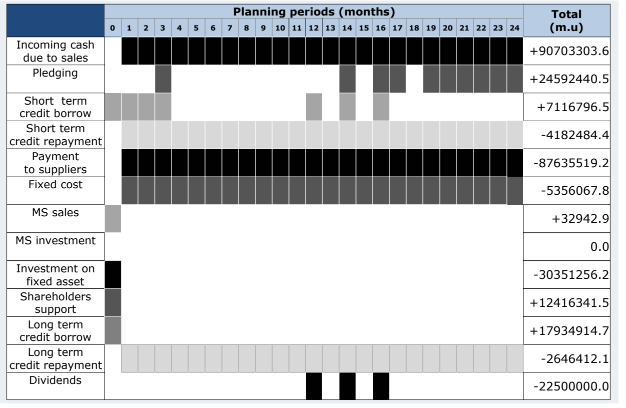
Quarter	Profit after sales	Δ accounts receivable	Δ accounts payable	Net investment	Other expenses	Change in invested capital	Discounted free cash flows
0	0.000	0.000	0.000	-30.344	0.000	-30.344	-30.344
1	5.011	-13.996	3.473	0.759	-0.805	-10.570	-5.409
2	5.113	-1.556	-1.524	0.759	-0.490	-2.811	2.149
3	5.047	0.000	-1.949	0.759	-0.158	-1.349	3.294
4	5.016	0.000	0.000	0.759	-0.122	0.637	4.869
5	5.029	0.000	0.000	0.759	-0.105	0.653	4.699
6	5.034	0.000	0.000	0.759	-0.116	0.643	4.514
7	5.005	0.000	0.000	0.759	-0.071	0.687	4.338
8	5.060	0.000	0.000	0.759	-0.036	0.723	4.231
9	5.049	0.000	0.000	0.759	0.002	0.760	4.081
10	5.054	0.000	0.000	0.759	0.039	0.797	3.946
11	5.011	0.000	0.000	0.759	0.077	0.835	3.786
12	5.084	0.000	0.000	0.759	0.111	0.869	3.701
13	5.047	0.000	0.000	0.759	0.149	0.908	3.554
14	5.065	0.000	0.000	0.759	0.186	0.944	3.444
15	5.031	0.000	0.000	0.759	0.224	0.982	3.308
16	5.068	0.000	0.000	0.759	0.260	1.019	3.215
17	5.046	0.000	0.000	0.759	0.298	1.057	3.095
18	5.095	0.000	0.000	0.759	0.334	1.092	3.012
19	5.026	0.000	0.000	0.759	0.373	1.131	2.878
20	1.386	15.552	3.462	0.759	0.172	19.945	9.554

that the solutions computed by maximizing profit or NPV as single objectives are far away from the optimal one (i.e., the best solution in terms of CV). Certainly, the maximum CV solution is almost 300% higher than the one computed by maximizing profit and 267% higher than the one accomplished when maximizing NPV. On the other hand, the maximum profit and NPV solutions are quite similar. Moreover, from these results, it is clear that in both cases a conflict exists between the different objectives (i.e., maximum corporate value and maximum profit or NPV). Numerical results show that an improvement in profit or NPV is only possible if the decision-maker is willing to compromise firm's CV. Certainly, SC configurations with better profits or NPVs can only be achieved at the expense of a reduction in the firm's CV.

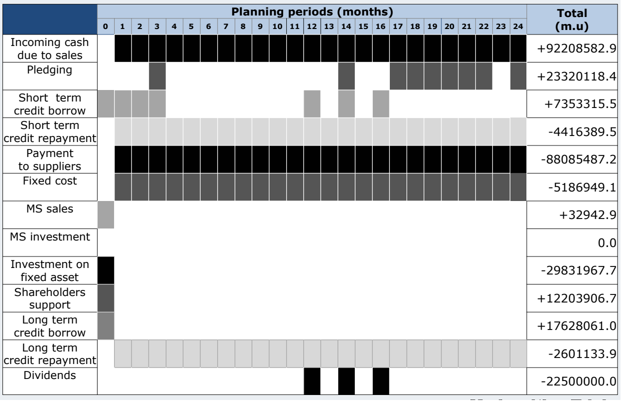
It is worth to mention that this case study represents a very specific situation where there is one market ($M2$) in which the product prices are slightly higher in comparison with the others (1.87%). At such market, accounts receivable are due within a large time period. Under this assumption, the design-planning model that accounts for the maximization of a biased KPI (either profit or NPV) that neglects the financial side of the problem decides to configure a supply chain network capable of easily fulfilling the demand of market $M2$ as much as possible (see Figure 4.7).The profit and the NPV are indeed blind KPIs in the sense that they are not capable of properly assessing the financial cost associated with net working capital. As a result, accounts receivables increase in certain periods of time in which the firm has to face important payments. The cash management model is then forced to pledge them, mainly during month 18 to 36 (quarters 6 to 12). Pledging is indeed a very expensive way of getting cash and because of that the firm reduces its capacity of creating value when applying it.

On the other hand, the integrated approach that accounts for the maximization of a suitable financial objective function (i.e., corporate value) is able to properly assess the trade off between the increment in profit that can be achieved by fulfilling demand at market $M2$ and the increment in net working capital that is required to carry out this decision. Hence, the integrated approach computes a SC configuration that does not fulfill the demand in $M2$ due to the poor payment conditions associated with its customers. Consequently, the net working capital needed is reduced significantly thus increasing the value accumulated during the whole planning horizon. This can be observed in Tables 4.5 to 4.7, which depict the behavior of the corporate value and the structure of the consumed value during the planning horizon for each optimum SC network configuration. For the purpose of facilitating their interpretation, the planning periods (months) have been aggregated into quarters in these tables. In figure 4.8, financial Gantt charts for each optimal SC configuration are shown. They describe how the cash is composed and utilized during the first 25 planning periods.

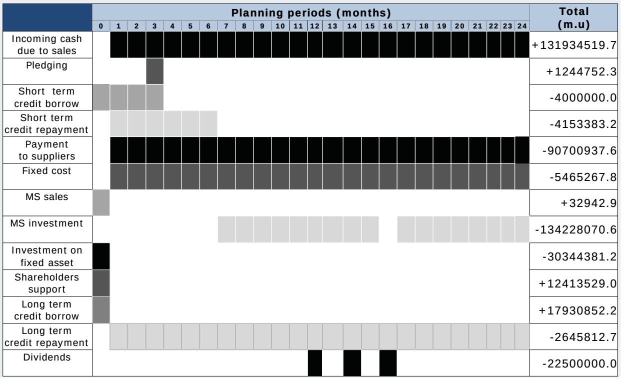
To demonstrate the advantages of using CV and its robustness to assess strategic decisions under different scenarios, the previous case study has been modified and solved. Two modifications have been done: 1) prices payed by



(a) Optimal profit



(b) Optimal NPV



(c) Optimal CV

Figure 4.8: Financial Gantt charts

Table 4.8: KPI values of optimal SC network configurations for second case study (m.u.)

Network Configuration	KPI		
	Total profit	NPV	CV
Optimal total profit	116,597,744.59	45,374,556.23	89,386,052.53
Optimal NPV	116,377,423.52	45,516,838.30	110,018,635.40
Optimal CV	105,955,397.81	42,068,183.09	145,023,155.58

market $M2$ are equal to those payed by rest of markets and 2) due time of account receivables in market $M2$ has the same conditions offered by market $M4$. The optimal SC network configurations obtained are quite similar to those resulting in the previous case study. In table 4.8, the values of each KPI are shown for each optimal configuration. Even for this second case, it can be observed that the maximum CV solution is 62% better than the one computed by maximizing profit and 32% superior than the one accomplished when maximizing NPV. It is clear from these two examples that the integrated model introduced in this chapter has a great potential when addressing the challenge of designing a SC capable to preserve and improve the firms' value.

4.6 Final considerations

This chapter has addressed the design and retrofit of chemical SCs taking into account financial concerns. The proposed framework applies mixed integer modeling techniques to develop holistic mathematical models for SCM that are able to optimize the strategic operations decisions in conjunction with the finances.

The main advantages of this approach have been highlighted through a case study, in which the integrated model has been compared with the traditional method. The former approach pursues the maximization of a suitable financial key performance indicator that is able to properly assess the expenses associated with the shortages of cash and the value penalty associated to increments in net working capital (i.e., the corporate value of the firm at the end of the time horizon). On the other hand, the latter strategy accounts for the maximization of a biased key performance indicator that is unable to assess the costs of the financing fixed and current assets. Numerical results show that the integrated solution not only ensures the feasibility of the strategic decisions from the financial viewpoint but also leads to a superior economic performance given its higher capacity of creating value for the firm.

The framework suggested in this work is thus in consonance with the new trends in PSE, which is going towards an enterprise wide optimization framework that aims to integrate all the functional decisions into a global model that should optimize an overall key performance measure. Here, it is proposed the corporate value measured through the discounted free cash flow method as a suitable first approach to this posed requirement.

It is not enough to have a static planning model reviewed only in certain periods. It will be necessary to maintain continuously updated an enterprise modeling system which should connect the SC strategic, tactical and operative levels. This modeling system must include the financial management of capital investments at the strategic level. The bottom level must incorporate a realistic cash flow management including net working capital analysis and also short term budget. The maximum corporate value as target and the holistic model itself constitute a first step forward in creating this ongoing planning system. To the best of our knowledge, a system based on an integrated model that takes into account a detailed financial analysis has not been implemented so far.

4.7 Nomenclature

Indices

e	suppliers
d	discount interval
i	products
j	plant equipment
m	markets
r	raw materials
s	manufacturing sites
t	planning periods
w	distribution centers

Sets

D_{er}	discounts intervals for each raw material r for which supplier e offers quantity discount
DR_e	raw materials for which supplier e offers quantity discounts
E_r	set of suppliers e that provide raw material r
I_j	products that can be processed in plant equipment j
I_r	products that consumed raw material r
J_i	equipment that can process product i
R_e	set of raw materials provided by supplier e
τ	planning periods in which investments on facilities are allowed

Parameters

A_{ert}	maximum availability of raw material r in period t associated with supplier e
$CLine^{max}$	upper bound of short term credit line
$Coef_{ett'}$	technical discount coefficient for payments to external supplier $e$executed in period t' on accounts incurred in period t
$\hat{d}_e$	maximum delay on payments of supplier e
$\tilde{d}_m$	maximum delay in receivables at market m
$\tilde{d}_M^{max}$	maximum delay in receivables at all markets
$D_{tt'}^{MS}$	technical coefficient for investments in marketable securities
DF_{erd}	discount factor associated with discount interval d for raw material r offered by external supplier e

Dem_{imt}	demand of product i at market m in period t
$disc_{erd}$	discount offered by supplier e for raw material r at interval d
$E_{tt'}^{MS}$	technical coefficient for sales of marketable securities
$E[ROE]$	expected return on equity
$FCFS_{jst}$	fixed cost per unit of capacity of plant equipment j at site s in period t
$FCFW_{wt}$	fixed cost per unit of capacity of distribution center w in period t
g_{ert}	cost of raw material r provided by supplier e in period t
ir_t^{LD}	interest rate of long term debt
ir_t^{SD}	interest rate of short term debt
I_{st}^{S}	investment required to open site s in period t
I_{wt}^{W}	investment required to open distribution center w in period t
Iu_{rt}^{RM}	value of inventory of raw material r in period t
Iu_{it}^{FP}	value of inventory of product i in period t
$MinCash$	lower bound of cash
$MinCSL$	lower bound of customer service level
$Other_t$	other expected outflows or inflows of cash in period t
$NetDebt_0$	net total debt at initial period
$Price_{imt}$	price of product i at market m in period t
$Price_{jst}^{FS}$	investment required per unit of capacity of equipment j increased at site s in period t
$Price_{wt}^{FW}$	investment required per unit of capacity of distribution center w increased in period t
rf	risk free rate of return
rp	risk premium rate
RR	return rate
S_t^{MS}	marketable securities of the initial portfolio maturing in period t
$trate$	tax rate
T	length of planning horizon

Binary variables

F_{ertd}	1 if the amount of raw material r purchased from supplier e in period t is within discount interval d, 0 otherwise
SB_{st}	1 if site s is opened in period t, 0 otherwise
V_{jst}	1 if the capacity of equipment j is increased at site s in period t, 0 otherwise
WB_{wt}	1 if distribution center w is opened in period t, 0 otherwise
X_{wt}	1 if the capacity of distribution center w is increased in period t, 0 otherwise

Continuous variables

$APay_t$	amount of accounts payable in period t
$ARec_t$	amount of accounts receivable in period t
$ASales_{tt'}$	sales executed in period t and receivable in period t'
$Borrow_t$	total amount borrowed from the short term credit line in period t
$Capital_t$	capital supported by shareholders in period t
$Cash_t$	cash in period t
$CLine_t$	short term debt in period t
CSL	customer service level calculated at the end of the planning horizon

CV	corporate value at the end of the planning horizon
Dep_t	depreciation in period t
$DFCF$	sum of discounted free cash flows at the end of the planning horizon
$ECash_t$	exogenous cash in period t
$EPurch_{et}$	economic value of purchases executed in period t to supplier e
$ESales_t$	economic value of sales carried out in period t
$FAsset_t$	increment in fixed assets in period t
FCF_t	free cash flows in period t
$FCost_t$	fixed cost in period t
FEx_t	other financial expenses and incomes in period t
FF_t	funds flow in period t
FS_{jst}	total capacity of plant equipment j during period t at site s
FSE_{jst}	capacity increment of plant equipment j during period t at site s
FW_{jst}	total capacity at distribution center w during period t
FWE_{jst}	capacity increment at distribution center w during period t
$LBorrow_t$	total amount of money borrowed from the long term credit line in period t
$LDebt_t$	long term debt in period t
$LRepay_t$	total amount repaid to the long term credit line in period t
Net_t^{CLine}	total amount of money borrowed or repaid to the short term credit line in period t
Net_t^{LDebt}	total amount of money borrowed or repaid to the long term credit line in period t
Net_t^{MS}	total amount received or paid in securities transactions in period t
$NetInvest_t$	net investment in period t
NPV	net present value computed for whole planning horizon
P_{ijst}	production rate of product i in equipment j at site s in period t
$Pay_{tt'}$	payments to external supplier e executed in period t' on accounts payable incurred in period t
$Pled_{tt'}$	amount pledged within period t' on accounts receivable maturing in period t
$Profit_t$	profit achieved in period t
$Purch_{et}^{rm}$	amount of money payable to supplier e in period t associated with consumption of raw materials
$Purch_{et}^{tr}$	amount of money payable to supplier e in period t associated with consumption of transport services
$Purch_{et}^{pr}$	amount of money payable to supplier e in period t associated with consumption of production utilities
$Purch_{erst}$	amount of raw material r purchased to supplier e at site s in period t
$Purch_{et}^{rm}$	amount of raw material r purchased in period t
q_{erdt}	amount of material r within discount interval d purchased to supplier e in period t
Q_{iwst}	amount of product i sent from site s to distribution center w in period t
$Repay_t$	total amount repaid to the short term credit line in period t
$Sales_{iwmt}$	amount of product i sold from distribution center w in market m in period t
SI_{rst}	amount of stock of raw material r at site s in period t

SO_{ist}	amount of stock of product i at site s in period t
SV	salvage value of facilities at the end of planning horizon
SW_{iwt}	amount of stock of product i at distribution center w in period t
$TProfit$	total profit achieved at end of planning horizon
$WACC_t$	weighted average cost of capital in period t
$Y_{tt'}^{MS}$	cash invested in period t' in marketable securities maturing in period t
$Z_{tt'}^{MS}$	security sold in period t' maturing in period t
$\Delta APay_t$	change in amount of accounts payable in period t
$\Delta ARec_t$	change in amount of accounts receivable in period t
ΔInv_t	change in inventory value in period t
ΔNWC_t	change in net working capital in period t

Greek symbols

α_{rij}	fixed coefficient for consumption of raw material r by product i
β_{sj}	minimum utilization of plant equipment j capacity allowed at site s
γ_w	minimum utilization of distribution center w capacity allowed
$\delta_{mtt'}$	fraction of sales carried out in period t that are receivable in period t' in market m
θ_{ij}	capacity utilization of plant equipment j by product i
λ_t	proportion of equity over total capital investment in period t
ρ_{eiws}^{tr1}	unitary transport costs of product i from plant s to warehouse w payable to external supplier e
ρ_{eiwm}^{tr2}	unitary transport costs of product i from warehouse w to market m
τ_{ijse}^{ut1}	cost associated with product i manufactured with equipment j in site s and payable to external supplier e
τ_{rse}^{ut2}	cost associated with handling the inventory of raw material r in site s and payable to external supplier e
τ_{ise}^{ut3}	cost associated with handling the inventory of final product i in site s and payable to external supplier e
τ_{iwe}^{ut3}	cost associated with handling the inventory of final product i in warehouse w and payable to external supplier e
υ_i	specific volume of product i
$\phi_{tt'}$	face value of accounts maturing in period t pledged in period t'
ψ_{ert}	price of raw material r offered by external supplier e in time period t

Superscripts

L	lower bound
U	upper bound

Chapter 5

Synchronizing SC and Product Development Decisions

5.1 Introduction

In today's highly competitive marketplace, SC and product development activities should be coordinated and synchronized so that market demand, product release and capacity requirements are matched in a financially sustainable fashion. In this chapter, an integrated model is developed which incorporates simultaneous treatment of SC design–planning and product development pipeline decisions in the pharmaceutical industry. Moreover, the aforementioned cross-functional model embeds a capital budgeting formulation enabling the quantitative assessment of the firms' value. The model also considers the endogenous uncertainty associated with product test outcomes during the development process. To tackle this problem, a scenario based multi-stage stochastic MILP formulation is proposed. This model includes risk constraints which allow finding optimal solutions within accepted risk levels. A decomposition technique is also applied in order to reduce the computational effort required for the solution of the monolithic model, thus facilitating the solution of realistic industrial problems of moderate scale.

5.2 The significance of product development and SC coordination

Enterprise-wide decision problems have increasingly become the focus of research and application for the process systems engineering (PSE) community. This expansion in the traditional scope of PSE research has been driven in part

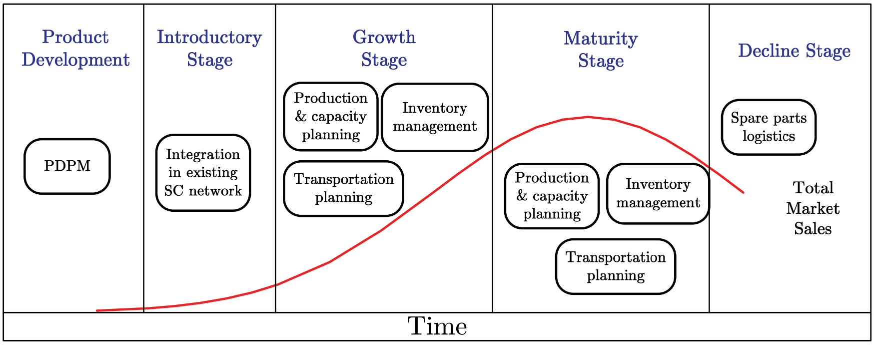


Figure 5.1: Product life cycle

by the availability of information systems that allow ready access to up-to-date information across the enterprise, in part by the ability to develop, solve and maintain large scale models, and partly because of a recognition that the globalization of enterprises requires that organizational decisions must take into account impact on a wider scale, both temporally and geographically. Additionally, the recognition of collective responsibility for the global environment has pushed into the forefront the issue of sustainability and thus consideration of all aspects of the life cycle of products and processes (see Fig. 5.1). Two enterprise-wide decision problems that have received the most intense attention have been SCM and product development pipeline management (PDPM). The former addresses the design and operational issues associated with the supplier, manufacturer, customer and logistics network by means of which an enterprise delivers its products to the market place. The latter addresses the set of decisions and network of tasks associated with turning a new discovery into a product and introducing it into the corporation's SC (Varma *et al.*, 2007).

Both of these enterprise-wide problems are resource intensive, involve large cash flows and thus their successful solution has a direct bearing on the viability of the enterprise. Both are large scale in terms of the number of state and decision variables that must be considered, involve activities at multiple time scales, are dynamic in nature, and are subject to a large number of exogenous and endogenous uncertainties. They, at root, constitute large-scale, multistage stochastic optimization problems. Given their importance to the viability of the enterprise, the quality of solutions to these decision problems must be measured in terms of enterprise-wide metrics such as cash flow, corporate value preservation and growth. Evaluation of these metrics in turn requires capture of the relevant financial flows and accounting details. However, there are substantive differences between the two. SCM encompasses the portion of the life cycle of a company's products from market launch to withdrawal, includes consideration of logistical functions associated with the movement of material through the SC and thus necessarily must include the management of feedstock supplier/producer and producer/customer relationships. PDPM covers

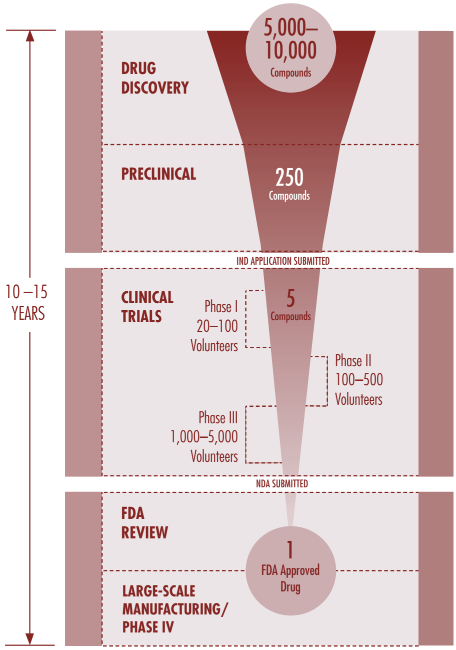


Figure 5.2: Research & development process (source: PhRMA, 2007)

only the development and launch portion of the product life-cycle and involves the critical decision of selection of product candidates that will constitute the development portfolio. One of the defining aspects of PDPM is that product candidates are likely to fail during development (see Fig. 5.2). When this occurs not only is the investment in the development of the failed product lost but the company incurs the opportunity cost of not having developed one of the alternate potential product candidates in its portfolio. Indeed studies have shown that the US industry average is only one commercial success per seven new product concepts in which development is invested. As a result as much as 50% of new product development resources are spent on failed or cancelled products. The success rate in the development of pharmaceutical products is even less than that and the investment per successful product is now reaching \$2 Billion (Hynes-III, 2008). It is thus no surprise that the management of pharmaceutical product development has been receiving special attention in the PSE literature in recent years. Given the high failure rate and large potential investment loss, the challenge is the valuation of product portfolios that properly takes into account not only the uncertainties and risks but also the decision flexibility that management can exercise during the course of the development path.

Since these two decision problems comprise complementary segments of the product life cycle, they do have areas of overlap. Specifically, in both cases the forecasting of uncertain demand, which may include forecasting of competitor action, is an important decision input. In both, capacity planning decisions are important, that is, whether to produce a new product for launch in an existing facility (and in which one) or whether to plan for new capacity. Moreover, the two are interdependent in that typically the cash flow from effective SCM provides all or a significant portion of the investment funding required for PDPM while SCM relies on a steady flow of new products from PDPM to drive SC growth or at least to sustain the enterprise in the face of competitor's product innovations.

Planning of new product development activities has been an active research topic in last decades. Schmidt and Grossmann (1996) address the optimal scheduling of testing tasks in the new product development process. They do not take into account the interaction with production capacity in their model. Maravelias and Grossmann (2001) consider the simultaneous optimization of resource-constrained scheduling of testing tasks in new product development and design/planning of batch manufacturing facilities. The authors adopt a two-stage stochastic optimization approach to account for the uncertainty in the outcome of the tests. Levis and Papageorgiou (2004) determine the product portfolio and the multi-site capacity planning in the face of uncertain clinical trials outcomes while taking into account the trading structure of the company. Recently, Colvin and Maravelias (2008) use a multistage stochastic approach to deal with the pharmaceutical R&D pipeline, accounting for the endogenous uncertainty of clinical trial outcomes. The above described approaches incorporate as objective function NPV and they do not account for financial issues nor do they incorporate capacity expansion decisions.

The PSE related research on the SCM problem has largely focused on issues related to process operations: assignment of physical resources and the scheduling and routing of material flows through the network. The supply and pricing of feedstocks are typically treated as deterministic and uncertain product demand is accommodated through production planning/scheduling and suitable allocation of inventory. Product pricing is usually assumed to be given. The work on the PDPM, which has almost exclusively concentrated on the pharmaceutical product domain, has focused on portfolio selection in the face of uncertainty due to product failure during development and to resource reassignment in response to termination of a product candidate. The variety of managerial actions, which can be taken at a tactical and operational level to mitigate risk by corrective action when uncertainties are realized, have not been fully exploited. In practice this may mean that the impacts of risks are over-estimated, performance metrics underestimated and thus poor strategic decisions advanced. Additionally, the treatment of financial factors is restricted to primary operating and fixed investment costs and, typically, some form of net present value with interest rate fixed over the time horizon is used as performance metric.

Additionally, as indicated by Varma *et al.* (2007) there is a need to model financial planning decisions, R&D resource allocation as well as capacity expansion decisions within an integrated model, so that capital and capacity allocation can be performed simultaneously with R&D projects selection and prioritization in order to enhance value generation. Certainly, R&D decisions necessarily impact the design and the regular activities of the entire SC. Thus, such operational impact should be considered and assessed at the time R&D and SC decisions are taken.

Then, so as to assure financial sustainability, enterprises must carefully assess the resource trade-offs between new product launches, capital budgeting and capacity allocation. This chapter deals with business strategic decisions related to product development and SC retrofitting/design. Here, it is developed an integrated model which incorporates simultaneous treatment of the SC design–planning and product development issues in a representative sector: the pharmaceutical industry. The endogenous uncertainty of product test outcomes during the development process are taken into account. Moreover, the aforementioned cross-functional model embeds a risk management and financial formulation enabling the quantitative assessment of the firm's value.

5.3 Problem statement

One of the industries for which R&D pipeline management is particularly significant is pharmaceuticals. No pharmaceutical product can be placed on the market without receiving prior authorization from the relevant public health agencies. For this type of businesses, solutions from holistic approaches are a necessity in order to support strategic decision making that will allow financial sustainability to be achieved.

New products in the development phase are required to go through strict tests. Generally, tests can be classified into pre-clinical tests; clinical trials (this stage is comprised of three phases); and regulatory approval (see Fig. 5.2). This study will be focused on the clinical trials phases.

The ultimate goal of clinical trials is to determine whether the drug works well enough in patients. The trials should address: whether the risk of toxic side effects outweighs the therapeutic benefit; which dose regimen provides the best response and the least number of side effects; whether the drug is better than existing treatments. As previously mentioned, clinical trials are divided in three phases (Robins-Roth, 2001):

Phase I This usually involves $20-100$ healthy volunteers treated with increasingly high doses. The goal is to study how the drug is metabolized, where it goes in the human body, whether it is safe to use it, and what is the best way to use it.

Phase II The goal of this phase is to provide more information about drug efficacy and how the drug behaves in people. These studies typically include $100-500$ patients, divided into several subgroups. The subgroups are administered the drug in different doses, by different routes, and on different schedules.

Phase III Here, $1000-5000$ patient volunteers are included and the aim is to generate statistically significant data, about effectiveness, patient subpopulations and dosing regiments that will lead FDA and the international regulatory agencies to approve the new drug. Note that the drug division of FDA often requires more than one Phase III trial.

Information regarding trial uncertainty (probability of success) and processing equipment requirements for large scale production is assumed to be known or estimated relying on results of previous tests and existing products.

It is given a set of existing products and a set of potential products. Failure to pass clinical trial implies termination of the development project. Each new product clinical trial has a probability of success, an associated duration and cost, which are assumed to be known. On the SC side it is assumed that various items of technological equipment are available to be installed in existing and potential facility sites. Regarding the financial area, the formulation endeavors to model cash management and value creation. To calculate corporate value (CV) the discounted-free-cash-flow (DFCF) method is utilized.

The model offers robust decision support to business managers; it determines the most appropriate subset of potential products to be launched, capacity expansion of production processes, and production profiles so as to optimize the expected CV.

5.4 Mathematical formulation

The problem is formulated as a multi-stage mixed integer linear programming (MILP). The variables and constraints of the model can be classified into five groups. The first group corresponds to the formulation of project selection. Process operations constraints given by the SC topology belong to the second group. The third one incorporates those constraints related to the integration of operations and product pipeline management. Finally, the fourth group is associated with the constraints required for allowing cash management and evaluating the objective function (CV).

5.4.1 Product pipeline management

The endogenous uncertainty associated with the outcome of clinical trials is modeled following the work of Colvin and Maravelias (2008). Figure 5.3 shows the scenario tree for a new product considering the three phases (I, II, III) of clinical trials. Notice that the number of scenarios is given by 4^N, where N is the number of potential new products. The four scenarios for a new product development project are: (i) failure during phase I clinical trial (I/F), (ii) failure

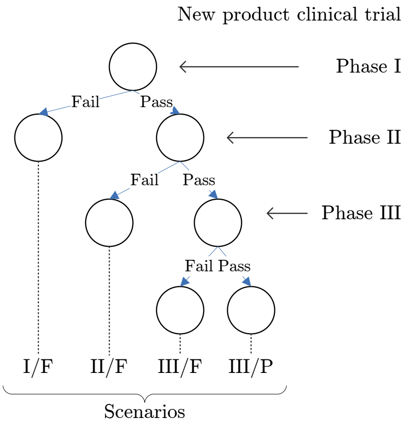


Figure 5.3: Scenario tree of clinical trials outcomes

during phase II clinical trial (II/F), (iii) failure during phase III clinical trial (III/F), and (iv) success in phase III clinical trial (III/P).

For a pair of scenarios (ς, ς') that become distinguishable in period $t^{\varsigma,\varsigma'}$ the decisions $\mathcal{D}$ in previous periods $(t < t^{\varsigma,\varsigma'})$ must be the same (see Section 3.7). In this case, $t^{\varsigma,\varsigma'}$ represents the period when these scenarios become distinguishable. This non-anticipativity condition can be expressed as follows:

$$\{\mathcal{D}_{t\varsigma} = \mathcal{D}_{t\varsigma'}\} \qquad \forall\ t < t^{\varsigma,\varsigma'}$$

The number of pairs of scenarios for which this non-anticipativity condition must be satisfied can be reduced to those pairs of scenarios which differ in the outcome of merely one potential product clinical trial (ϑ). This relationship between pair of scenarios is crucial for devising an ad hoc decomposition strategy. In Fig. 5.4, it is presented the 16 (4^2) scenarios for the case of two potential

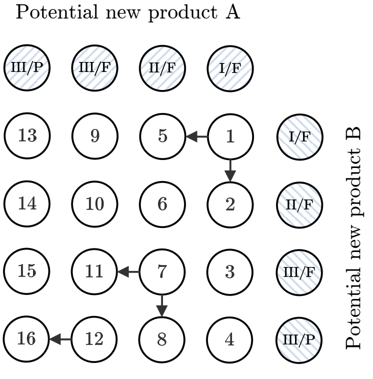


Figure 5.4: Relationship between scenarios

Table 5.1: Non-anticipativity relationships to be included for Figure 5.4 example

Pair of scenarios		Differentiating clinical trial		Pair of scenarios		Differentiating clinical trial	
		Product	Phase			Product	Phase
1	2	B	I	8	9	B	II
1	5	A	I	8	12	A	II
2	3	B	II	9	10	B	III
2	6	A	I	9	13	A	III
3	4	B	III	10	11	B	I
3	7	A	I	10	14	A	III
4	5	B	I	11	12	B	II
4	8	A	I	11	15	A	III
5	6	B	II	12	13	B	III
5	9	A	II	12	16	A	III
6	7	B	III	13	14	B	I
6	10	A	II	14	15	B	II
7	8	B	I	15	16	B	III
7	11	A	II				

new products, A and B. Note that nodes that are horizontally or vertically adjacent differ only in one product clinical trial outcome, consequently the non-anticipativity constraints should be expressed only for them. For instance, a non-anticipativity constraint must be included for the pair of scenarios $(1, 5)$. Notice that product A phase I clinical trial fails in scenario 1 (I/F), while this clinical trial must pass in scenario 5 so that product A phase II clinical trial fails (II/F). The outcome of product A phase I clinical trial is the only difference between scenario 1 and 5, thus it is the differentiating clinical trial for these two scenarios. Accordingly, one can distinguish these two scenarios when product A clinical trial I is completed. In general, the period when two scenarios become distinguishable ($t^{\varsigma,\varsigma'}$) is the period when the corresponding differentiating clinical trial is finished. It is important to point out that the relationships among non-adjacent nodes are implicitly enforced by the relationship between adjacent nodes. Table 5.1 summarizes the relationships that are required for the example presented in Fig. 5.4.

Equation (5.1) is to track completion of clinical trials. This is compulsory in order to define the non-anticipativity constraints. Variable $\Omega_{ict\varsigma}$ indicates the periods following the phase c clinical trial completion for new product i. Here, $\eta_{ict\varsigma}$ is a binary variable that indicates the period when product i phase c clinical trial starts for scenario ς. Note that ε_{ic} and $\mathcal{N}$ are the trial duration and the set of potential new products, respectively.

$$\Omega_{ict\varsigma} = \Omega_{ict-1\varsigma} + \eta_{ict-\varepsilon_{ic}\varsigma} \qquad \forall\ i \in \mathcal{N}, c, t, \varsigma \tag{5.1}$$

Equation (5.2) assures that no clinical trial c can be executed more than once. Also, phase c clinical trial cannot start until phase $c-1$ is completed. This condition is expressed in Eq.(5.3).

$$\sum_t \eta_{ict\varsigma} \leq 1 \qquad \forall\ i \in \mathcal{N}, c, \varsigma \tag{5.2}$$

$$\sum_{t'<t} \eta_{ic+1t\varsigma} \leq \Omega_{ict\varsigma} \qquad \forall\ i \in \mathcal{N}, t, \varsigma, c \in \{I, II\} \tag{5.3}$$

Product development resource utilization is modeled using Eq. (5.4). Here, j^{rd} and $Cap_{j^{rd}}$ represent the resources dedicated to product development and their corresponding maximum capacity per period, respectively. To go on, $\theta^{rd}_{icj^{rd}}$ indicates the resource j^{rd} utilization factor for product i phase c clinical trial.

$$\sum_{i\in\mathcal{N}} \sum_{t'=t-\varepsilon_{ic}+1}^{t} \theta^{rd}_{icj^{rd}} \eta_{ict'\varsigma} \leq Cap^{\max}_{j^{rd}} \qquad \forall\ t, J^{rd} \tag{5.4}$$

Finally, as previously discussed, non-anticipativity constraints should be active until the differentiating trial of a pair of scenarios is finished ($\Omega_{i'c't\varsigma}$). This condition is expressed as an integer constraint in Eq. (5.5). Notice that set ϑ includes those pair of scenarios (ς, ς') that differ in merely the outcome of one product clinical trial, while ι_ϑ represents the differentiating product i' phase c' clinical trial for a specific pair of scenarios (ς, ς') belonging to ϑ.

$$-\Omega_{i'c't\varsigma} \leq \eta_{ict\varsigma} - \eta_{ict\varsigma'} \leq \Omega_{i'c't\varsigma} \qquad \forall\ i \in \mathcal{N}, c, (\varsigma, \varsigma') \in \vartheta, (i', c') \in \iota_\vartheta, t \tag{5.5}$$

5.4.2 Design and planning model

The design-planning approach and its integration with finances follows the model presented in Chapter 4, *Enhancing Corporate Value in the Design of Supply Chains*. The formulation has been extended to account for the different scenarios associated to clinical trial outcomes. For that purpose, simply an extra index, ς, has been added to each variable of that formulation (Eqns. 4.1 to 4.28). In that manner a design–planning model is straightforwardly generated for each scenario ς. In order to avoid redundancy the equations concerning such a model are not enumerated herein. The reader is referred to Sections 4.4.1 and 4.4.2 for details regarding this formulation.

5.4.3 Integration of product pipeline management and SC operations

The integration between formulations is carried out by the non-anticipativity constraints associated with capacity allocation variables (Eqns. (5.6) to (5.9)). Any "extra" expansion in capacity induced by product development projects should satisfy these constraints. Recall that $V_{jst\varsigma}$ and $X_{wt\varsigma}$, take a value of 1 if the facility being represented (either the equipment j at processing site s or the distribution center w) is expanded in capacity in period t, being 0 otherwise. Continuous variables $FSE_{jst\varsigma}$ and $FWE_{wt\varsigma}$ denote the expansion in capacity of the different network facilities during period t. In Eqns. (5.8) and (5.9) M represents a large quantity.

$$-\,\Omega_{ict\varsigma} \leq V_{jst\varsigma} - V_{jst\varsigma'} \leq \Omega_{ict\varsigma} \qquad \forall\ (\varsigma,\varsigma') \in \vartheta, (i,c) \in \iota_{\vartheta}, j, s, t \tag{5.6}$$

$$-\,\Omega_{ict\varsigma} \leq X_{wt\varsigma} - X_{wt\varsigma'} \leq \Omega_{ict\varsigma} \qquad \forall\ (\varsigma,\varsigma') \in \vartheta, (i,c) \in \iota_{\vartheta}, w, t \tag{5.7}$$

$$-\,M\Omega_{ict\varsigma} \leq FSE_{jst\varsigma} - FSE_{jst\varsigma'} \leq M\Omega_{ict\varsigma} \qquad \forall\ (\varsigma,\varsigma') \in \vartheta, (i,c) \in \iota_{\vartheta}, j, s, t \tag{5.8}$$

$$\begin{aligned} -M\Omega_{ict\varsigma} \leq FWE_{wt\varsigma} - FEW_{wt\varsigma'} \leq M\Omega_{it\varsigma} \\ \forall\ (\varsigma,\varsigma') \in \vartheta, (i,c) \in \iota_{\vartheta}, w, t \end{aligned} \tag{5.9}$$

Additionally, Eq. (5.10) states that production rates prior to trial completion must be equal to zero for every successful new product in scenario ς. No production for products that fail trials in scenario ς ($i \notin I_{\varsigma}^{suc}$) is allowed as defined by Eq. (5.11).

$$P_{ijst\varsigma} \leq M\Omega_{ict\varsigma} \qquad \forall\ \varsigma, c = III, i \in I_{c,\varsigma}^{suc}, j, s, t \tag{5.10}$$

$$P_{ijst\varsigma} = 0 \qquad \forall\ \varsigma, i \notin I_{III,\varsigma}^{suc}, j, s, t \tag{5.11}$$

5.4.4 Financial management

Similarly to the Design–planning formulation, the financial formulation follows that presented in Chapter 4 (Eqns. (4.29)–(4.60)). Such formulation uses the discounted-free-cash-flow (DFCF) method in order to carry out the firm's valuation. Again, the formulation has been extended to consider the different scenarios associated to clinical trial outcomes by adding the extra index ς to each variable. However, some modifications are required to incorporate the costs of development projects ($RDcost(\eta_{ict\varsigma}, \varepsilon_{i,c})_{t\varsigma}$) and some equations must be included so as to calculate the expected CV as well. This set of modified and new equations are described next.

Free cash flow at every period t ($FCF_{t\varsigma}$) is defined by a function that depends on net operating profit after taxes, change in net working capital ($NWC_{t\varsigma}$), net change in investments ($NetInvest_{t\varsigma}$) and now costs of development projects ($RDcost_{t\varsigma}$) as well. This can be seen in Eq. (5.12). This equation should replace Eq. (4.51) of Chapter 4.

$$\begin{aligned} FCF_{t\varsigma} = Profit_{t\varsigma}\,(1 - trate) - \\ NetInvest_{t\varsigma} - \Delta NWC_{t\varsigma} - RDcost_{t\varsigma} \qquad \forall\ t, \varsigma \end{aligned} \tag{5.12}$$

Finally Eq. (5.13) is to compute the total expected CV. For financial formulation details the reader is referred to Sections 4.4.3 and 4.4.4.

$$E[CV] = \sum_{\varsigma} prob_{\varsigma} CV_{\varsigma} \tag{5.13}$$

Here, $prob_{\varsigma}$ denotes the scenario ς probability of occurrence. Given the product i trial c probability of success $\hat{p}_{i,c}$, the scenario ς can be calculated as follows.

$$prob_{\varsigma} = \left(\prod_{c} \prod_{i \in I^{suc}_{c\varsigma}} \hat{p}_{i,c} \right) \left(\prod_{c} \prod_{i \notin I^{suc}_{c\varsigma}} (1 - \hat{p}_{i,c}) \right)$$

Financial risk management

The risk management formulation is presented next. Financial risk associated with a planning project can be defined as the probability of not meeting a certain target performance level referred to as Γ (Barbaro & Bagajewicz, 2004). Notice that for this problem, the performance is measured by the CV. Eqns. (5.14) to (5.16) have been added to constraint the risk of obtaining CVs less than target Γ. According to Eq. (5.14), ϱ_{ς} is a binary variable which takes a value of 1 if CV of scenario ς is less than Γ, being 0 otherwise. $Risk_{\max}$ indicates the maximum risk that decision makers are willing to accept for target level Γ.

$$\Gamma - M\varrho_{\varsigma} \leq CV_{\varsigma} \leq \Gamma + M(1 - \varrho_{\varsigma}) \qquad \forall\, \varsigma \tag{5.14}$$

$$Risk(\Gamma) = \sum_{\varsigma} prob_{\varsigma} \varrho_{\varsigma} \tag{5.15}$$

$$Risk(\Gamma) \leq Risk^{\varsigma}_{\max} \qquad \forall\, \varsigma \tag{5.16}$$

The overall mathematical program to tackle the simultaneous SC design-retrofitting and product development pipeline planning so as to maximize the expected CV ($E[CV]$) can be posed as follows:

$$\begin{gathered} \underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\, E[CV] \\ \text{subject to} \\ \text{Eqns. (4.1)–(4.50);(4.52)–(4.60)}\ \forall\, \varsigma \\ \text{Eqns. (5.1)–(5.16)} \\ \mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R} \end{gathered}$$

Here $\mathscr{X}$ denotes the model binary variables set, while $\mathscr{Y}$ represents the model continuous variable set.

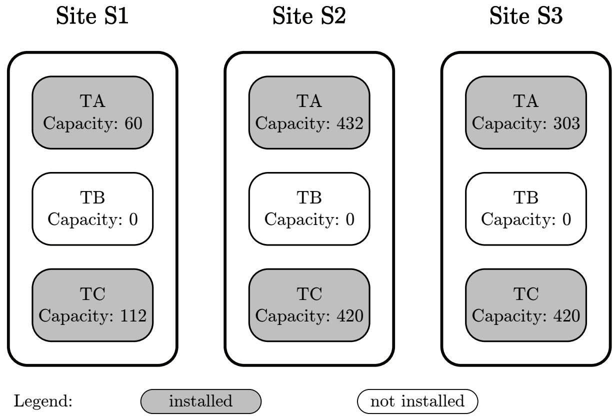


Figure 5.5: SC initial configuration (1x10^3 c.u.)

5.5 Example

The advantages of the proposed approach are demonstrated by solving a SC retrofitting–planning problem; which contains three processing sites ($S1 - S3$), S1 and S3 are already operational), three distribution centers ($W1 - W3$) and three market locations. Six products ($P1 - P6$) can be manufactured on three different equipments types (TA to TC). The SC initial configuration is presented in Fig. 5.5. A time horizon of 15 years is considered. This is composed of 15 periods with a length of one year each. In this example, products $P4 - P6$ are regarded as new products. For comparison purposes, the problem has been also solved using the traditional sequential approach. Under the sequential scheme, financial and other functional decisions are made following a hierarchical decision-making process. Firstly the SC and product development decisions are made and then the financial ones are determined. The operational decisions are typically obtained by optimizing NPV, while the financial decisions are computed by maximizing the CV using the model previously described.

Table 5.2: Corporate value for each scenario

Probability	Sequential approach	Integrated approach	$Risk(\Gamma = 0)$
0.594	-412.47	15990.60	14532.30
0.198	13040.00	15991.20	14205.00
0.066	-279.92	15520.60	11485.00
0.022	12955.10	15523.30	11086.40
0.081	1636.12	2505.39	8461.00
0.027	2292.79	2505.39	6783.38
0.009	-285.36	-81.54	1901.63
0.003	-175.56	-81.52	0.00
E[CV](1x10^6 m.u.)	2794.79	14300.35	13094.11

Product	P4	P6			P5
Year	1	2	3	4	5

(a) Sequential approach

Product	P6			P5	
Year	1	2	3	4	5

(b) Integrated approach

Figure 5.6: New product project selection

Numerical results show that the solution calculated by the integrated approach offers improved performance over the sequential approach. Certainly, the optimal expected CV from the integrated approach (IA) is considerably higher than the one computed by utilizing sequential approach (SA). The IA renders an expected CV of 14.3x10^9m.u.; while a CV of 2.79x10^9m.u. is obtained by applying the SA (see Table 5.1). The two approaches also yield different project selection decisions as shown in Figure 5.6. The SA launches the product development process for $P4$ in first period, P6 in second period and $P5$ in fifth period, while the IA launching policy is $P6$ in first period and then waits until the fourth period to launch $P5$. It is important to point out that the sequential approach selects the projects based on the NPV.

In Table 5.3, the NPVs obtained for each scenario are presented. Notice that the sequential approach obtains the highest NPV in the most probable scenario by developing the three products, however this requires significant amounts of net working capital which leads to a poor CV result for such scenario. Indeed, the expected CV is low compared to the integrated approach due to this reason.

Furthermore, the SC capacity allocation decisions are different. The SA proposes to install TA (40x10^3 c.u.) and TB (22x10^3 c.u.) in site $S2$, while the IA proposed to install merely TA (5x10^3 c.u.) in the same site. As shown in Figure

Table 5.3: NPV for each scenario

Probability	Sequential approach	Integrated approach
0.594	2464.235	2228.036
0.198	1727.445	2228.036
0.066	2423.956	2205.542
0.022	1684.258	2205.542
0.081	1248.441	72.85142
0.027	8.873884	72.85142
0.009	1138.557	-56.1196
0.003	-100.269	-56.1218
E[NPV](1x10^6 m.u.)	2114.13	1965.89

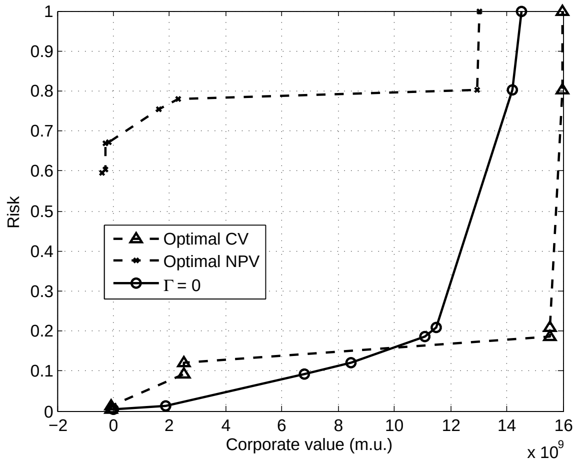


Figure 5.7: Risk curves for motivating example

5.7, a significant risk reduction is achieved by using the IA, the probability of obtaining negative CVs is reduced from 59% to 1.5%. Moreover, risk management constraints have been applied to the IA assuming that no negative CVs are desired ($\Gamma = 0$). For this case, no equipment capacity expansion is proposed. It is worth noticing that the expected CV has decreased to 13.1x10^9m.u. by using the risk constraints. Nevertheless, there is a reduction in the risk associated to those CVs which are lower than 10.0x10^9m.u. as depicted in Fig. 5.7.

The integrated formulation leads to an MILP model with 59,173 equations, 52,603 continuous variables, and 2,520 discrete variables. The problem was solved in 148 CPU seconds. In order to tackle medium size problems, a decomposition strategy is devised in the next section.

5.6 Decomposition strategy

The Optimal Condition Decomposition (OCD), which is a particular case of the Lagrangian relaxation procedure, is applied to overcome the computational cost of solving the monolithic problem which integrates SC design–retrofitting and product development pipeline management formulations. Further details about this decomposition strategy can be found in Section 3.8.1.

Here, the non-anticipativity (Eqns. (5.4)–(5.9)) constraints are preventing the overall problem to be solved by blocks, each block representing the equations of each scenario ς. The non-anticipativity constraints are the complicating constraints of the problem. However, Guignard and Kim (1987) have proved that bounds and convergence can be substantially improved by transforming mathematical programs so that every constraint of the original problem is preserved in one of the subproblems. In order to do so, new equations should be added to come to be the new complicating constraints. These new equations are constructed by duplicating the "complicating" variables.

For instance, for this problem the non-anticipativity condition represented by Eq. (5.4) might be rewritten in terms of variables belonging to one unique scenario if variable $\eta_{ict\varsigma'}$ could be duplicated in terms of scenario ς. Here, it is important to recall that there is one unique pair of scenarios considered which differs in the outcome of a specific potential product clinical trial (see Fig. 5.4). Then, Eq. (5.4) can be reformulated by replacing it by Eq.(5.17) and Eq. (5.18).

$$\tilde{\eta}_{icti'c'\varsigma} - \eta_{ict\varsigma'} = 0 \qquad \forall\ i \in \mathcal{N}, c, \varsigma < \varsigma', (\varsigma, \varsigma') \in \vartheta, (i', c') \in \iota_\vartheta, t \tag{5.17}$$

$$-\Omega_{i'c't\varsigma} \leq \eta_{ict\varsigma} - \tilde{\eta}_{icti'c'\varsigma} \leq \Omega_{i'c't\varsigma} \qquad \forall\ \varsigma, i \in \mathcal{N}, (i', c') \in \hat{\iota}_\varsigma, t \tag{5.18}$$

Here, $\tilde{\eta}_{icti'c'\varsigma}$ is the copy or duplicated variable of $\eta_{ict\varsigma'}$. Following a similar reasoning, the other non-anticipativity constraints can be reformulated as follows.

$$\tilde{V}_{jstic\varsigma} - V_{jst\varsigma'} = 0 \qquad \forall\ j, s, \varsigma < \varsigma', (\varsigma, \varsigma') \in \vartheta, (i, c) \in \iota_\vartheta, t \tag{5.19}$$

$$-\Omega_{ict\varsigma} \leq V_{jst\varsigma} - \tilde{V}_{jstic\varsigma} \leq \Omega_{ict\varsigma} \qquad \forall\ \varsigma, (i, c) \in \hat{\iota}_\varsigma, j, s, t \tag{5.20}$$

$$\tilde{X}_{wtic\varsigma} - X_{wt\varsigma'} = 0 \qquad \forall\ w, \varsigma < \varsigma', (\varsigma, \varsigma') \in \vartheta, (i, c) \in \iota_\vartheta, t \tag{5.21}$$

$$-\Omega_{ict\varsigma} \leq X_{wt\varsigma} - \tilde{X}_{wtic\varsigma} \leq \Omega_{ict\varsigma} \qquad \forall\ \varsigma, (i, c) \in \hat{\iota}_\varsigma, w, t \tag{5.22}$$

$$F\tilde{S}E_{jstic\varsigma} - FSE_{jst\varsigma'} = 0 \qquad \forall\ j, s, \varsigma < \varsigma', (\varsigma, \varsigma') \in \vartheta, (i, c) \in \iota_\vartheta, t \tag{5.23}$$

$$-M\Omega_{ict\varsigma} \leq FSE_{jst\varsigma} - F\tilde{S}E_{jstic\varsigma} \leq M\Omega_{ict\varsigma} \qquad \forall\ \varsigma, (i, c) \in \hat{\iota}_\varsigma, j, s, t \tag{5.24}$$

$$F\tilde{E}W_{wtic\varsigma} - FEW_{wt\varsigma'} = 0 \qquad \forall\ w, \varsigma < \varsigma', (\varsigma, \varsigma') \in \vartheta, (i, c) \in \iota_\vartheta, t \tag{5.25}$$

$$\begin{aligned} -M\Omega_{ict\varsigma} \leq FWE_{wt\varsigma} - F\tilde{E}W_{wtic\varsigma} \leq M\Omega_{it\varsigma} \\ \forall\ \varsigma, (i, c) \in \hat{\iota}_\varsigma, w, t \end{aligned} \tag{5.26}$$

By doing this reformulation, the complicating constraint turn to be the equalities (5.17), (5.19), (5.21), (5.23), and (5.25). The main difference between the OCD and the classical Lagrangian decomposition is that the OCD does not dualize all the complicating constraints. Here, a subproblem is constructed for every scenario (ς). Let us define ς as the scenario that is being evaluated in each subproblem. Then, the Lagrangian decomposition is applied by dualizing those complicating constraints that belong to other subproblems. Notice that the following subproblem is decomposable when the Lagrange multipliers ($\pi^I, \pi^{II}, \pi^{III}, \pi^{IV}, \pi^V$) and the duplicated variables for other scenarios are fixed to a given value. Also it noteworthy that complicating constraints related to the scenario being evaluated (ς) are left into the subproblem, so that their corresponding dual variables (i.e., $\pi^I, \pi^{II}, \pi^{III}, \pi^{IV}, \pi^V$) are obtained and updated using the subproblem solution.

$$
\begin{aligned}
&\text{maximize} \quad prob_\varsigma CV_\varsigma + \\
&\sum_{\varsigma'<\varsigma \wedge (\varsigma,\varsigma')\in\vartheta} \sum_{i\in\mathcal{N}} \sum_{c} \sum_{(i',c')\in\iota_\vartheta} \sum_{t} \left(\pi^I_{\varsigma',\varsigma,i,c,i',c',t} \left(\tilde{\eta}_{icti'c'\varsigma'} - \eta_{ict\varsigma}\right) \right) + \\
&\sum_{\varsigma'<\varsigma \wedge (\varsigma,\varsigma')\in\vartheta} \sum_{j} \sum_{s} \sum_{(i,c)\in\iota_\vartheta} \sum_{t} \left(\pi^{II}_{\varsigma',\varsigma,j,s,i,c,t} \left(\tilde{V}_{jstic\varsigma'} - V_{jst\varsigma}\right) + \right. \\
&\qquad \left. \pi^{IV}_{\varsigma',\varsigma,j,s,i,c,t} \left(F\tilde{S}E_{jstic\varsigma'} - FSE_{jst\varsigma}\right) \right) + \\
&\sum_{\varsigma'<\varsigma \wedge (\varsigma,\varsigma')\in\vartheta} \sum_{w} \sum_{(i,c)\in\iota_\vartheta} \sum_{t} \left(\pi^{III}_{\varsigma',\varsigma,w,i,c,t} \left(\tilde{X}_{wtic\varsigma'} - X_{wt\varsigma}\right) + \right. \\
&\qquad \left. \pi^{V}_{\varsigma',\varsigma,w,i,c,t} \left(F\tilde{E}W_{wtic\varsigma'} - FEW_{wt\varsigma}\right) \right) \\
&\text{subject to} \\
&\text{Eqns. (4.1)–(4.50);(4.52)–(4.60); (5.1)–(5.4);(5.10)–(5.26)} \qquad \forall\ \varsigma
\end{aligned}
\tag{5.27}
$$

The decomposition procedure is described in Algorithm 5.1. The decomposition subproblems complexity for this case study is presented in Table 5.4. As shown, this kind of problems can be solved with reasonable computational cost by using the OCD strategy. The problems were solved in an Intel 2 Core Duo-2.0 GHz - 2 GB RAM with a 3% integrality gap. The risk curves for the 16 and 64 scenarios cases are depicted in Figs. 5.8 and 5.9, respectively.

5.7 Final considerations

A model integrating product development pipeline management and SC design/retrofitting is presented. This approach incorporates the endogenous nature of trial uncertainties during the development process. By utilizing this

Table 5.4: Complexity comparison between monolithic (M) and decomposed problems (D-S)

Scen.	Equations		Cont. Var.		Dis. Var.		E[CV] (109)		Total CPU sec	
	M	D-S	M	D-S	M	D-S	M	D-S	M	D-S
16	62102	7282	68897	5562	3064	210	7.03	7.06	165	95
64	290662	22735	279377	6422	13584	240	8.21	8.15	24370	1026

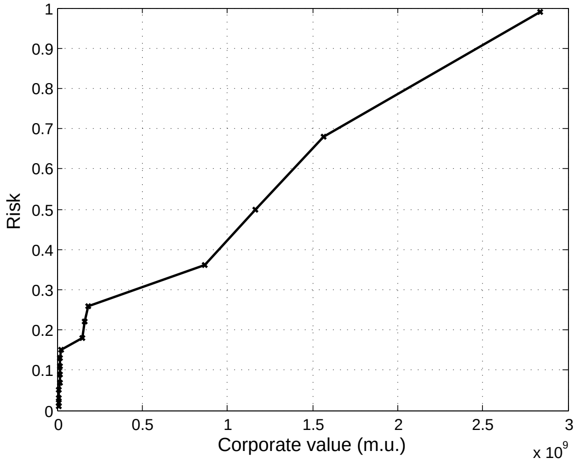


Figure 5.8: Risk curve for the case study including 16 scenarios

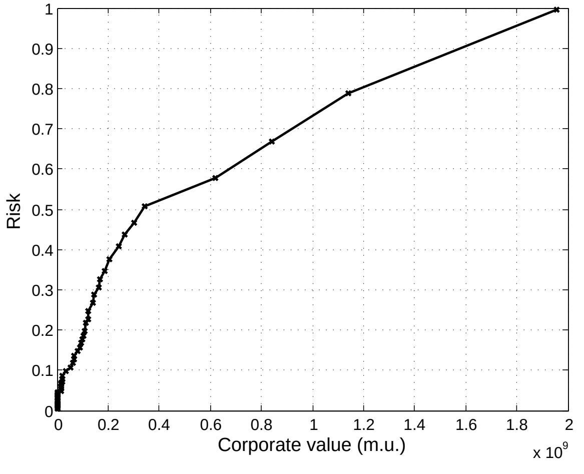


Figure 5.9: Risk curve for the case study including 64 scenarios

Algorithm 5.1: Optimal Condition Decomposition algorithm

Data: Initial values for complicating variables, multipliers $(\pi^{I}, \pi^{II}, \pi^{III}, \pi^{IV}, \pi^{V})$, gap tolerance ($tolerance$).
Result: The optimal solution $E[CV], \mathscr{X}, \mathscr{Y}$.
begin
  $gap \longleftarrow \infty$;
  $k^{a} \longleftarrow 0$;
  while $gap > tolerance$ **do**
    forall ς **do**
      forall $\varsigma' \neq \varsigma$ **do**
        $\eta_{ict\varsigma'} \longleftarrow \hat{\eta}^{k}_{ict\varsigma'}$;
        $V_{jst\varsigma'} \longleftarrow \hat{V}^{k}_{jst\varsigma'}$;
        $FE_{jft\varsigma'} \longleftarrow \hat{FE}^{k}_{jst\varsigma'}$;
        $X_{wt\varsigma'} \longleftarrow \hat{X}^{k}_{wt\varsigma'}$;
        $FEW_{wt\varsigma'} \longleftarrow \hat{FEW}^{k}_{wt\varsigma'}$;
        $\tilde{\eta}_{icti'c'\varsigma'} \longleftarrow \hat{\tilde{\eta}}^{k}_{icti'c'\varsigma'}$;
        $\tilde{V}_{jstic\varsigma'} \longleftarrow \hat{\tilde{V}}^{k}_{jstic\varsigma'}$;
        $F\tilde{S}E_{jftic\varsigma'} \longleftarrow F\hat{\tilde{S}}E^{k}_{jstic\varsigma'}$;
        $\tilde{X}_{wtic\varsigma'} \longleftarrow \hat{\tilde{X}}^{k}_{wtic\varsigma'}$;
        $F\tilde{E}W_{wtic\varsigma'} \longleftarrow F\hat{\tilde{E}}W^{k}_{wtic\varsigma'}$;
        $\pi^{I}_{\varsigma',\varsigma,i,c,i',c',t} \longleftarrow \hat{\pi}^{I,k}_{\varsigma',\varsigma,i,c,i',c',t}$;
        $\pi^{II}_{\varsigma',\varsigma,j,s,i,c,t} \longleftarrow \hat{\pi}^{II,k}_{\varsigma',\varsigma,j,s,i,c,t}$;
        $\pi^{III}_{\varsigma',\varsigma,j,s,i,c,t} \longleftarrow \hat{\pi}^{III,k}_{\varsigma',\varsigma,j,s,i,c,t}$;
        $\pi^{IV}_{\varsigma',\varsigma,w,i,c,t} \longleftarrow \hat{\pi}^{IV,k}_{\varsigma',\varsigma,w,i,c,t}$;
        $\pi^{V}_{\varsigma',\varsigma,w,i,c,t} \longleftarrow \hat{\pi}^{V,k}_{\varsigma',\varsigma,w,i,c,t}$;
      Solve sub-problem (5.27);
      $\hat{\mathscr{X}}_{\varsigma}^{k+1} \longleftarrow \mathscr{X}_{\varsigma}^{*b}$;
      $\hat{\mathscr{Y}}_{\varsigma}^{k+1} \longleftarrow \mathscr{Y}_{\varsigma}^{*}$;
      forall $\varsigma' \neq \varsigma$ **do**
        $\hat{\pi}^{I,k+1}_{\varsigma,\varsigma',i,c,i',c',t} \longleftarrow \pi^{I*}_{\varsigma,\varsigma',i,c,i',c',t}$;
        $\hat{\pi}^{II,k+1}_{\varsigma,\varsigma',j,s,i,c,t} \longleftarrow \pi^{II*}_{\varsigma,\varsigma',j,s,i,c,t}$;
        $\hat{\pi}^{III,k+1}_{\varsigma,\varsigma',w,i,c,t} \longleftarrow \pi^{III*}_{\varsigma,\varsigma',w,i,c,t}$;
        $\hat{\pi}^{IV,k+1}_{\varsigma,\varsigma',j,s,i,c,t} \longleftarrow \pi^{IV*}_{\varsigma,\varsigma',j,s,i,c,t}$;
        $\hat{\pi}^{V,k+1}_{\varsigma,\varsigma',w,i,c,t} \longleftarrow \pi^{V*}_{\varsigma,\varsigma',w,i,c,t}$;
    $gap \longleftarrow \|[\hat{\mathscr{X}}^{k+1} - \hat{\mathscr{X}}^{k}]^{T} | [\hat{\mathscr{Y}}^{k+1} - \hat{\mathscr{Y}}^{k}]^{T}\|$;
    $k \longleftarrow k+1$;
end

[a] k refers to the iteration number
[b] An * indicates the optimal variable value

model, the new product launching decisions are made in tandem with the capacity expansion and production planning decisions. The model evaluates the capacity requirements of the whole business product portfolio (i.e, existing and potential new products). Both, existing and new products, compete for the enterprise resources which include cash flows and capacity among others. The allocation of such resources is made so that the expected corporate value is maximized. The corporate value has been computed using a discounted-free-cash-flow method which considers the business fixed and currents assets (net working capital). Performance comparison with the traditional sequential decision approach is also made, demonstrating the significant economic benefits of holistic approaches.

The results show that improvements can be achieved when these decisions, usually taken by different functions, are integrated into a single model. Moreover, the model is able to account for financial risk restrictions that may be imposed by stockholders. It is shown that probabilities of low SC performance are considerable reduced by incorporating the risk management formulation. Finally, an ad-hoc Lagrange decomposition has been developed to successfully reduce the significant computational burden associated with solving this kind of problems.

Further work is focused on applying the decomposed problem in a parallel computing scheme so that large industrial size cases can be tackled using the proposed model.

5.8 Nomenclature

Indices

c	clinical trial phase
i	products
j	plant equipment
s	manufacturing sites
t	planning periods
w	distribution centers
ς	scenarios

Sets

I_j	products that can be processed in plant equipment j
$I_{c\varsigma}^{suc}$	set of products i whose clinic trial c is successful for scenario ς
J_i	equipment that can process product i
J_{rd}	equipment used for product development tasks
$\mathcal{N}$	set of new products
ϑ	set of related pair of scenarios
$\hat{\iota}_\varsigma$	differentiating product i clinical trial c for the relationship for scenario ς
ι_ϑ	differentiating product i clinical trial c for pair of scenarios ϑ

Parameters

Cap_{jrd}^{max}	maximum capacity of equipment j
M	a large value
$\hat{p}_{ic}$	product i clinical trial c probability of success
$prob_{\varsigma}$	scenario ς probability of occurrence
$Risk_{\max}$	maximum acceptable risk at level Γ
$trate$	tax rate
$\varepsilon_i c$	duration of product i clinical trial c
Γ	level of performance for risk determination
θ_{icj}^{rd}	capacity utilization of equipment j by product i clinical trial c

Binary variables

$V_{jst\varsigma}$	1 if the capacity of equipment j is increased at site s in period t for scenario ς, 0 otherwise
$\tilde{V}_{jstic\varsigma}$	copy of $V_{jst\varsigma}$
$X_{wt\varsigma}$	1 if the capacity of distribution center w is increased in period t for scenario ς, 0 otherwise
$\tilde{X}_{wtic\varsigma}$	copy of $X_{wt\varsigma}$
$\eta_{ict\varsigma}$	1 if the product i clinical trial c starts in period t for scenario ς, 0 otherwise
$\tilde{\eta}_{icti'c'\varsigma}$	copy of $\eta_{ict\varsigma}$
ϱ_{ς}	1 if CV_{ς} is less than level Γ
$\Omega_{ict\varsigma}$	1 if the product i clinical trial c is already completed in period t for scenario ς, 0 otherwise

Continuous variables

CV_{ς}	corporate value at the end of the planning horizon for scenario ς
$E[CV]$	expected corporate value
$FCF_{t\varsigma}$	free cash flows in period t for scenario ς
$FSE_{jst\varsigma}$	capacity increment of plant equipment j during period t at site s for scenario ς
$F\tilde{S}E_{jst\varsigma}$	copy of $FSE_{jstic\varsigma}$
$FWE_{jst\varsigma}$	capacity increment at distribution center w during period t for scenario ς
$F\tilde{W}E_{jst\varsigma}$	copy of $FWE_{jstic\varsigma}$
$NetInvest_{t\varsigma}$	net investment in period t for scenario ς
$P_{ijst\varsigma}$	production rate of product i in equipment j at site s in period t for scenario ς
$Profit_{t\varsigma}$	profit achieved in period t for scenario ς
$Risk(\Gamma)$	financial risk for level Γ
$RDCost_{t\varsigma}$	development costs in period t for scenario ς
$\Delta NWC_{t\varsigma}$	change in net working capital in period t for scenario ς

Chapter 6

Linking Marketing and SC Models for Improved Business Strategic Decision Support

6.1 Introduction

Nowadays, a supply chain management model incorporating business strategic components is becoming of paramount importance to gain a competitive edge in the market place. To be successful, the enterprise model has to contemplate not only the supply chain, but also the demand chain. Understanding the market and customer behavior is extremely crucial for developing a good business policy. Marketing is a boundary-spanning activity, linking selling entities with buyers and intermediate channels. To operate most effectively, marketing activities must be coordinated with other functional areas of the firm. The marketing – SC management interface is an issue that deserves further research. Business managers should evaluate the existing trade-off between marketing and SC planning decisions in order to enhance the performance of the overall business metric: the shareholders value. Recently, there is a significant trend driving business managers to implement marketing science models for reaching more rational and holistic decisions. In this chapter, a mathematical model is presented for the enterprise that accounts for the three main business functionalities (i.e., operations, finances and marketing). The posed problem is tackled by developing a holistic MINLP model which optimizes in tandem the SC and marketing strategic decisions. Moreover, a financial model that allows to quantitatively assessing the enterprise value is also incorporated. Finally, the main advantages of coordinated decisions are discussed through an illustrative example.

Figure 6.1: Marketing mix

6.2 The SC operations and marketing interface

Typically, the business strategy is modeled as a hierarchical process in which functional strategies, such as operations, logistics, marketing, and finance are driven by a higher level strategy (Fine & Hax, 1985). A key element of the strategic framework involves coordinating functional level plans to work in concert so as to achieve the overall business strategy rather than to locally optimize outcomes for individual functions, business units, plants, or stores. One of the primary challenges in implementing an effective strategy involves achieving consensus within the business organization. Undoubtedly, business functional decisions must be integrated and coordinated in order to tackle the critical decision of resource allocation among the different business activities. Unfortunately, while this concept is clearly sound on a conceptual level, actual implementation is typically very difficult (Bozarth & Berry, 1997).

One important strategic issue that needs more research is the integration of SC production-distribution operations and marketing activities. According to the American Marketing Association[1], Marketing is the process of planning and executing the conception, pricing, promotion, and distribution of ideas, goods, and services in order to create exchanges that satisfy individual and organizational objectives. This activities, usually regarded as Marketing mix (see Fig. 6.1), refers to the primary elements that must be attended in order to properly trade a product or service. On the other hand, SCM's focus is on the synchronization of production and distribution activities along the different entities comprising the SC network. The main objective is typically to minimize the total SC cost. Although several authors have highlighted the conflicting goals of SC and marketing managers (Eliashberg & Steinberg, 1997; Shapiro, 2006), it is still typically assumed that under a decentralized decision making scheme, marketing decisions are made first; determining demand forecasts which are later considered by the SC model to support production-distribution related

[1] http://www.marketingpower.com/

decisions. By deploying this sequential procedure, the firm may be significantly under-estimating its overall performance. Integrating marketing and operations is a challenge in any business, since there is a natural tension between these two functional areas (Bozarth & Berry, 1997). At best, the tension between these two functions results in a dampening of marketing's tendency to over-promise to lure customers and a push on operations to move beyond an internal focus on reducing costs without a clear vision of end-consumer needs.

Usually, the primary objective of marketing function is maximizing revenues creation by satisfying customers through the products and services offered. On the other hand, SCM's objective is to minimize the total SC cost as previously mentioned. In general, conflicts arise between marketing and SC because of these contrasting performance indicators which eventually are used to develop incentive structures for managers and their corresponding employees. For instance, one classical conflict between these two functions is the one associated to the inventory management. SC managers strive to keep low stock levels, while marketing managers long for high stock levels to guarantee that most of customer orders are met, thus improving revenue generation. Nevertheless, the enterprise main goal is to create and maximize shareholders value which actually is a function of revenues, cost and other economic factors (see Section 4.4.4). Consequently, business managers are in need of an integrated analytical decision support tool that is capable of appraising the trade-off between operations and marketing while evaluating and maximizing shareholders value.

Nowadays, there are more and more companies that are continuously searching for competitive advantages in order to get a better position in markets. One way of doing so may be by aligning functionalities strategic/tactical decisions towards the optimization of the overall business performance metric. In this chapter, it is presented a novel approach to address this challenge. Here, it is developed a MINLP model that tackles SC network design and marketing strategic decisions in tandem. Then, such model is coupled with the financial formulation presented in Chapter 4, *Enhancing Corporate Value in the Design of Supply Chains*, which allows calculating shareholders value by means of the discounted-free-cash-flow (DFCF) method.

6.3 Problem statement

This chapter also deals with the optimal design and operation of SC network. The network consists of a number of existing multi-product manufacturing sites at fixed locations, a number of distribution centers, and finally a number of customer zones at fixed locations. In general, each product can be produced at several plants using different equipment at different locations. The production capacity of each manufacturing site is modeled in terms of a set of linear constraints relating the mean production rate per product to the availability of the equipment plant. Distribution centers are described by upper and lower bounds on their material handling capacity and they can be supplied from more than one manufacturing plants and can supply more than one market place. Each market demands one or more products. These demands are assumed to be influenced by marketing activities such as product pricing and advertising. A market may be served by more than one distribution center.

Operational costs include those associated with production, handling of material, transportation and raw materials. Transportation costs are assumed to be linear functions of the actual flow of the product from the source echelon to the destination echelon. Revenue is obtained from the selling of products. It is noteworthy that the problem does not consider product prices as a given parameter, instead it is a decision variable to be determined. Investments on facilities and equipment are also taken into account.

The proposed model is intended to support managers on the decision making about SC and marketing decisions. On the marketing side, the model assists managers on deciding the product pricing, the amount of advertising expenditures and its most appropriated allocation along time. The relationship among pricing, advertising and demand is considered in order to propose how equipment capacity should be expanded along the SC. Additionally, the production and distribution planning is also carried out to better satisfy market demand. This includes product portfolio per production plant, production amounts, utilization level, and transportation links to establish in the network along side with material flows. All this decisions will be taken such that the corporate value evaluated at the end of a predefined planning horizon is maximized.

6.4 The mathematical formulation

The problem is formulated as a mixed integer nonlinear programming (MINLP). The variables and constraints of the model can be classified into four groups. The first group corresponds to the formulation of marketing activities. SC design and operations constraints given belong to the second group. The third one incorporates those constraints related to the financial formulation. Finally, the fourth group is associated with the integration of operations and marketing decisions.

6.4.1 Strategic marketing modeling

Using marketing models can be valuable for the industry in order to achieve improvement in the business bottom line. For instance, the 2006 R&D expenditures by North American pharmaceutical companies were \$55.2 billion or 19.4% of sales (PhRMA, 2007). By comparison, the marketing expenditures in 2006 by these companies were \$27.3 billion or about 10% of sales (IMS-Health, 2006). Given this substantial level of spending, there is an increasing use of and need for analytic and data driven models for strategic marketing decisions in this particular industry. However, this is a necessity that spans over other type of industries as well.

According to Lilien (ISBM-Newsletter, 1998), marketing is no longer based primarily on conceptual content. Marketing resembles design engineering by putting together data, models, analyses, and computer simulations to design effective marketing plans. One of the most influential developments for marketing modeling has been the e-commerce and the bar-code scanners. Today firms have access to more market and customer data than they can use. Having too much data without the models and systems for analyzing what is important and what can be discarded can be as bad as or even worse than having too little data. Increasingly marketing managers are being asked to clear the same budget-justification hurdles imposed on other types of investment firms make. It is not surprising, therefore, that more managers are seeking help in turning their data and knowledge into improved decision making (Lilien & Rangaswamy, 2001). The systematic approach to harness data and knowledge to drive marketing decision making and implementation through a technology-enabled and model-supported interactive decision process is what it is recently regarded as marketing engineering. The marketing engineering approach to decision making helps transform objective and subjective data about the marketing environment into decisions and decision implementations.

Here, BRANDAID, a marketing decision making model is used. This kind of models are designed for helping marketing managers make better decisions. They recommend optimal marketing mix decisions for the manager. These models have been developed for each marketing variable and for the entire marketing mix program which includes pricing, distribution and promotion decisions.

The BRANAID model

Marketing managers make decisions about price, advertising, promotion, and other marketing variables on the basis of factual data, and assumptions about how the market works. BRANDAID is a model for assembling these elements to describe the market and evaluate strategies. This flexible strategic marketing mix model is basically comprised of three sub-models, namely: advertising sub-model, pricing sub-model and sales force sub-model. It is noteworthy that the model is (i) modular, so managers determine which sub-models to take into account according to their needs and (ii) customizable, since managers may introduce into the sub-models those functions that best describe their own marketing processes. The model is briefly presented next following the work of Little (1975). Two sub-models are considered in this chapter; however other marketing influences or activities can be handled in the same manner.

The main model structure The model is based on the two following expressions. Eq. (6.1) expresses firm's target market demand (Dem_{imt}) as a function of market share ($MktShare_{imt}$) and total market demand (D_{imt}), while Eq. (6.2) computes market share as a reference value (S^{o}_{im}) modified by the effect of marketing activities (e.g., pricing, advertising, promotions, sales force) and other considered influences ($\zeta_{i,ma,m,t}$) such as competitors actions.

$$Dem_{imt} = MktShare_{imt}D_{imt} \qquad \forall\ i, m, t \tag{6.1}$$

$$MktShare_{imt} = S^o_{im} \prod_{ma} \zeta_{i,ma,m,t} \qquad \forall\ i, m, t \tag{6.2}$$

The quantity S^o_{im} introduce the idea of reference conditions. An established product has an existing situation and planning is primarily concerned with changes from that situation. Accordingly, a set of reference conditions are defined, usually from sales and marketing activities in the recent past. The terms $\zeta_{i,ma,m,t}$ are called effect indices. As used here, an index is a number with nominal value 1.0 that expresses fractional changes from a reference value. The use of a multiplicative form in Eq. (6.2) implies a specific assumption about the interaction of marketing effects in the neighborhood of reference values. It says that an improvement in the effect of one marketing variable increases the improvement that can be obtained from another. Other degrees of interaction can be provided by adding effect indices that depend on more than one marketing activity.

Advertising sub-model This module assumes that there exists an advertising rate that maintains sales at target level. If a brand starts out with its sales rate at its reference value and marketing conditions other than advertising at their reference values, then there is some advertising rate that will maintain sales at reference. This advertising will be designated as the maintenance or reference advertising rate. If advertising is less than reference, the sales rate will presumably sag, and, after a while, level off at a new lower value. Advertising consists of messages delivered to individuals by exposures in media paid for by monetary unit. The next equations describe this procedure. It is assumed $ma = 1$ to describe advertising activities.

$$\zeta_{i1mt} = \varpi_1 \zeta_{i1mt-1} + (1 - \varpi_1) Adver_{imt} \qquad \forall\ i, m, t \tag{6.3}$$

$$Adver_{imt} = f(h_{imt}, k_{imt}, AdvExp_{imt}) \qquad \forall\ i, m, t \tag{6.4}$$

$$Adver_{imt} = \frac{h_{imt} k_{it} AdvExp_{imt}}{h^o_{im} k^o_{im} AdvExp^o_{im}} \qquad \forall\ i, m, t \tag{6.5}$$

Here, ϖ_1 represents the carryover effect of advertising on target demand per period. The value of ϖ_1 determines how quickly demand is affected by advertising activities. The advertising rate ($Adver_{imt}$) is usually considered as a function of media efficiency (h_{imt}), copy effectiveness (k_{imt}) and advertising expenditures ($AdvExp_{imt}$) as expressed in Eq. 6.4. In marketing, copy is understood as the printed text or spoken words in an advertisement. As previously mentioned, this function can be estimated by each particular case by

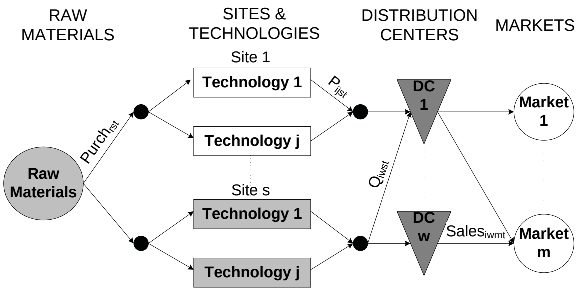


Figure 6.2: Model supply chain structure

examining the data available regarding this marketing activity. Hence, particular and current market-media trends can be taken into account by constructing an adequate descriptive model. For the illustrative example a function similar to Eq. (6.5) is used. In that equation, h^o_{im}, k^o_{im}, and $AdvExp^o_{im}$ are reference values of the abovementioned parameters.

Pricing sub-model Price is a sensitive control variable and a frequently used one. The price under consideration is the basic price charged by the firm. Price elasticity of demand is considered in this chapter for this sub-model. Again, more complicated descriptive models can be used to describe the specific product behavior of price-demand. It is assumed $ma = 2$ to describe pricing activities. Here the linear function (6.6) is used. Ξ_{im} denotes the elasticity coefficient.

$$Price^o_{im}(1 - \zeta_{i2mt}) = \Xi_{im}(Price_{imt} - Price^o_{im}) \qquad \forall\, i, m, t \tag{6.6}$$

6.4.2 The SC design–planning model

The design-planning approach is based on the model developed in Chapter 4. In that formulation (Eqns.(4.1)–(4.28)), a four echelon SC is considered as shown in Figure 6.2. In this chapter, the equation that expresses that part of the demand can be left unsatisfied because of limited production capacity (Eq. (4.4))becomes one of the integrating equations as stated in section 6.4.4.

6.4.3 The financial formulation

Similarly to the Design–planning formulation, the financial formulation follows the one presented in Chapter 4 (Eqns. (4.29)–(4.60)). Such formulation uses the discounted-free-cash-flow (DFCF) method in order to carry out the firm's valuation. However, some modifications are required to incorporate the advertising expenditures ($AdvExp_{imt}$). This set of modified and new equations are described next.

Free cash flow at every period t (FCF_t) is defined by a function that depends on net operating profit after taxes, change in net working capital (NWC_t), net change in investments ($NetInvest_t$) and now advertising expenditures ($AdvExp_{imt}$) as well. This can be seen in Eq. (6.7). This equation should replace Eq. (4.51) of Chapter 4.

$$FCF_t = Profit_t \,(1 - trate) - \left(\Delta NWC_t + NetInvest_t + \sum_i \sum_m AdvExp_{imt} \right) \qquad \forall\, t \tag{6.7}$$

6.4.4 Integration among models

Additionally to Eq. (6.7), integration among models is carried out by demand and revenue ($ESales_t$). As it can be observed a better balance between the demand generated by means of advertising and the available capacity proposed by the SC model can be achieved by utilizing Eq. (6.8).

$$\sum_w Sales_{iwmt} \le Dem_{imt} \qquad \forall\, i, m, t \tag{6.8}$$

$$ESales_t = \sum_i \sum_w \sum_m Sales_{iwmt} Price_{imt} \qquad \forall\, t \tag{6.9}$$

Notice that price and demand are problem variables instead of parameters: Recall that it is assumed that products i should be transported to final market from distribution centers w.

The overall mathematical program to tackle the simultaneous SC design-retrofitting and marketing strategic planning so as to maximize the Corporate Value (CV) can be posed as follows:

$$\begin{gathered} \underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\, CV \\ \text{subject to} \\ \text{Eqns.(4.1)–(4.3); (4.5)–(4.16); (4.18)–(4.50); (4.52)–(4.60); (6.1)–(6.9)} \\ \mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R} \end{gathered}$$

The model binary variables set is denoted by $\mathscr{X}$ denotes , while $\mathscr{Y}$ represents the model continuous variable set.

6.5 Example

The advantages of the proposed approach are demonstrated by solving an illustrative SC design–planning problem; which contains three processing sites ($S1$–$S3$), three distribution centers ($W1 - W3$) and three market locations

Table 6.1: Capacity requirement per product for each technology equipment (c.u.)

	TA	TB	TC
$P1$	20.00	21.25	12.50
$P2$	17.50	22.50	18.75
$P3$	22.50	12.50	18.75

Table 6.2: Performance comparison between integrated and sequential approaches

Approach	Revenues	Advertising expenditures	Net revenues	Corporate value	Investment in capacity
Sequential	$522.32\text{x}10^6$	$86.11\text{x}10^6$	$436.21\ \text{x}10^6$	$84.35\text{x}10^6$	$79.77\ \text{x}10^6$
Integrated	$512.94\text{x}10^6$	$85.15\text{x}10^6$	$427.79\ \text{x}10^6$	$123.93\text{x}10^6$	$43.42\ \text{x}10^6$

($M1-M3$). A set of potential equipment technologies are assumed to be available for the processing sites. Three product families ($P1-P3$) can be manufactured on three different equipments types (TA to TC). A time horizon of 5 annual periods is considered. For all markets and products, the elasticity coefficient and the reference advertising expenditures are assumed to be 0.85 and $3.0\text{x}10^6$ c.u., respectively. The capacity requirements for each product and technology are presented in Table 6.1. The integrated formulation leads to an MINLP with 1,811 equations, 2,587 continuous variables, and 90 discrete variables. It takes 4 CPU seconds to reach the optimal solution for the integrated problem on an Intel Core 2 Duo at 2.0 GHz computer using DICOPT solver.

For comparison purposes, the problem has been also solved using the traditional sequential approach (SA) described in section 6.2. First marketing decisions are taken and then the SC and financial decisions are determined. The marketing decisions are typically obtained by optimizing net revenues (subtracting advertising expenditures from total revenues), while the financial and SC decisions are computed by maximizing the CV. Numerical results show that

Table 6.3: Sequential approach network design

		Time period (t) 1	2	3	4
Manufacturing sites					
s	j	Capacity increment (c.u.)			
S1	TA	400,000.0	258,351.4	0.0	0.0
	TB	255,950.6	0.0	0.0	0.0
	TC	400,000.0	0.0	0.0	0.0
S2	TA	0.0	400,000.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	0.0	0.0	0.0
S3	TA	400,000.0	400,000.0	0.0	0.0
	TB	400,000.0	0.0	0.0	0.0
	TC	400,000.0	0.0	0.0	0.0

Table 6.4: Integrated approach network design

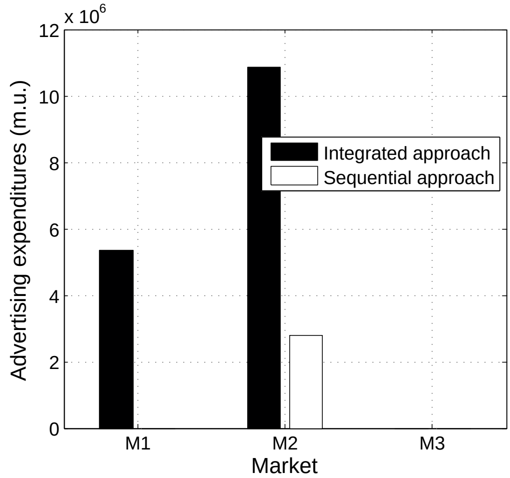
		Time period (t)			
		1	2	3	4
Manufacturing sites					
s	j	Capacity increment (c.u.)			
S1	TA	400,000.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	400,000.0	0.0	0.0	0.0
S2	TA	0.0	0.0	0.0	0.0
	TB	0.0	0.0	0.0	0.0
	TC	0.0	0.0	0.0	0.0
S3	TA	400,000.0	0.0	0.0	0.0
	TB	340,689.8	0.0	0.0	0.0
	TC	400,000.0	314,466.7	0.0	0.0

the solution calculated by the integrated approach (IA) offers improved performance over the SA solution. Certainly, the optimal CV from IA is 47% higher than the one obtained by utilizing SA. The IA obtains such performance by a 2% decrease in net revenues (see Table 6.2).

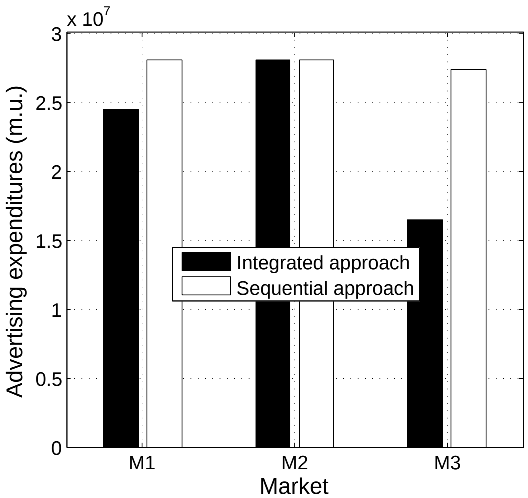
The two approaches also yield different SC design decisions. The SC network configurations obtained by following the integrated and sequential approach are summarized in Tables 6.4, and 6.3. For the first year, the sequential approach proposes to install all equipment technologies in sites $S1$ and $S3$, while the integrated approach proposes to install TA and TC in location $S1$ and all technologies in $S3$. The pricing decisions are the same for both approaches: 77.56 m.u., 87.47 m.u., and 74.4 m.u. for products $P1$, $P2$, and $P3$, respectively. Figure 6.3 shows the advertising expenditures for each product. Table 6.5 shows the product demands induced by marketing activities and their corresponding sales for both approaches. Notice that in order to achieve a greater revenue, the sequential approach induces higher sales for $P2$, the more expensive product. However, it does not consider that the capacity requirements for this product are higher than the other products (see TB and TC). TA is the more efficient

Table 6.5: Induced demand and sales carried out for both approaches (1x10^3 units)

	Markets							
	M1		M2		M3		Total	
Product	Sales	Demand	Sales	Demand	Sales	Demand	Sales	Demand
Sequential approach								
P1	10.2	51.2	226.0	272.0	5.1	25.6	241.3	348.8
P2	1824.5	1866.0	2162.3	2211.5	1763.5	1804.5	5750.3	5881.9
P3	3.1	15.5	3.7	18.4	1.5	7.7	8.3	41.6
Integrated approach								
P1	375.0	415.9	808.0	854.0	5.1	25.6	1188.1	1295.5
P2	1580.3	1621.7	2162.4	2211.5	1061.0	1102.0	4803.7	4935.2
P3	3.1	15.5	3.7	18.4	1.5	7.7	8.3	41.6



(a) Product $P1$



(b) Product $P2$

Figure 6.3: Advertising expenditures

technology equipment for producing $P2$ (see Table 6.1). These are the reasons for proposing greater investments in capacity and for expanding TA technology in the second year. These decisions lead to a lower corporate value. From another standpoint, the integrated approach simultaneously assesses the revenue obtained from the products to be sold and the capacity requirements to do so. The integrated model evaluates such a trade-off and finds a balanced solution which maximizes the corporate value. As shown in Table 6.2, a significant improvement in terms of corporate value can be achieved by using the integrated approach.

6.6 Final considerations

The intent of this chapter is to motivate and draw attention to the need of further research in this kind of decision problems which are interfacing SC operations and marketing functions. A MINLP model considering simultaneously SC design/retrofitting, financial and marketing decisions is presented. Performance comparison with the traditional sequential decision approach is made, which demonstrates the economic benefits that the holistic approach may provide. The aim is to emphasize the relevance of a correct appraisal of the trade-off existing between the demand (which can be induced by marketing activities) and the SC capacity investments required to meet such demand. Such decisions have an important impact in the firm's value as it has been demonstrated. Finally, it is worthy to point out the potential of response surface and data mining techniques in this field. By using these techniques, descriptive models for the marketing activities can be obtained to be used later in an optimization scheme.

6.7 Nomenclature

Indices

i	products
t	planning periods
m	markets
ma	marketing activities
w	distribution centers

Parameters

$AdvExp^o_{im}$	reference value for advertising expenditures for product i in market m
D_{imt}	total demand in market m for product i during period t
h_{imt}	media efficiency for product i in market m during period t
h^o_{im}	reference value for the media efficiency for product i in market m
k_{imt}	copy effectiveness for product i in market m during period t
k^o_{im}	reference value for the copy effectiveness for product i in market m
$Price^o_{im}$	reference value for price of product i in market m

S_{im}^{o}	market share reference value for product i in market m
$trate$	tax rate
ϖ_1	carry-over rate for advertising effect on demand target
Ξ_{im}	demand elasticity of product i in market m

Continuous variables

$Adver_{imt}$	advertising rate for product i in maket m during period t
$AdvExp_{imt}$	advertising expenditures for product i in market m during period t
CV	corporate value at the end of the planning horizon
Dem_{imt}	target demand in market m for product i during period t
$ESales_t$	economic value of sales carried out during period t
FCF_t	free cash flows in period t
$MktShare_{imt}$	share in market m for product i during period t
$NetInvest_t$	net investment in period t f
$Price_{imt}$	product i price in market m at period t
$Profit_t$	profit achieved in period t f
$Sales_{iwmt}$	amount of product i sold from warehouse w to market m during period t
ΔNWC_t	change in net working capital in period t
$\zeta_{i,ma,m,t}$	influence of marketing activity ma on share in market m for product i during period t

Part III

Operations Strategic and Tactical Issues

Chapter 7

Flexible Design – Planning of SC Networks

7.1 Introduction

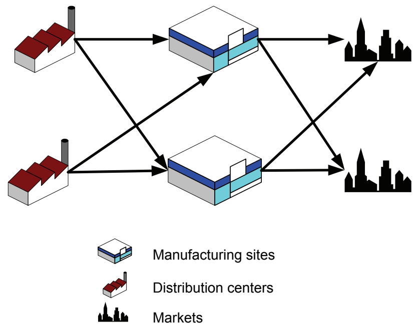
Nowadays market competition is essentially associated to supply chain (SC) improvement. Therefore, the locus of value creation has shifted to the chain network. The strategic decision of determining the optimal SC network structure plays a vital role in the later optimization of SC operations. This chapter focuses on the design and retrofit of SCs. Traditional approaches available in literature addressing this problem usually utilize as departing point a rigid pre-defined network structure which may restrict the opportunities of adding business value. Instead, a novel flexible formulation approach which translates a recipe representation to the SC environment is proposed to solve the challenging design-planning problem of SC networks. The potential of the presented approach is highlighted through illustrative examples of increasing complexity, where results of traditional rigid approaches and those offered by the flexible framework are compared. The implications of exploiting this potential flexibility to improve the SC performance are highlighted.

7.2 Flexible SC design and planning

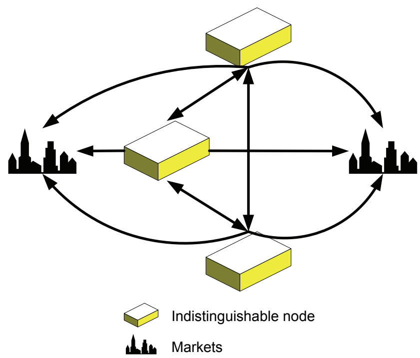
The SC modeling problem is very complex. In practice, it is usually helpful to use the time dimension to establish a hierarchical order so as to facilitate SC coordination as indicated in Chapter 2. The need to support decision making and improve operations over all hierarchical levels has lead to the development of several SC models. A review of the approaches devised so far to tackle this kind of problems is found also in 2. The current chapter is focused on modeling the strategic-tactical decision level of SCM which has been an active research topic in the last two decades. For the purposes of this chapter, the works of Bok *et al.* (2000); You and Grossmann (2008); and Ferrio and Wassick (2008) are revisited here. Bok *et al.* (2000) propose a multi-period SC optimization model for operational planning of continuous flexible process networks, where sales, intermittent deliveries, production shortfalls, delivery delays, inventory profiles and job changeovers are taken into account. It is important to point out that intermediate product flows among manufacturing sites are considered in the process networks, however process allocation to sites and SC components links are fixed since a planning problem is being addressed. Recently, the flexible process networks framework is extended to tackle SC design problems by You and Grossmann (2008). They address SC optimization under demand uncertainty considering responsiveness and net present value as the objectives to be maximized. The authors quantitatively analyze how network configurations may have an effect on the responsiveness to market changes. By using a probabilistic model for stock-out, the expected lead time is proposed as a quantitative measure of SC responsiveness. The production process network (from raw material to final products) may be decoupled in various processing "sub-trains". These sub-trains can take place at different locations, however a potential process SC network superstructure must be given a priori. Ferrio and Wassick (2008) present an approach which is aimed to the redesign of existing SC networks. Their model consists in a single period network design MILP model for multi-product SCs considering three echelons (processing plants, distribution centers and customers). Direct shipping and product flows among plants and/or distribution centers are taken into account, but the potential linkages must be predefined. Their approach does not take into account the process network required to produce the final products.

Reviews of works related to strategic SC models can be found in Vidal and Goetschalckx (1997), Beamon (1998), Schmidt and Wilhelm (2000), Meixell and Gargeya (2005) and Shah (2005).

Evidently, a SC network is comprised by lateral links, reverse loops, two way exchanges and so forth, encompassing the upstream and downstream activity (Lamming, 2000). Notwithstanding, common characteristics of most existing SC approaches are that among SC components exclusively vertical flows that have only one direction are considered (see Fig. 7.1(a)) and a predefined superstructure is necessary. Vertical flows are understood as those flows between SC components that belong to consecutive echelons type (e.g. flows that go from wholesalers to retailers, from production plants to wholesalers). Instead, this chapter proposes a flexible SC design-planning formulation (see Fig. 7.1(b)) whose distinctive features are that (i) considers all feasible links and material (raw material, intermediate and final products) flows among the potential SC components inherently and (ii) does not need any pre-established process network superstructure so that the sub-trains (if any) in which production process is decoupled and their location are determined by the model. Regarding the latter feature, the model does merely require as input the SC production pro-



(a) Traditional framework



(b) Flexible framework

Figure 7.1: Approaches for SC Design

cess recipe representation. The abovementioned features provide opportunities to select a value-efficient allocation of production-distribution activities which may lead to more advantageous SC designs. Furthermore, a more appropriate description of manufacturing processes at the SC level is achieved by translating a recipe representation to the SC environment.

Finally, it is important to mention that flexibility has been recognized as a key strategy for efficiently improving responsiveness of production systems facing demand uncertainty. Jordan and Graves (1995) analyze the process flexibility which can be understood as the ability to build different types of products in the same capacitated processing resource at the same time. They propose guidelines to identify the best way to add process flexibility to a network of plants and conclude that it is creating longer product-plant "chains" what results in flexibility benefits, instead of building diverse products in a single plant. The authors define a "chain" as a group of products and plants which are all connected, directly or indirectly, by product assignment decisions. All products within a chain share that chain's capacity, even without each plant building all products. Later on, Graves and Tomlin (2003) extend this work to understand the role of process flexibility in general multistage SCs. Their analysis disregards economic issues, then comparisons among different configurations are carried out using capacity utilization and demand satisfaction as performance indicators. The proposed approach is similar in the sense that includes the analysis of which products should be processed at each plant but also considering economic issues. Besides this approach is deterministic, hence demand uncertainty is not taken into account. Certainly, the presented approach can be further extended to a stochastic model so that more responsive SC designs can be obtained; however that extension is out of the present chapter scope and objectives. This chapter focuses on how improved SC designs are obtained by more properly considering: the connectivity among SC components and the selection of processes (i.e., stages) to be installed at each location.

7.3 Problem statement

The scope of the SC network design problem is typically to determine the optimal manufacturing and distribution network for the entire product line of a company according to a pre-established economic objective. As it has been already mentioned in the introduction, the majority of works in the PSE field related to chemical SC network design relies on the concept of fixed "echelons" (Fig. 7.1(a)); they assume a given fundamental structure for the network in terms of the echelons involved (i.e., consecutive SC components connected by vertical flows). Thus, a rather rigid structure is imposed on the SC network and the design procedure focuses on the determination of the number of components in each echelon and the connectivity between components in adjacent echelons. However, changes in the fundamental structure of the network may sometimes lead to economic benefits that far exceed what can be achieved merely by changing the number of components and/or the connectivity within an existing structure (Shah, 2005).

The multi-period deterministic model that is developed next provides a flexible framework for the design of SCs. The model assumes that equipment is available for eventual installation at potential locations and assists in their selection. Furthermore, the model allows for the expansion of plant equipment capacities, not only in the first planning period but also during any other period in which managers believe that opportunities for investing on facilities may result in a more favorable performance. The problem can be stated as follows:

The following data is assumed to be known in advance.

- A fixed time horizon;
- A set of products;
- A set of markets in which products are available to customers and their nominal demand;
- A set of potential geographical sites for locating facilities;

- A set of potential equipment for manufacturing the different products;
- Lower and upper bounds for the increment of equipment and storage capacity;
- Product recipes (mass balance coefficients and utilization of production resources);
- Suppliers capacity ;
- Minimum utilization rate of installed capacity.
- Direct cost parameters such as production, handling, transportation and raw material costs;
- Price for every product in each market during the time horizon;
- Relationship between capital investment and facility capacity;
- Relationship between indirect expenses and facility capacity;

The goal is to determine:

- The facilities to be opened;
- The increase in facility capacity in each time period;
- The linkages among facilities;
- The assignment of manufacturing and distribution tasks to the network nodes;
- The amount of final products to be sold;

such that an economic performance metric to be evaluated at the end of the planning horizon is maximized.

The model utilizes a uniform discrete time formulation. It is assumed that demand is satisfied (i.e., sales execution) at the end of each time period in which the planning horizon is divided. It is also noteworthy to mention that it is assumed that some of the demand can be left unsatisfied because of limited production capacity.

7.4 Mathematical formulation

The model variables and constraints can be grouped in two categories: (i) those related to the SC strategic and tactical operations, and (ii) those that allow computing an economic indicator. Both categories are explained in detail next.

7.4.1 Design and planning model

The State-Task-Network (STN) representation (Kondili, Pantelides, & Sargent, 1993) has been utilized to formulate the problem of production scheduling in multipurpose plants as an MILP problem. An important feature of this representation is that both the individual operations (i.e., tasks) and the feedstocks, intermediate and final products (i.e., states) are included explicitly as network nodes. Processes involving sharing of raw materials and intermediates, batch splitting and mixing and recycles of material, can be represented unambiguously in such networks (see Fig. 7.2). In this work, the STN concept

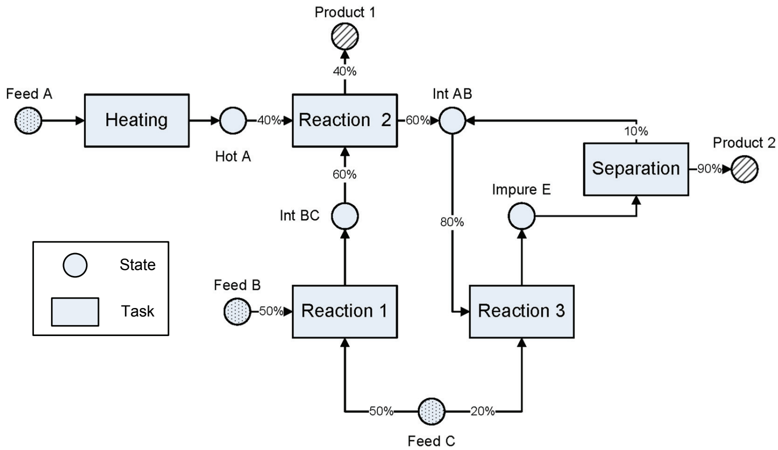


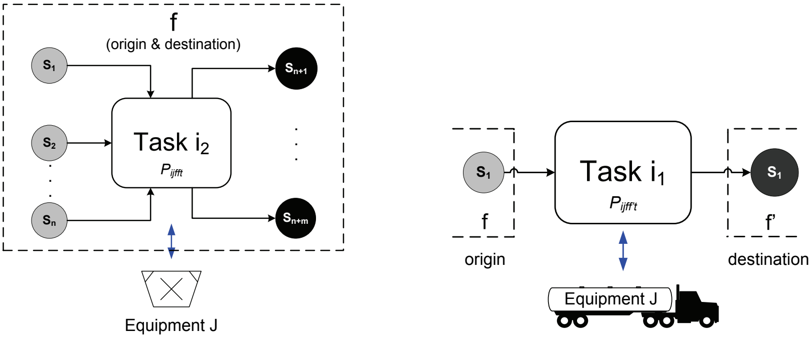
Figure 7.2: STN example

is expanded to formulate the flexible design-planning SC network model. The proposed model implements the flexible echelons concept. Hence, the connectivity between echelons is not imposed and a facility may play the role of either a processing and/or a distribution site. Material flows among facilities are allowed even if they belong to the same echelon type. Moreover, raw, intermediate and final material flows between facilities are allowed. The STN formulation has been enhanced to handle multiple site locations so that the abovementioned aspects can be addressed. These aspects rely on the definition of variable $P_{ijff't}$ which is analog to the batch size in Kondili's original scheduling model. $P_{ijff't}$ represents the amount of task i performed in equipment j which receives input materials from site f and "delivers" output materials to site f' during period t. Furthermore, production ($i \notin Tr$) and distribution ($i \in Tr$) tasks are strictly separated. Figure 7.3a depicts how the production rates are managed by the model. Certainly, a production task receives and delivers material within the same site. In case of distribution tasks, facilities f and f' must be different (Fig. 7.3b). As the reader can observe, a key characteristic of the model is that each task is associated to an origin and a final site location (f, f'). Thereby, a distribution center f can be easily identified since all its associated production rates are equal to zero ($P_{ijfft} = 0$).

The design-planning model is explained in detail next. The equations have been categorized into four groups; namely (i) mass balances, (ii) design, (iii) capacity, and (iv) markets and suppliers constraints.

Mass balances

Mass balances must be satisfied at each of the nodes that integrate the SC network. Equation (7.1) denotes the material balance for each state s in every facility f at period t. Inventory change $(S_{sft} - S_{sft-1})$ of consecutive peri-



(a) Production task (b) Distribution task

Figure 7.3: SC activities State-Task representation

ods $(t-1,t)$ must be equal to the difference between the amount of material s $(\alpha_{sij}P_{ijf'ft})$ produced/transported by tasks $(i \in T_s)$, whose destination is facility f, and the amount $(\bar{\alpha}_{sij}P_{ijff't})$ consumed by tasks $(i \in \bar{T}_s)$, whose origin is facility f. Here, α_{sij} and $\bar{\alpha}_{sij}$ represent the mass fraction coefficients of material s for task i performed in equipment j. It is noted that this equation should be merely applied to those equipment technologies which are suitable to perform task i (J_i) and only if these technologies can be installed on the corresponding facility $(\hat{J}_f)$. M and Sup are the subsets of locations where markets and suppliers are placed, respectively.

$$
\begin{aligned}
S_{sft} - S_{sft-1} = \sum_{f'} \sum_{i \in T_s} \sum_{j \in (J_i \cap \hat{J}_{f'})} \alpha_{sij} P_{ijf'ft} \\
- \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (J_i \cap \hat{J}_f)} \bar{\alpha}_{sij} P_{ijff't} \qquad \forall\ s, f \notin (Sup \cup M), t
\end{aligned}
\tag{7.1}
$$

In the process industry, there might be cases in which some intermediate material s cannot be transfered between facilities due to its instability. Distribution tasks associated to these materials can be restricted within the model by using the following constraint. Here, S^I represents the unstable materials set.

$$
P_{ijff't} = 0 \qquad \forall\ s \in S^I, i \in (Tr \cup T_s), f' \neq f, t \tag{7.2}
$$

Design constraints

Capacity and facilities location constraints are stated next. A similar formulation can be found in Chapter 4. Here, FJ_{jft} and FS_{ft} represent the equipment j total capacity in site f and the total storage capacity in site f accounting for decisions made until period t, respectively. Moreover, variables FJE_{jft} and

FSE_{ft} denote the facilities capacity expansion decision at period t. In these variables, it is important to notice that period t reflects the period when the expansion decision is taken. The model is general enough to address not only the design-planning of a new SC, but also the retrofitting of an existing SC network. In the latter case, the problem should be formulated by fixing at the initial period ($t = 0$) the value of the variables representing the facilities capacity according to the initial network topology. No installation/construction time is considered for the initial network.

Equations (7.3) and (7.4) are added to control the changes in the facilities capacity over time. These constraints include binary variables V_{jft} and X_{ft}, which take a value of 1 if the facility being represented (either the equipment j at site f or the storage) is expanded in capacity, otherwise is set to zero. The capacity increments are bounded in the range $[FJE^L_{jft}, FJE^U_{jft}]$ and $[FSE^L_{ft}, FSE^U_{ft}]$, which represent the realistic intervals where they must fall.

$$V_{jft}FJE^L_{jft} \leq FJE_{jft} \leq V_{jft}FJE^U_{jft} \qquad \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, t \tag{7.3}$$

$$X_{ft}FSE^L_{ft} \leq FSE_{ft} \leq X_{ft}FSE^U_{ft} \qquad \forall\ f \notin (Sup \cup M), t \tag{7.4}$$

Equations (7.5) and (7.6) are added to update the total capacity (FJ_{jft} and FS_{ft}) by the amount increased during planning period t (FJE_{jft} and FSE_{ft}).

$$FJ_{jft} = FJ_{jft-1} + FJE_{jft} \qquad \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, t \tag{7.5}$$

$$FS_{ft} = FS_{ft-1} + FSE_{ft} \qquad \forall\ f \notin (Sup \cup M), t \tag{7.6}$$

Capacity constraints

Equation (7.7) forces the total production/distribution rate in each facility to be greater than a minimum desired capacity utilization ($\beta_{jf}FJ_{jft-\pi_{jf}}$) and lower than the available capacity ($FJ_{jft-\pi_{jf}}$). In this equation, $\theta_{ijff'}$ represents the capacity utilization factor of equipment j by task i. To go on, β_{jf} expresses the minimum percentage of utilization of equipment j at site f. Finally, π_{jf} reflects the necessary time to install and set up equipment j in facility f. It is noteworthy that the model considers that task i is to be performed in equipment that is installed on the facility of "origin". Notice that those expansion decisions made in period $t - \pi$ are available to be utilized in period t.

$$\beta_{jf}FJ_{jft-\pi_{jf}} \leq \sum_{f'}\sum_{i \in I_j} \theta_{ijff'}P_{ijff't} \leq FJ_{jft-\pi_{jf}} \qquad \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, t \tag{7.7}$$

Parameter $\theta_{ijff'}$ is one of the key factors to be determined when addressing aggregated planning problems, considering strategic and tactical decisions.

The presented operational model may be applied in continuous as well as in semi-continuous processes. Firstly, consider the continuous process. For this case, the capacity utilization factor is a conversion factor, which allows taking into account the equipment j capacity in site f in terms of task i kg of produced material per production time unit. In this way the factor is the maximum throughput per planning period. On the other hand, this parameter is closely related to tasks operation time in the case of semicontinuous (i.e., batch) processes. Notice that in this kind of production processes the time period scale utilized in aggregated planning is usually larger than the time a task (production/distribution activity) requires to be performed. It is important to bear in mind that capacity is expressed as equipment j available time during one planning period, then $\theta_{ijff'}$ represents the time required to perform task i in equipment j per unit of produced material. Thus, once operation times are determined this parameter can be easily estimated.

In addition, total inventory in facility f is constrained to be equal to or lower than the available capacity $(FS_{ft-\hat{\pi}_f})$ in each period t by Eq. (7.8). In this equation, $\hat{\pi}_f$ is the time required to install storage and material handling equipment, while u_s holds for specific volume of material s.

$$\sum_{s} \upsilon_s S_{sft} \leq FS_{ft-\hat{\pi}_f} \qquad \forall\ f \notin (Sup \cup M), t \tag{7.8}$$

Markets and suppliers

With regards to markets and suppliers, the model assumes that markets and suppliers are placed at "different" locations from facilities. Hence, for modeling purposes dummy locations are needed in case facilities can be installed on the same site a market and/or supplier is. In this way, it is followed the distribution tasks representation $(P_{ijff't})$ which is based on distinguishing the origin and destination locations. It is emphasized that despite the previous assumption the model permits different suppliers to be located at the same site. By Eq.(7.9) sales of final product $s \in FP$ carried out from facility location f' to market $f \in M$ are estimated. Eq.(7.10) states that sales in markets during period t must be less than or equal to the demand. Also, a minimum customer service level (CSL) target for each product, which must be attained in all periods, is imposed by Eq.(7.11).

$$Sales_{sf'ft} = \sum_{i \in (T_s \cap Tr)} \sum_{j \in (J_i \cap \hat{J}_f)} P_{ijf'ft} \qquad \forall\ s \in FP, f \in M, f' \notin M, t \tag{7.9}$$

$$\sum_{f' \notin M} Sales_{sf'ft} \leq Dem_{sft} \qquad \forall\ s \in FP, f \in M, t \tag{7.10}$$

$$\frac{\sum_{f \in M} \sum_{f' \notin M} Sales_{sf'ft}}{\sum_{f \in M} Dem_{sft}} \geq MinCSL_s \qquad \forall\ s \in FP, t \tag{7.11}$$

Finally, the model also assumes a maximum availability of raw materials. Therefore, Eq.(7.12) forces the amount of raw material, $s \in RM$, purchased from location $f \in Sup$ at each period t to be lower than an upper bound, A_{sft}, given by physical limitations. In this expression, R_f denotes the set of raw materials that can be provided from location f.

$$\sum_{f' \notin Sup} \sum_{i \in (\bar{T}_s \cap Tr)} \sum_{j \in J_i} \bar{\alpha}_{sij} P_{ijff't} \leq A_{sft} \qquad \forall\ f \in Sup, s \in R_f, t \tag{7.12}$$

7.4.2 Economic performance metrics formulation

Many economic performance metrics have been utilized for determining the goodness of a SC network design. The most traditional metrics are profit, net present value (NPV), and total cost. The current business environment has led managers to become aware of the financial dimension of decision making. Thus, business managers are becoming more driven by the goal of enhancing shareholder value. By recognizing this fact corporate value has been proposed in Chapter 4 as a suitable financial indicator that is able to properly assess the trade-off between net operating income (i.e., profit) and capital efficiency (i.e., fixed assets and net working capital). In this section expressions that provide the essential input to compute the aforementioned economic indicators are presented. In this way the model is general enough to suit different metrics. Indeed, these expressions are the ones that allow the integration between the proposed design-planning model and the financial and corporate value formulations presented in Chapter 4. Slight modifications and/or extra equations will be required depending on the indicator selected as objective function. For the sake of clarity and in order to straightly evidence the proposed model advantages, the equations to compute the NPV are included here.

In the next subsections, expressions have been classified in three groups: (i) operating revenue, (ii) operating cost, and (iii) capital investment.

Operating revenue

Revenue is calculated by means of net sales which are the income source related to the normal SC activities. Thus, the total revenue incurred in any period t can be easily computed from the sales of products executed in period t as it is stated in Eq. (7.13).

$$ESales_t = \sum_{s \in FP} \sum_{f \in M} \sum_{f'} Sales_{sf'ft} Price_{sft} \qquad \forall\ t \tag{7.13}$$

Operating cost

Indirect cost The total fixed cost of operating a given SC structure can be computed using equation (7.14). $FCFJ_{jft}$ and $FCFS_{ft}$ are the fixed unitary capacity cost for production equipment and storage, respectively. Regarding the installation times, a reasoning similar to the one in section 7.4.1 is followed.

$$FCost_t = \sum_f \sum_{j \in \hat{J}_f} FCFJ_{jft} FJ_{jft-\pi_{jf}} + \sum_f FCFS_{ft} FS_{ft-\hat{\pi}_f} \qquad \forall\ t \quad (7.14)$$

Direct cost The cost of purchases from supplier e, which is computed through Eq. (7.15), includes purchases of raw materials, transportation, and production resources. Notice that e refers to supplier entity and not to supplier location f ($f \in Sup$).

$$EPurch_{et} = Purch_{et}^{rm} + Purch_{et}^{tr} + Purch_{et}^{prod} \qquad \forall\ e, t \qquad (7.15)$$

The purchases ($EPurch_{et}$) associated to raw materials made to supplier e can be computed through Eq. (7.16). ψ_{est} is the cost associated to raw material s purchased from supplier e. Since it is assumed that several suppliers of raw materials may exists, Eq. (7.17) expresses that the total quantity of raw materials purchased in period t must be equal to the sum of the amounts purchased from each supplier e.

$$Purch_{et}^{rm} = \sum_{s \in RM_e} \sum_{f \in Sup} Purch_{esft} \psi_{est} \qquad \forall\ e, t \qquad (7.16)$$

$$\sum_{f'} \sum_{i \in (\bar{T}_s \cap Tr)} \sum_{j \in J_i} \bar{\alpha}_{sij} P_{ijff't} = \sum_{E_s} Purch_{esft} \qquad (7.17)$$
$$\forall\ s \in RM, f \in Sup, t$$

Otherwise, for the sake of simplicity external transportation services as well as production resources are assumed to be "acquired" each of them from one unique supplier (i.e., $|\tilde{E}_{tr}| = |\hat{E}_{prod}| = 1$) . This assumption can be easily relaxed to address more general cases. Production and transportation costs are determined by Eqns. (7.18) and (7.19), respectively. Here, $\rho_{eff'}^{tr}$ denotes the unitary transportation cost associated with sending products from location f to location f'. τ_{ijfe}^{ut1} represents the unitary production cost associated to perform task i in processing equipment j, whereas τ_{sfe}^{ut2} represents the unitary inventory costs.

$$Purch_{et}^{tr} = \sum_{i \in Tr} \sum_{j \in J_i} \sum_f \sum_{f'} P_{ijff't} \rho_{eff'}^{tr} \qquad \forall\ e \in \tilde{E}_{tr}, t \qquad (7.18)$$

$$Purch_{et}^{prod} = \sum_{f} \sum_{i \notin Tr} \sum_{j \in (J_i \cap \hat{J}_f)} P_{ijfft} \tau_{ijfe}^{ut1} + \sum_{s} \sum_{f \notin (Sup \cup M)} S_{sft} \tau_{sfe}^{ut2} \qquad \forall\ e \in \hat{E}_{prod}, t \tag{7.19}$$

Capital investment

Finally, the total investment on fixed assets is computed through Eq. (7.20). This equation includes the investment made to expand the equipment j capacity in facility site f at period t ($Price_{jft}^{FJ} FJE_{jft}$), plus the investment required to open a manufacturing plant in location f, in case it is opened at period t ($I_{ft}^{J} JB_{ft}$), plus the investment required to support distribution center capacity increase ($Price_{ft}^{FS} FSE_{ft}$), plus the investment required to set a distribution center if it is opened at period t ($I_{ft}^{S} SB_{ft}$). Here, JB_{ft} and SB_{ft} are binary variables which take value of 1 in case the facility being represented, processing site or distribution center, starts construction in period t.

$$\begin{aligned} FAsset_t = & \sum_{f} \left(\sum_{j} Price_{jft}^{FJ} FJE_{jft} + I_{ft}^{J} JB_{ft} \right) + \\ & \sum_{f} \left(Price_{ft}^{FS} FSE_{ft} + I_{ft}^{S} SB_{ft} \right) \qquad \forall\ t \end{aligned} \tag{7.20}$$

The following disjunctive expressions allow to define binary variables JB_{ft} and SB_{ft}. The equivalent logic conditions state that if no equipment was decided to be installed in previous periods ($t' < t$) and some equipment is decided to be installed at the current period t, then decision to open facility f is made at period t.

$$\left[\neg \bigvee_{t' < t} JB_{ft'} \right] \wedge \left[\bigvee_{j \in \hat{J}_f} V_{jft} \right] \Rightarrow JB_{ft} \qquad \forall\ f \notin (Sup \cup M), t$$

$$\left[\neg \bigvee_{t' < t} SB_{ft'} \right] \wedge X_{ft} \Rightarrow SB_{ft} \qquad \forall\ f \notin (Sup \cup M), t$$

Next, the previous disjunctions are transformed in mixed integer constraints. Equations (7.21) and (7.22) are to force definition of variable JB_{ft}, while Eqns. (7.23) and (7.24) restrict variable SB_{ft}.

$$\sum_{j \in J_f} \left(\sum_{t' \leq t} JB_{ft'} - V_{jft} \right) \geq 0 \qquad \forall\ f \notin (Sup \cup M), t \tag{7.21}$$

$$\sum_{t} JB_{ft} \leq 1 \qquad \forall\, f \notin (Sup \cup M) \tag{7.22}$$

$$\sum_{t' \leq t} SB_{ft'} - X_{ft} \geq 0 \qquad \forall\, f \notin (Sup \cup M), t \tag{7.23}$$

$$\sum_{t} SB_{ft} \leq 1 \qquad \forall\, f \notin (Sup \cup M) \tag{7.24}$$

Equation (7.25) represents the calculation of profit at period t. To conclude, NPV is computed by means of Eq. (7.26).

$$Profit_t = ESales_t - (FCost_t + \sum_{e} EPurch_{et}) \qquad \forall\, t \tag{7.25}$$

$$NPV = \sum_{t} \left(\frac{Profit_t - FAsset_t}{(1 + rate)^t} \right) \tag{7.26}$$

Thus, the SC network design-planning problem whose objective is to optimize NPV can be mathematically posed as follows:

$$\begin{gathered} \underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\, NPV \\ \text{subject to} \\ \text{Eqns. (7.1) to (7.26)} \\ \mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R} \end{gathered}$$

Here $\mathscr{X}$ denotes the model binary variables set, while $\mathscr{Y}$ represents the model continuous variable set.

7.5 Examples

The capabilities of the flexible model are illustrated by solving three SC design – planning problems. The first three problems are illustrative examples which intend to demonstrate some of the special features of the flexible model. The last one constitutes a more sophisticated case study based on a real problem. The resulting MILP models have been solved to optimality in GAMS using CPLEX (11.0) on a computer with an Intel Core 2 Duo 2.0 GHz and 2GB RAM.

7.5.1 Illustrative examples

Example 1

A SC design-planning problem comprising four potential locations for the processing sites and the distribution centers is presented. A planning horizon of five annual periods is considered. The STN representation of the production

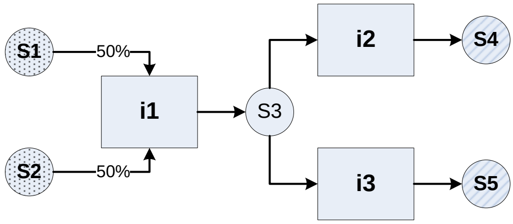
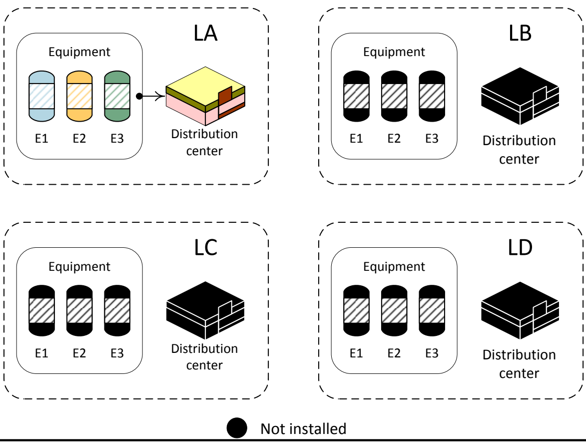


Figure 7.4: STN notation for example 1

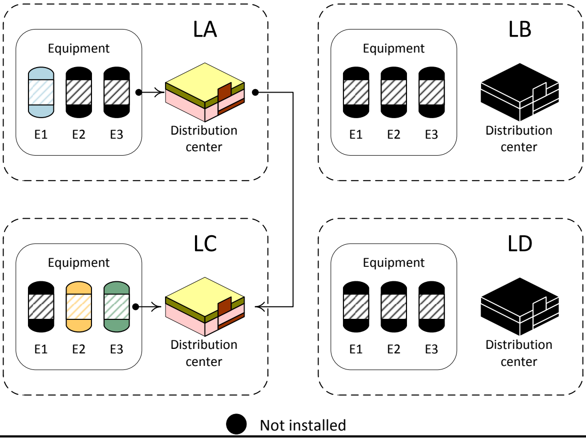
process is depicted in Fig. 7.4. Two final products ($S4$ and $S5$) can be sold in two markets ($M1$ and $M2$). $S1$ and $S2$ are raw materials. A set of three equipment technologies ($E1$-$E3$) are assumed to be available for the processing sites. It is assumed that task $i1$ can be performed in equipment $E1$, task $i2$ in equipment $E2$, and task $i3$ in equipment $E3$. The discount rate has been taken equal to 35%. Input data associated to this example can be found in Appendix C.1.

The SC network configurations obtained by the traditional and flexible formulation are summarized in Figures 7.5 and 7.6. Numerical results show that



Net present value (NPV)					479.086 m.u.
Capacity increment (c.u.)					
Manufacturing sites		Equipment technology j			
l	t	$E1$	$E2$	$E3$	
LA	1	145.0	126.0	55.0	
LB	1	0.0	0.0	0.0	
LC	1	0.0	0.0	0.0	
LD	1	0.0	0.0	0.0	
Distribution centers					
	t	LA	LB	LC	LD
	1	50.0	0.0	0.0	0.0

Figure 7.5: Traditional network design of illustrative example 1



Net present value (NPV)					584.652 m.u.
Capacity increment (c.u.)					
Manufacturing sites		Equipment technology j			
l	t	$E1$	$E2$	$E3$	
LA	1	163.0	0.0	0.0	
LB	1	0.0	0.0	0.0	
LC	1	0.0	142.0	62.0	
LD	1	0.0	0.0	0.0	
Distribution centers					
	t	LA	LB	LC	LD
	1	50.0	0.0	50.0	0.0

Figure 7.6: Flexible network design of illustrative example 1

the solution computed by the flexible formulation has higher performance in terms of NPV than the optimal traditional solution. Certainly, the optimal flexible model solution shows an NPV 22% greater than the one calculated by using the traditional approach. As shown in the figures, the traditional approach solution proposes to establish a processing site and a distribution center in one unique location (LA), while the flexible approach proposes to establish facilities in two locations (LA and LC). Notice that the flexible approach takes advantage of the capability of (i) splitting processes in different sites and (ii) transferring intermediate products among sites belonging to the same echelon type. Indeed, the flexible solution advises to install $E1$ at LA in order to produce state $S3$. A flow of state $S3$ exists from LA to LC. Equipment $E2$ and $E3$ are installed in LC where $S3$ is transformed into final products $S4$ and $S5$. Products are sent to the markets from LC. On the other hand, the traditional approach establishes all equipment technologies in the low-investment location LA since no intermediate material flows among facilities of same echelon type are allowed.

Figure 7.7 exhibits the economic characterization of each approach. As expected, the flexible model renders higher total transportation cost due to the transferring of $S3$; whereas the total production cost is lower because each

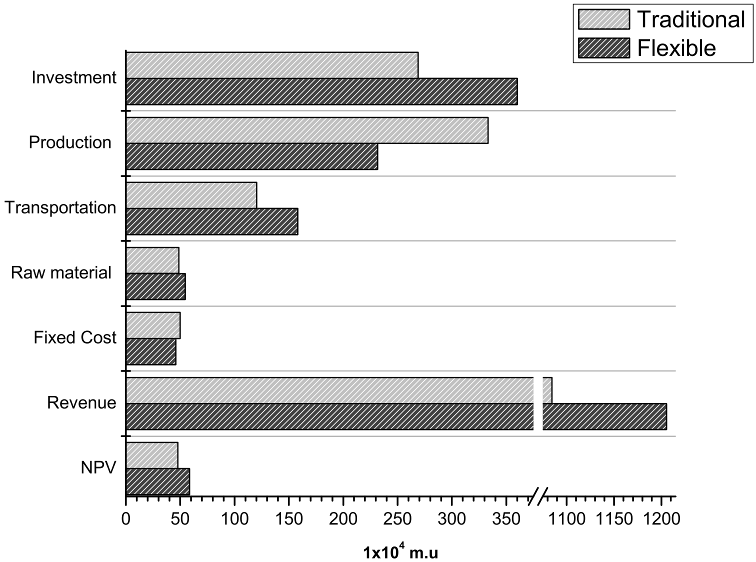


Figure 7.7: Economic characterization of illustrative example 1

equipment technology is installed to its corresponding lowest operating cost location. The lower production cost and higher revenue counterbalance the increase on investment and transportation costs.

This flexible model example consists of 4,391 equations, 935 continuous variables and 64 binary variables. The total CPU time is 0.34 CPU seconds and the integral optimal solution is found after 1,434 iterations. The LP-relaxed solution gives a value of 1,762,204 m.u. for the objective function.

Example 2

A SC design-planning problem comprising four potential locations for the processing sites and the distribution centers in a planning horizon of five annual periods is considered. The STN representation of the process is depicted in Fig. 7.8. Now, two final products ($S1$ and $S2$) and one intermediate product ($S3$) may be sold in six markets ($M1$-$M6$). $S7$, $S8$, and $S9$ are raw materials. A set of four equipment technologies (H, $R1$, $R2$, S) are available for the processing sites. It is assumed that task $i1$ can be performed in equipment H, task $i2$ in equipment $R1$, tasks $i3$ and $i4$ in equipment $R2$ and finally $i5$ in equipment S. The discount rate has been considered equal to 35%. Input data associated to this example can be found in Appendix C.2.

The resulting supply network configurations for this example are shown in Figures 7.9 and 7.10. In the traditional approach plant sites and distribution centers are opened in three different locations (LB, LC, and LD). For this

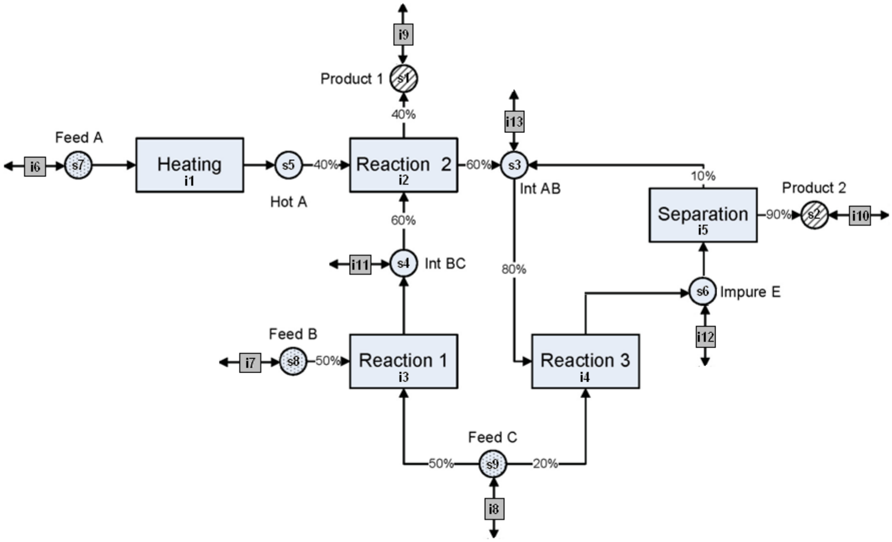


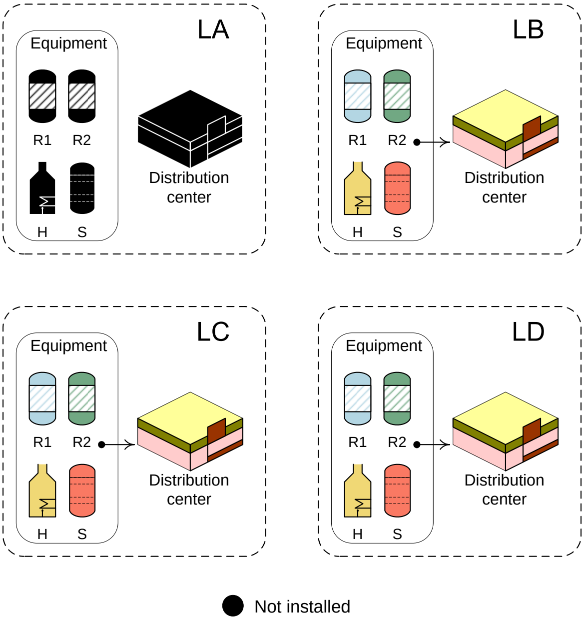
Figure 7.8: STN notation for illustrative example 2

approach, the four equipment technologies are installed at every location. On the other hand, the flexible model establishes two plant sites at locations LB and LD. In location LB all equipment technologies are installed while the separation technology S is not installed at location LD. The flexible model opens three distributions centers which are located at LA, LB and LC. In the flexible solution a flow of material $S3$ appears. $S3$ is transferred from distributions centers located at LB and LD to the distribution center located at LA.

The flexible approach solution results in an improvement of 13.7% over the traditional approach. Figure 7.11 shows the economic results of both solutions. As one can notice, the flexible solution leads to cost reductions, but it also results in a revenue reduction of approximately 6x10^6 m.u. Consequently, the profit contribution to the NPV is reduced about 25% by using the flexible approach. However, the flexible model investment on facilities is 36.5 % lower in comparison to the traditional one. Therefore, the SC configuration proposed by the flexible model renders a better economic performance. The flexible model for this example consists of 3,117 equations, 26,800 continuous variables and 136 binary variables. The total CPU time is 12.41 CPU seconds and the integral optimal solution is found after 20,310 iterations. The LP-relaxed solution gives a value of 6,587,803 m.u. for the objective function.

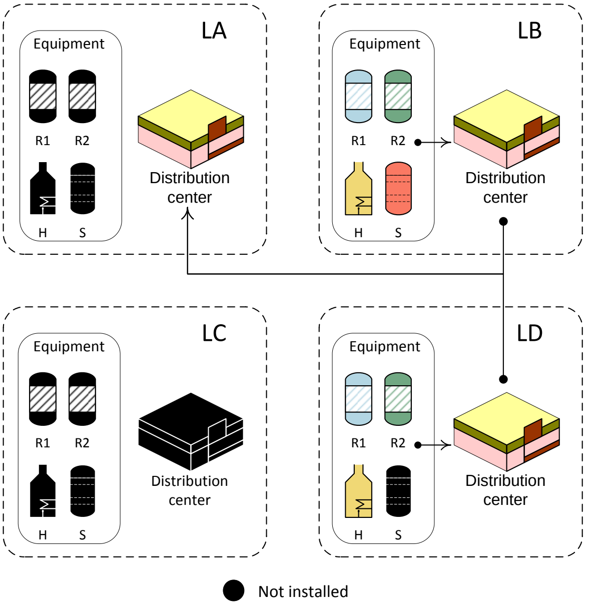
Example 3

Here, a more complex SC design-planning problem of eight potential locations ($fc1$-$fc8$) for the processing sites and the distribution centers is addressed. A planning horizon of 48 monthly periods is examined. The production process



Net present value (NPV)					2.498.276 m.u.
Capacity increment (c.u.)					
Manufacturing sites		Equipment technology j			
l	t	$R1$	$R2$	H	S
LA	1	0.0	0.0	0.0	0.0
LB	1	78.0	202.0	244.0	56.0
LC	1	96.0	230.0	244.0	50.1
LD	1	96.0	230.0	300.0	50.0
Distribution centers					
	t	LA	LB	LC	LD
	1	0.0	51.0	62.0	62.0

Figure 7.9: Traditional network design of illustrative example 2



Net present value (NPV)					2.839.709 m.u.
Capacity increment (c.u.)					
Manufacturing sites			Equipment technology j		
l	t	$R1$	$R2$	H	S
LA	1	0.0	0.0	0.0	0.0
LB	1	96.0	230.0	300.0	50.0
LC	1	0.0	0.0	0.0	0.0
LD	1	96.0	180.0	300.0	0.0
Distribution centers					
	t	LA	LB	LC	LD
	1	50.0	62.0	64.0	0.0

Figure 7.10: Flexible network design of illustrative example 2

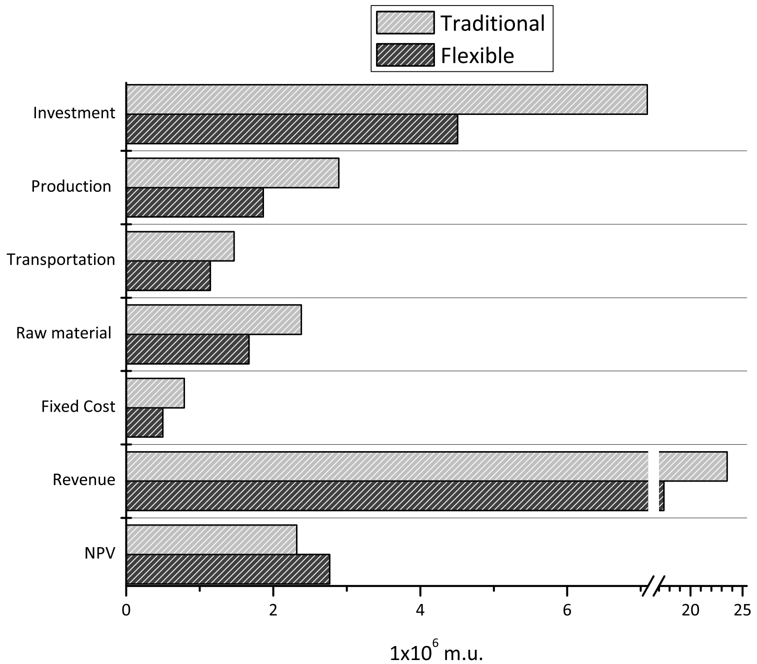
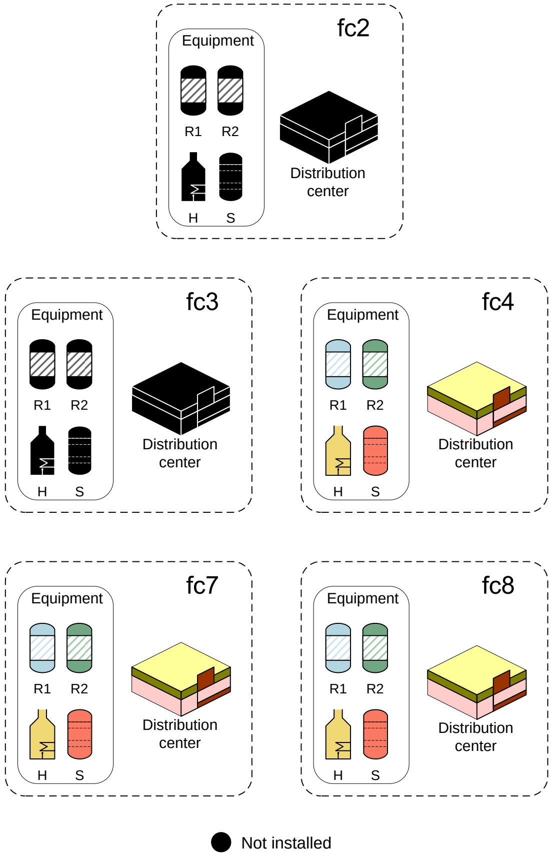


Figure 7.11: Economic characterization of illustrative example 2

is the same of example 2 which is depicted in Fig. 7.8. Two final products ($S1$ and $S2$) and two intermediate product ($S3$ and $S4$) may be sold in six markets ($fc12$-$fc17$). $S7$, $S8$, and $S9$ are raw materials. A set of four equipment technologies (H, $R1$, $R2$, S) are available for the processing sites. It is assumed that task $i1$ can be performed in equipment H, task $i2$ in equipment $R1$, tasks $i3$ and $i4$ in equipment $R2$ and finally $i5$ in equipment S. The discount rate has been taken equal to 35%. Example 3 input data can be found in Appendix C.3.

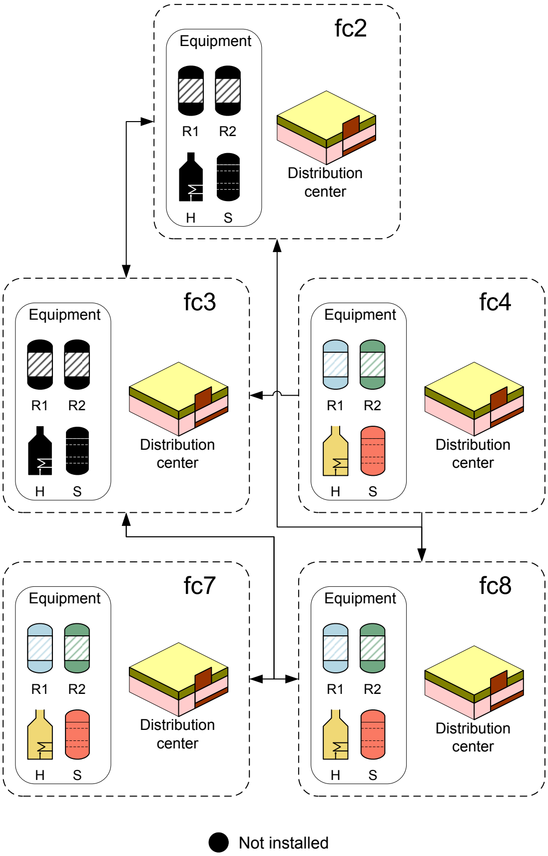
The distinct configurations of the traditional SC design-planning and the flexible model are shown in Fig. 7.12 and Fig. 7.13. In the traditional SC design-planning case three facility locations are established; $fc4$, $fc7$ and $fc8$. Processing plants and distribution centers are installed at all established sites. In the flexible SC design-planning case five facility locations are established; $fc2$, $fc3$, $fc4$, $fc7$ and $fc8$. Processing plants and distribution centers are installed at sites: $fc4$, $fc7$ and $fc8$ while in sites $fc2$ and $fc3$ are established only distribution centers. The attached tables of Fig. 7.12 and Fig. 7.13 illustrate the capacity increase for every equipment technology installed in each planning period at each manufacturing site. The main flexible design-planning model characteristic is the significant material flow between production plants. Moreover, material flows between distribution centers also exist. Fig. 7.13 de-



Net present value (NPV)					70.883.086 m.u.
		Capacity increment (c.u.)			
Manufacturing sites		Equipment technology j			
fc	t	$R1$	$R2$	H	S
$fc4$	1	66.37	243.41	207.40	83.31
$fc7$	1	73.15	250.00	228.60	86.33
$fc8$	1	80.00	250.00	250.00	69.36
	13	50.48	146.41	157.75	55.85

Distribution centers					
t	$fc2$	$fc3$	$fc4$	$fc7$	$fc8$
1	0.00	0.00	49.69	55.48	62.57
13	0.00	0.00	0.00	0.00	29.81

Figure 7.12: Traditional SC network design of illustrative example 3



Net present value (NPV)						73.383.512 m.u.
			Capacity increment (c.u.)			
Manufacturing sites			Equipment technology j			
fc	t	$R1$	$R2$	H	S	
$fc4$	1	74.26	250.00	232.05	59.49	
	13	0.00	0.00	0.00	25.00	
$fc7$	1	70.42	250.00	220.06	79.89	
	13	0.00	0.00	0.00	25.00	
$fc8$	1	80.00	250.00	250.00	97.62	
	13	45.32	139.47	141.63	32.40	
Distribution centers						
	t	$fc2$	$fc3$	$fc4$	$fc7$	$fc8$
	1	25,00	25,00	55,05	52,35	75,83
	13	0,00	0,00	0,00	0,00	25,00

Figure 7.13: Flexible SC network design of illustrative example 3

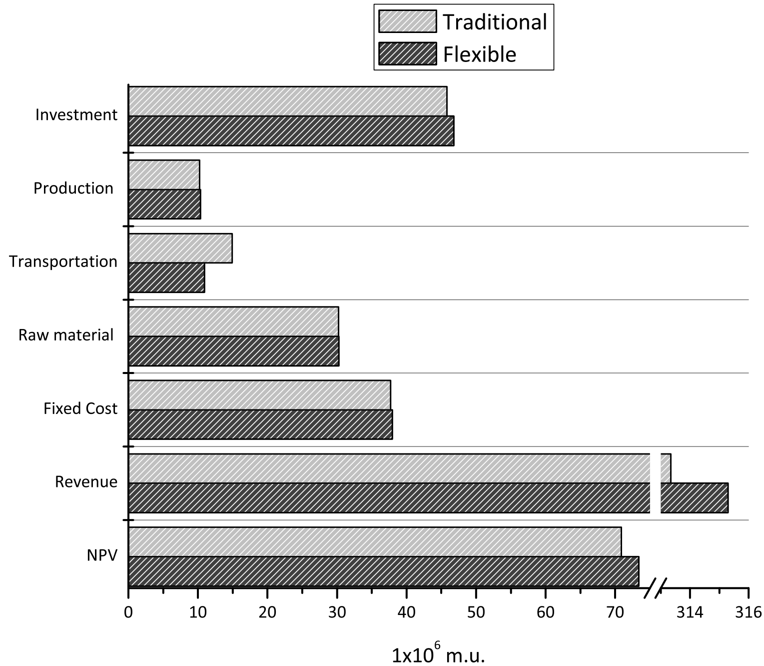


Figure 7.14: Economic characterization of example 3

picts the aforementioned flow connections between the SC echelons.

In Fig. 7.14 the economic characterization of both cases follows. The flexible approach results into investment and fixed costs slightly higher than the traditional approach. However, the flexible SC design-planning gives significantly lower transportation costs. This constitutes the main fact that contributes to higher revenue and NPV values. Fig. 7.15 presents the NPV contribution per semester of both cases. The flexible SC design-planning model gives better NPV for all semesters except for the first one where the capital investment is higher (two additional sites are established) than the one of the traditional approach. Finally, it is worth mentioning that the traditional approach results into a NPV equal to $70,883,086$ m.u. while the flexible one gives a NPV equal to $73,383,512$ m.u.; a 3.53% of improvement. This larger flexible model example consists of 29,825 equations, 223,185 continuous variables and 992 binary variables. The total CPU time is 1,980 CPU seconds and the integral optimal solution is found after 495,714 iterations. The LP-relaxed solution gives a value of 91,011,406.61 m.u. for the objective function.

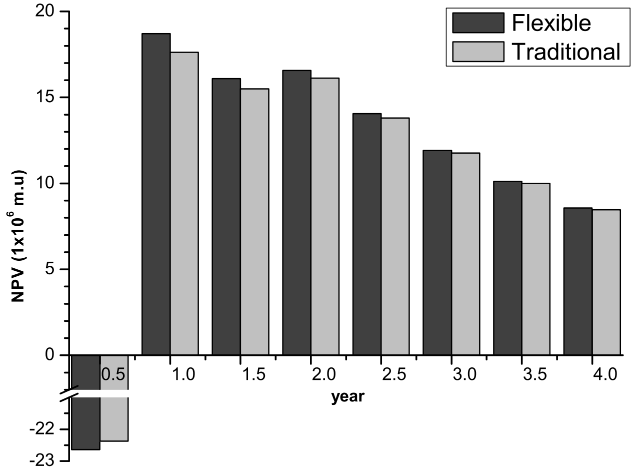


Figure 7.15: NPV contribution per semester for example 3

7.5.2 Case study

Consider the following case study which is an adapted version of the one introduced by You and Grossmann (2008). This case study was motivated by a real world application concerning a polystyrene SC design. The polystyrene production process is shown in Figure 7.16. Styrene monomers are produced from ethylene and benzene, then styrene is processed to obtain five final products: three different types of solid polystyrene (SPS) and two types of expandable polystyrene (EPS). Potential benzene suppliers are located in Texas (TX), Louisiana (LA), and Alabama (AL); while ethylene suppliers are located in Illinois (IL), TX and Mississippi (MS). Customers are aggregated into nine sale regions according to their geographical proximity. Distribution centers and processing plants may be established in eight different states which are Michigan (MI), TX, California (CA), LA, Nevada (NV), Georgia (GA), Pennsylvania (PA), and Iowa (IA). Figure 7.17 shows the SC components location. The potential SC superstructure that was considered by You & Grossmann is depicted in Fig. 7.18.

The case study has been modified in order to consider all production activities in every potential facility location. In order to prevent biased data, cost associated to those activities that are not considered in the given pre-established superstructure have been randomly determined by using a uniform probability distribution whose lower limit is equal to the superstructure most costly option. Following this procedure, those options which have not been included in the superstructure do imply a higher cost/investment. Additionally, transportation cost has been calculated taking into consideration the distances between facilities, sales regions and suppliers. The problem has been solved for

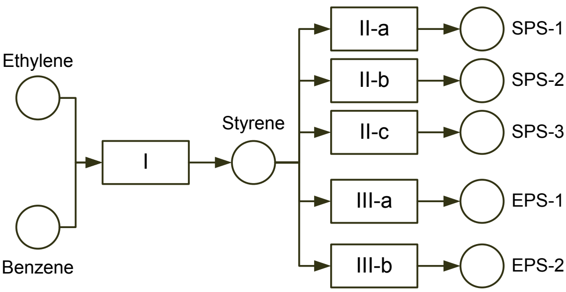


Figure 7.16: STN for the case study

a planning horizon of 48 monthly periods. Discount rate for this case study has been taken equal to 20%.

Figure 7.19 shows the optimal SC configuration obtained using the pre established superstructure. The traditional approach proposes to produce styrene in the sites located at TX and LA, while equipment technologies to produce final products are installed at MI, CA and LA. Two inter-site material flows are included from TX to CA and from LA to MI for the styrene monomer shipment. This SC network configuration supplies the customers from four different distribution centers. In the flexible approach case, the optimal SC configuration involves three production sites (TX, CA and LA) and three distribution centers (TX, GA and IA) as shown in Figures 7.20 and 7.21. An inter-site styrene flow exists from TX site to LA site. It is interesting to observe that the flexible solution has established a distribution center at TX that transfers final products to

Figure 7.17: Location map for the case study

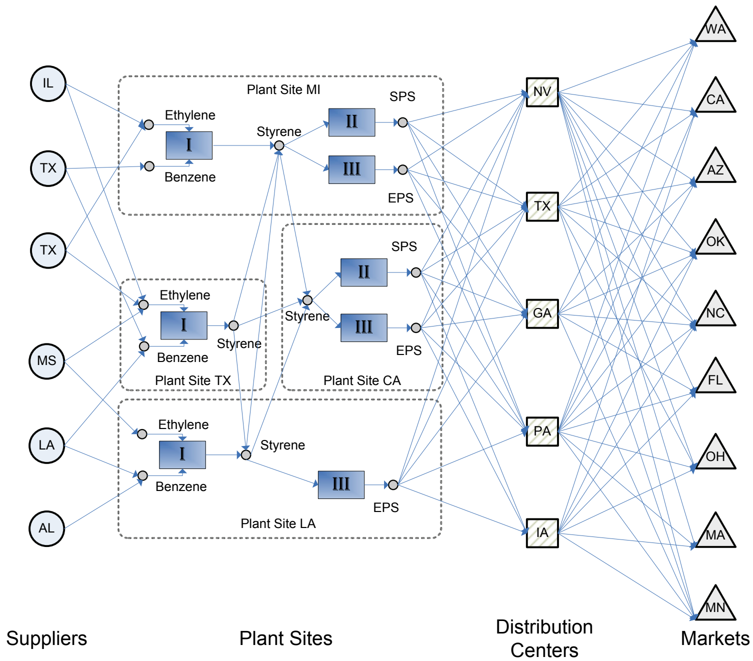


Figure 7.18: Potential process SC network superstructure for the case study given in a traditional approach

customers located in Washington (WA) but it also receives raw materials from suppliers to be sent to the production site at CA. Raw materials are usually not considered to be handled by distribution centers, however improvements can be achieved by doing so. Moreover, production plants are directly shipping final products to some markets which has not been considered in the SC superstructure. Additionally, it should be noticed that technologies I and II are installed at CA and TX sites, respectively. However, the allocation of these technologies to those sites is not considered in the SC superstructure (see Fig. 7.18). The flexible approach has installed them in spite of being more costly than the other available options, since the trade-off between the required higher investment and the transportation cost results in an overall NPV increase. The economic outcomes of both solutions are presented in Fig. 7.22. The flexible approach solution leads to an NPV improvement of 74.6% over the traditional approach. Such improvement is achieved mostly by reducing the total transportation cost. This case study flexible model consists of 43,027 equations, 693,025 continuous variables and 1008 binary variables. The total CPU time is 14 CPU seconds and the integral solution is obtained after 24,412 iterations. The LP-relaxed solution gives a value of 1,186x10^6 m.u. for the objective function.

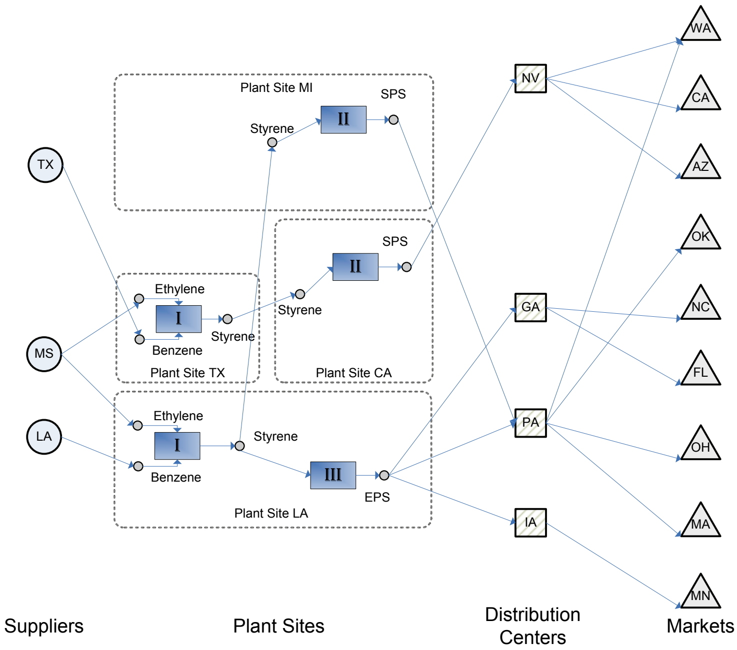


Figure 7.19: Optimal SC network design for the case study considering the pre-established superstructure, NPV = 676x10^6 m.u.

7.6 Final considerations

This chapter has addressed the strategic problem of designing a SC network. The proposed approach utilizes a SC design and planning model that permits material flows of any kind (raw and intermediate materials, final products) between any kind of facilities. What is more, only potential locations are provided to the model as input data; decisions regarding the installation of a processing plant, a distribution center or both of them at a location are made during the optimization procedure. It is noteworthy that a main feature of the flexible model is that it does not require a pre-established process network superstructure thus allowing to optimally define the sub-trains in which production process is decoupled and their respective locations. As a result, processing facilities outputs may be intermediate materials. This is one key feature in modeling the complex global SCs behavior.

The examples presented have evidenced that a great potential to improve the firm's economic performance can be gained by exploring the whole range of available alternatives when designing a SC. The flexible model proposed in this work enables to do this exploration in a straightforward manner. In the worst scenario, the flexible approach would find the same optimal solution as traditional approaches. The flexible model can be also implemented to exploit

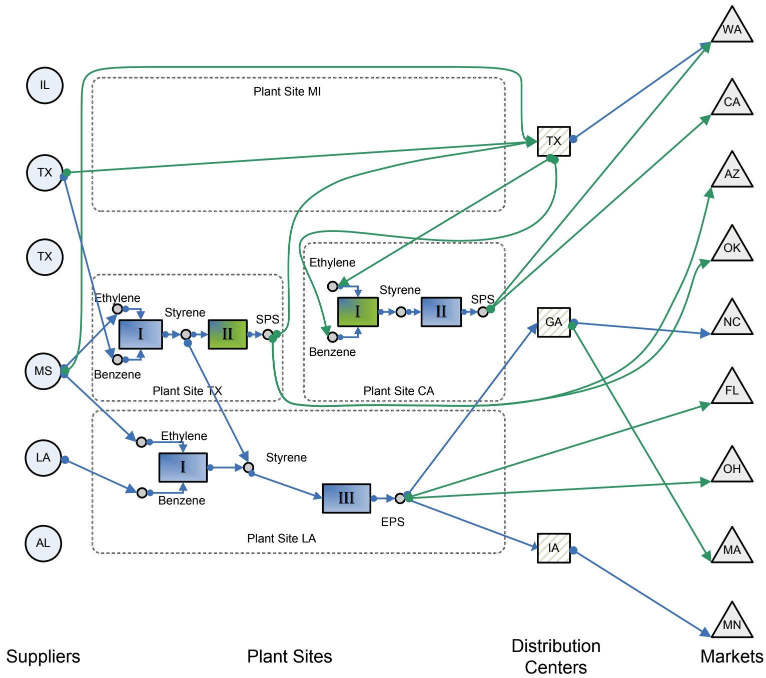


Figure 7.20: Optimal SC network design for the case study by using the flexible approach, NPV = $1180\text{x}10^6$ m.u.

Figure 7.21: SC network in the location map for the flexible solution

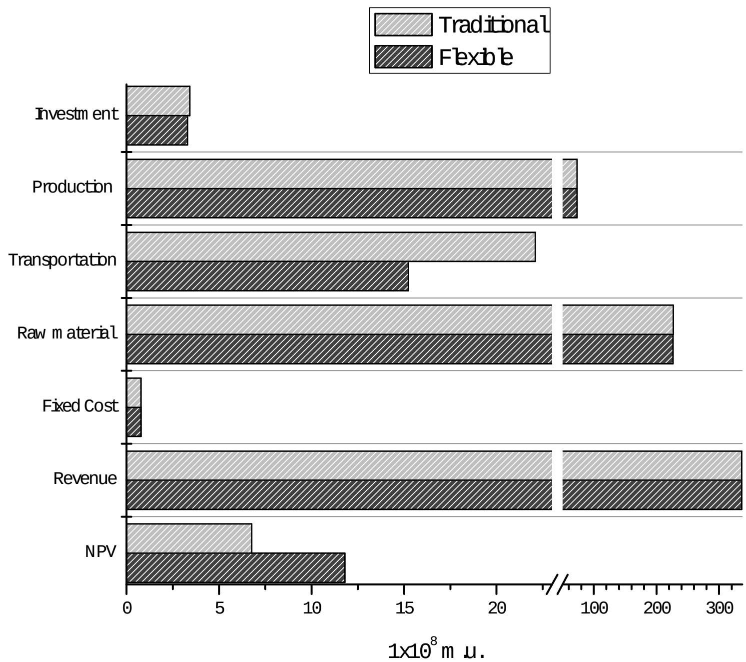


Figure 7.22: Case study economic characterization

flexibility in strict operations planning when the SC network configuration is already fixed. For this case, the model supports task allocation and the definition of links among network nodes taking into account capacity constraints.

Shah (2005) states that it has not really been shown what is an appropriate description of manufacturing processes at the SC level. By translating the STN concept to the whole SC environment an adequate representation of all operations and materials entailed in a production system can be achieved. It should be also emphasized that the proposed model simplifies the representation of batch and/or continuous process SCs into the same framework. Moreover, given that the proposed SC model is an extension of a classical multipurpose plant scheduling formulation it may eventually facilitate the consideration of scheduling decisions while designing a SC. This issue constitutes one important subject that is addressed afterward.

While dealing with SC design problems, managers usually have considerable more time availability to come out with a final decision (i.e. SC configuration) than in the case of planning and scheduling problems. Despite this fact it is necessary to devote research efforts to develop decomposition strategies in order to tackle industrial scale problems. In this regard, spatial and temporal decompositions schemes based on Lagrangian decomposition have proven to considerably reduce the computational burden associated with the solution of this kind of problems (Jackson & Grossmann, 2003). Future work should be focused on developing decomposition schemes applicable to the model presented in this chapter.

7.7 Nomenclature

Indices

e	suppliers
f	facility locations
i	tasks
j	plant equipment
s	states
t	planning periods

Sets

E_s	set of suppliers e that provide raw material s
$\hat{E}_{prod}$	set of suppliers e that provide production services
$\tilde{E}_{tr}$	set of suppliers e that provide transportation services
FP	set of states s that are final products
$\hat{J}_f$	equipment j that can be installed at location f
J_i	equipment that can perform task i
M	set of market locations
R_f	set of raw materials that can be provided from location f
RM	set of states s that are raw materials
RM_e	set of raw materials that are offered by supplier e
S^I	set of unstable materials which cannot be transfered between facilities
Sup	set of supplier locations
Tr	set of distribution tasks
T_s	set of tasks producing state s
$\bar{T}_s$	set of tasks consuming state s

Parameters

A_{sft}	maximum availability of raw material s in period t at location f
Dem_{sft}	product s demand at market f in period t
$FCFJ_{jft}$	fixed cost per unit of capacity of plant equipment j at location f in period t
$FCFS_{ft}$	fixed cost per unit of distribution center capacity at location f in period t
I^J_{ft}	investment required to establish a processing facility in location f in period t
I^S_{ft}	investment required to establish a distribution center in location f in period t
$MinCSL_s$	lower bound of customer service level for product s
$Price_{sft}$	price of product s at market f in period t
$Price^{FJ}_{jft}$	investment required per unit of capacity of equipment j increased at facility f in period t

$Price^{FS}_{ft}$	investment required per unit of distribution center capacity increased at facility f in period t
$rate$	discount rate

Binary Variables

JB^{l}_{ft}	1 if a processing site at location f is established in period t, 0 otherwise
SB^{l}_{ft}	1 if a distribution center at location f is established in period, 0 otherwise t
V_{jft}	1 if the equipment j capacity is increased at location f in period t 0, otherwise
X_{ft}	1 if the distribution center capacity at location f is increased at period t, 0 otherwise

Continuous Variables

$EPurch_{et}$	economic value of purchases executed in period t to supplier e
$ESales_{t}$	economic value of sales executed in period t
$FAsset_{t}$	investment on fixed assets in period t
$FCost_{t}$	fixed cost in period t
FS_{ft}	total distribution center capacity at location f during period t
FSE_{ft}	distribution center capacity increment at location f during period t
FJ_{jft}	plant equipment j total capacity during period t at location f
FJE_{jft}	plant equipment j capacity increment at location f during period t
NPV	net present value
$P_{ijff't}$	production rate of task i in equipment j in period t whose origin is location f and destination location f'
$Profit_{t}$	profit achieved in period t
$Purch^{pr}_{et}$	amount of money payable to supplier e in period t associated with production activities
$Purch^{rm}_{et}$	amount of money payable to supplier e in period t associated with raw materials consumption
$Purch^{tr}_{et}$	amount of money payable to supplier e in period t associated with transport services
$Purch_{esft}$	amount of raw material s purchased to supplier e from location f in period t
$Sales_{sff't}$	amount of product s sold from location f in market f' in period t
S_{sft}	amount of state s stock at location f in period t

Greek symbols

α_{sij}	mass fraction of task i for state s production in equipment j
$\bar{\alpha}_{sij}$	mass fraction of task i for state s consumption in equipment j
β_{jf}	minimum utilization rate of plant equipment j capacity that is allowed at location f
$\theta_{ijff'}$	capacity utilization factor of task i performed in plant equipment j whose origin is location f and destination location f'
π_{jf}	time to install and set up equipment j in facility f
$\hat{\pi}_{f}$	time to install and set up a distribution center in location f
$\rho^{tr}_{eff'}$	unitary transportation costs from location f to location f'

τ^{ut1}_{ijfe}	unitary cost associated with task i performed in equipment j from location f and payable to external supplier e
τ^{ut2}_{sfe}	unitary cost associated with handling the inventory of material s in location f and payable to external supplier e
υ_s	specific volume of product s
ψ_{est}	raw material unitary cost s offered by external supplier e in period t

Superscripts

L	lower bound
U	upper bound

Chapter 8

Mapping Environmental Impacts within SCM

8.1 Introduction

Corporate approaches to improve environmental performance cannot be undertaken in isolation, so a concerted effort along the SC entities is needed which poses another important challenge to managers. This chapter addresses the optimization of SC planning and design considering economical and environmental issues. The strategic decisions considered in the model are facility location, processing technology selection and production-distribution planning. A Life Cycle Assessment (LCA) approach is envisaged to incorporate the environmental aspects of the model. IMPACT 2002+ methodology is selected to perform the impact assessment within the SC, thus providing a feasible implementation of a combined midpoint-endpoint evaluation. The proposed approach reduces the value-subjectivity inherent to the assignment of weights in the calculation of an overall environmental impact by considering end-point damage categories as objective function. Additionally, the model performs an impact mapping along the comprising SC nodes and activities. Such mapping allows focusing financial efforts to reduce environmental burdens to the most promising subjects. Furthermore, consideration of CO_2 trading scheme and temporal distribution of environmental interventions are also included with the intention of providing a tool that may be utilized to evaluate current regulatory policies or pursue more effective ones. The mathematical formulation of this problem becomes a multi-objective MILP (moMILP). Criteria selected for the objective function are damage categories impacts, overall impact factor and net present value (NPV). Main advantages of this model are highlighted through a case study of a maleic anhydride SC production and distribution network.

8.2 Green supply chain management

A proper handling of SC should be concerned with the sharing of responsibility from various aspects of performance which includes environmental matters. It has been realized that significant improvements in terms of environmental performance and market competitiveness may be achieved by concentrating efforts from all SC partners. Actually, managerial practice related to environmental issues has expanded from a narrow focus on pollution control within a single firm to include a larger set of inter-organizational management decisions, programs, tools, and technologies that prevent pollution before its generation (Klassen & Johnson, 2004). Consequently, these issues are being considered in recent works and call for further research in the integration of environmental management with ongoing SC operations.

The aforementioned integration may be achieved through the emerging concept regarded as "Green Supply Chain Management" (GrSCM), defined as the integration of environmental thinking into SCM, including product design, raw materials sourcing and selection, manufacturing process selection, delivery of final product to the consumers as well as end of life management of the product after its useful life (Srivastava, 2007). Traditionally, in the PSE community the optimization models devised to assist operation and design in the chemical processing industry have focused on finding the solution that maximizes a given economic performance indicator while satisfying a set of operational constraints imposed by the processing technology and the topology of the plant. In recent years, however, there has been a growing awareness of the importance of including environmental and financial aspects associated to the business decision support levels (Puigjaner & Guillén-Gosálbez, 2007). In fact, there are some documented successful stories of enterprises that have integrated environmental and SC management. Hart (1997) has presented the Xerox's Asset Recycle Program which redirects 90% of all materials and components for its photocopiers through reuse, remanufacturing, and recycling; in this case annual savings are estimated in US$300 million. Hoeffer (1999) has reported a scrap management system deployed by Daimler-Chrysler which allows for an annual saving of US$4.7 million. These examples illustrate the potential benefits that can be achieved by integrating environmental aspects along the SC.

The environmental science and engineering community have developed several systematic methodologies for the detailed characterization of the environmental impacts of chemicals, products, and processes. All of these methodologies have embodied the concepts of life cycle, i.e., they are based on an LCA which is described in a series of ISO documents (IRAM-ISO-14040, 1997). This framework includes the entire product life cycle, process or activity, encompassing extraction and processing of raw materials; manufacturing, transport and distribution; re-use, maintenance recycling and final disposal. Most importantly, it encompasses a holistic approach, bringing the environmental impacts into one consistent framework, wherever and whenever these impacts have occurred or will occur (Guinee *et al.*, 2001).

Examples of these methodologies in the chemical engineering field are the Minimum Environmental Impact (MEI) methodology (Stefanis, Livingston, & Pistikopoulos, 1995), the Waste Reduction (WAR) algorithm (Young & Cabezas, 1999), the Optimum LCA Performance (OLCAP) framework (Azapagic, 1999; Azapagic & Clift, 1999b), the Environmental Fate and Risk Assessment tool (EFRAT) (Chen & Shonnard, 2004) and the methodologies proposed by Alexander, Barton, Petrie, and Romagnoli (2000) and by Guillén-Gosálbez, Caballero, and Jiménez (2008). All these methodologies are based on the incorporation of an optimization step to the four classical phases in an LCA study (i.e., goal definition, life cycle inventory-LCI, life cycle impact assessment-LCIA and interpretation), which optimizes process conditions or topology considering a single SC echelon.

Because an LCA ideally covers a cradle-to-grave approach, it can be clearly seen that LCA fits as a suitable tool for quantitatively assessing the environmental burdens associated with designing and operating a SC. Two possible LCA approaches can be carried out, namely, comparison/selection and improvement (Klassen & Greis, 1993). The former approach focuses on identifying environmentally preferable products or processes alternatives as an attempt to leverage market-place/financial forces to displace environmentally harmful activities (Klöpffer & Rippen, 1992). The latter one uses LCA as a tool to identify the SC stages that have a particularly strong negative impact on the environment, and thus, where improvements would be most beneficial. This last alternative allows to improve the allocation of limited management time and financial resources within the SC (Freeman, Harten, Springer, Randall, Curran, & Stone, 1992). Both types of analysis are performed in this work by means of a SC design-planning optimization model. Recently, Mele, Hernández, and Bandoni (2008) have shown a quantitative tool for decision making support in the design of sugar cane to ethanol SCs. Also, Hugo and Pistikopoulos (2005) have shown how a set of SC network designs can form an environmentally conscious basis for the investment decisions associated with strategic SC level.

From another standpoint, as the planet warms up, so does legislation to reduce greenhouse gas (GHG) emissions worldwide. Within this scenario much of the opportunity to manage carbon (CO_2) emissions effectively relies on the organization's capacity to have an overall view of its specific responsibility and associated cost, from a life cycle point of view. With estimated economic damage of about US$85 for each ton of CO_2, capping GHG emissions and establishing a price tag on them became inevitable (Stern, 2006). Indeed, such a setup is already in effect in some countries and for certain industries under the European Union Emissions Trading Scheme-(EU ETS). The idea behind the scheme is to make firms pay for their carbon emissions so that a financial incentive to decrease carbon emissions is provided. A cap is set on emissions, businesses are allowed to buy or sell from each other the right to emit GHGs. Firms exceeding their emissions cap have to buy extra credits to cover the excess, providing an incentive for them to operate under the capped level, while those that do not use up all their allowances can sell them, providing the least-polluting firms with an extra revenue and an incentive to further reduce emissions (Young, 2008). Similar schemes are popping up across the United States and in other major industrial economies worldwide. Going forward, organizations should expect to be charged for their CO_2 emissions. Much of the opportunity to address CO_2 emissions rests on SCM, compelling companies to look for new approaches to manage carbon emissions effectively. And most certainly, this charge will force a change in the way organizations run their SCs (Butner, Geuder, & Hittner, 2008). One of the key aspects to have a successful policy is the definition of the free emissions allowance cap for each industry type.

Several institutions (e.g., the California Climate Action Registry (CCAR), The Climate Registry (TCR), the World Resources Institute (WRI), World Business Council for Sustainable Development (WBCSD)) have determined protocol definitions for carbon registries in order to help organizations analyze their CO_2-footprints. Nevertheless, according to Matthews, Hendrickson, and Weber (2008) the scope of these protocols varies, generally suggests estimating only direct emissions (Tier 1) and emissions from purchased energy (Tier 2), with less focus on the SC context which will lead to large underestimates of the overall CO_2 emissions. The authors propose a footprint estimation that includes the total SC up to the production gate, also known as cradle-to-gate approach (Tier 3). Furthermore, the authors refer to Tier 4 emission estimations when the whole product life cycle is taken into account by considering emissions occurring during distribution and product end of life. This extended scope is expected to better aid effective environmental strategies since both firms and consumers have an important influence over the carbon footprints through their "purchase" decisions. It is pointed out that tools, specifically LCA models, should be useful in pursuing more effective climate change policies and international trade should be included within this analysis. Finally, it is noteworthy that climate change policies are applied based on the temporal distribution of emissions. Usually SC environmental impacts are evaluated at the end of the planning horizon, and in the case of an LCA the temporal distribution is disregarded at all. Consequently, the incorporation of constraints associated to the temporal emission distributions is necessary when studying climate change policies in a SC planning model.

Recalling all the aspects that have been mentioned before, this chapter presents a novel approach for SC design and planning focusing on environmental impact and its sources. An optimization step is included allowing for selecting the appropriate technology, and the appropriate raw material/service supplier. In this respect the proposed approach calculates tier 3 and partially tier 4 related emissions. It encompasses direct emissions, purchased energy emissions, raw materials production emissions and transport distribution emissions. LCA concepts are fully embedded in the approach. Furthermore, in order to attain a comprehensive LCA application, not merely an overall environmental impact indicator is calculated but partial environmental impact categories are studied. Additionally, the impact associated to every SC echelon is mapped aiming at discovering possible opportunities to focus management efforts and resources for environmental impact reduction. Moreover, the temporal emission distribution is considered for the calculation of environmental and financial metrics, accounting for possible emissions trading. In this way the current LCA scheme is further extended by including emissions temporal distribution.

8.3 Problem statement

This work represents a comprehensive step over the approaches presented by Mele, Espuña, and Puigjaner (2005b) and Hugo and Pistikopoulos (2005) by assisting in the planning and design of a SC under economical and environmental impacts considerations. The resulting model is solved by using an moMILP algorithm, which allows observing possible environmental tradeoffs between damage categories and the economic indicator. This approach reduces the value-subjectivity inherent to the assignment of weights in the calculation of an overall SC environmental impact, which is also calculated. The analysis of partial environmental impacts for every echelon is performed with the aim of discovering improvement opportunities; this analysis also provides information about where to focus emission control activity and hints on possible strategies for emission reduction at source. The temporal emissions distribution and trading schemes considerations contributes to understand how regulatory schemes may induce environmental impact reductions. The problem can be stated as follows.

Given:

Process operations planning data

- A fixed time horizon;
- A set of materials: products, raw materials and possible intermediates;
- A set of markets in which products should be available to customers and their expected nominal demand;
- A set of potential geographical sites for facilities location;
- A set of potential equipment technologies for different processing stages;
- Lower and upper bounds for feasible equipment and storage capacity increments;
- Product recipes, manufacturing and transport requirements (such as, mass balance coefficients and resources utilization);
- Minimum/maximum utilization rate installed capacity bounds;
- Suppliers capacity bounds;

Economic data

- Direct cost parameters such as production, handling, transport and raw material costs;
- Price for every product in each market during the time horizon;
- Relationship between capital investment and facilities capacity;
- Relationship between indirect expenses and facilities capacity.
- GHG emission prices.

Environmental data

- Product manufacturing environmental interventions (including GHG emissions).
- Maximum GHG free emission allowance
- Raw material production environmental interventions
- Distribution environmental interventions
- Environmental setting for characterization and aggregation of environmental interventions

The goal is to determine:

- The active SC nodes and links;
- The facilities capacity in each time period;
- The assignment of the manufacturing and distribution tasks to the network nodes;
- The amount of final products to be sold;
- The environmental impact associated to each SC node;

such that economic and environmental metrics are optimized at the end of the planning horizon. The model assumes that processing technologies are available for eventual installation at potential locations and assists in their selection. Within this model, and in order to avoid emission double counting, raw material emissions are not aggregated to product manufacturing, similarly transport and energy consumption are considered separately.

8.4 Mathematical formulation

The mathematical formulation of the LCA – SC problem is briefly described next. The variables and constraints of the model can be roughly classified into three groups. The first one concerns process operations constraints given by the SC topology. The second one deals with the environmental model used, while the third refers to the economical metric applied.

8.4.1 Supply Chain Design-planning model

Here, the flexible design–planning approach presented in Chapter 7 is utilized. This model is suitable to collect all SC node information through a single variable, which eases environmental formulation. This way SC node characteristics are modeled with a single equation set, since manufacturing nodes and distribution centers are treated in the same way as well as production and distribution activities. The model's details are in Chapter 7.

8.4.2 Environmental model

The results of the LCI, which gathers all SC environmental interventions (i.e., emissions or natural raw material consumptions), can be interpreted by means of different environmental metrics. These metrics differ in their position along the environmental damage chain (environmental mechanism). Environmental interventions are translated into metrics related to environmental impact as endpoints or midpoints metrics by the usage of characterization factors (CF). Two main schools of methods have evolved, namely, problem oriented methods which restrict quantitative modeling to early stages in the cause-effect chain (mid-points), and damage oriented methods which attempt to model the cause-effect chain up to the damage itself (end-points). In this model the environmental metric IMPACT 2002+ (Humbert, Margni, & Jolliet, 2005) is used, which presents an implementation working at both midpoint and damage levels. For each environmental intervention two CFs are proposed, which eases model implementation.

IMPACT 2002+ is mainly a combination between IMPACT 2002 (Pennington, Margni, Amman, & Jolliet, 2005), Eco-indicator 99 (Goedkoop & Spriensma, 2001) using egalitarian factors, classical impact assessment methods (CML) (Guinee *et al.*, 2001) and Intergovernmental Panel on Climate Change (IPCC) considerations. IMPACT 2002+ has grouped similar category endpoints into a structured set of damage categories by combining two main schools of impact model methods: CML and damage oriented methods (Eco-indicator 99). This methodology proposes a feasible implementation of a combined midpoint/damage-oriented approach. It links all types of LCI results via 15 midpoint categories (human toxicity, respiratory effects, ionizing radiation, ozone layer depletion, photochemical oxidation, aquatic ecotoxicity, terrestrial ecotoxicity, terrestrial acidification/nitrification, aquatic acidification, aquatic eutrophication, land occupation, global warming, non-renewable energy, mineral extraction) to four damage categories (human health, ecosystem quality, climate change-global warming potential, resources).

This approach contains the advantages of being able to calculate both mid and endpoint indicators. In this model, damage categories are used as objective functions since these metrics are easier to comprehend compared to mid-point values.

The equations of the environmental model are briefly described next. Equation (8.1) models IC_{aft} which represents the midpoint a environmental impact associated to site f which rises from activities in period t; $\psi_{ijff'a}$ is the a environmental category impact CF for task i performed using technology j, receiving materials from node f and delivering it at node f'.

$$IC_{aft} = \sum_{j \in \tilde{J}_f} \sum_{i \in I_j} \sum_{f'} \psi_{ijff'a} P_{ijff't} \qquad \forall\ a, f, t \tag{8.1}$$

The value of $\psi_{ijff'a}$ is fixed and constant, provided that all environmental impacts are directly proportional to the activity performed in that node (i.e., variable P_{ijfft} of the SC design–planning model). This issue is common practice in LCA, where all direct environmental impacts are considered linear with respect to the functional unit (Heijungs & Suh, 2002).

It should be noted that environmental impacts associated to materials transport are assigned to their origin node. The study of environmental impacts associated to transport or production can be performed by setting the indices summation over the corresponding tasks (i.e., $i \in Tr$ or $i \in NTr$). Furthermore the value of $\psi_{ijff'a}$ can be calculated by Eq. (8.2) in the case of transportation. Here ψ^{T}_{ija} represents the a environmental category impact CF for the transportation of a mass unit of material over a length unit.

$$\psi_{ijff'a} = \psi^{T}_{ija} distance_{ff'} \qquad \forall\ i \in Tr, j \in J_i, a, f, f' \tag{8.2}$$

Equation (8.3) introduces $DamC_{gft}$ which are a weighted sum of all midpoint environmental interventions combined using g endpoint damage factor ζ_{ag} and then further normalized with $NormF_g$ factors. Equation (8.4) is to compute the g normalized endpoint damage along the whole SC ($DamC^{SC}_{g}$).

$$DamC_{gft} = \sum_{a \in A_g} NormF_g \zeta_{ag} IC_{aft} \qquad \forall\ g, f, t \tag{8.3}$$

$$DamC^{SC}_{g} = \sum_{f} \sum_{t} DamC_{gft} \qquad \forall\ g \tag{8.4}$$

CO_2 emissions trading is modeled by introducing Eq. (8.5). The climate change damage category accounts for all the equivalent CO_2 kg. Eq. (8.5) states that the total equivalent CO_2 emission occurring in the SC (Tier 4 minus product use and end of life emissions) in period t to be equal to the free allowance emissions cap ($MaxCO_{2t}$) plus the extra rights bought to emit ($Buy_t^{CO_2}$) minus the sold rights ($Sales_t^{CO_2}$) in period t. T_L is the subset of those periods when the emission trading is executed, usually every year. In this model it is assumed that any amount of rights can be sold or obtained at the emissions market. L is the number of periods that accounts for the emission trading interval (e.g., in case that emissions trading occurs yearly and each period t represents one month, L is equal to 12).

$$\sum_{f} \sum_{a \in A_g} \sum_{t'=t-L+1}^{t} \zeta_{ag} IC_{aft'} = MaxCO_{2t} + Buy_t^{CO_2} - Sales_t^{CO_2} \qquad \forall\ g = ClimateChange, t \in T_L \tag{8.5}$$

Equations (8.6) and (8.7) sum up the environmental damage category results for each site f and for the whole SC, respectively.

$$Impact^{2002}_{f} = \sum_{g} \sum_{t} DamC_{gft} \qquad \forall\ f \tag{8.6}$$

$$Impact^{2002}_{overall} = \sum_{f} \sum_{g} \sum_{t} DamC_{gft} \tag{8.7}$$

$DamC_g^{SC}$ or $Impact_{overall}^{2002}$ are both used as objective functions in the moMILP formulation.

8.4.3 Economic model

Many economic performance indicators have been proposed to assess the economic performance of a SC network design. The most traditional indicators are profit, net present value (NPV), and total cost. However, other more holistic measures have been proposed which take into account the dynamic change of net working capital (see Chapter 4). Similarly to the SC operations model, the reader is referred to section 7.4.2 where the equations belonging to the economic model are found. Notice that for this case, the CO_2 emissions trading must be taken into account in the economic model.

The Net income ($Net_t^{co_2}$) due to emissions trading is calculated by Eq.(8.8). Here, $Cost^{co_2}$ and $Price^{co_2}$ represent the emission right cost and price respectively.

$$Net_t^{co_2} = Price_t^{co_2} Sales_t^{co_2} - Cost_t^{co_2} Buy_t^{co_2} \qquad \forall\, t \in T_L \tag{8.8}$$

Accordingly, the profit calculation at period t represented in Equation (8.9) incorporate such an issue. To conclude, NPV is computed by means of Eq. (8.10).

$$Profit_t = ESales_t + Net_t^{co_2} - (FCost_t + \sum_e EPurch_{et}) \qquad \forall\, t \tag{8.9}$$

$$NPV = \sum_t \left(\frac{Profit_t - FAsset_t}{(1 + rate)^t} \right) \tag{8.10}$$

Thus, the SC network design-planning problem whose objective is to optimize a given set of objective functions can be mathematically posed as follows:

$$\begin{gathered} \underset{\mathscr{X},\mathscr{Y}}{\text{Minimize}} \left\{ -NPV, DamC_g^{SC}, Impact_{overall}^{2002} \right\} \\ \text{subject to} \\ \text{Eqns. (7.1)–(7.24); (8.1)–(8.10);} \\ \mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R}^+ \end{gathered}$$

Here $\mathscr{X}$ denotes the binary variables set, while $\mathscr{Y}$ corresponds to the continuous variable set.

8.5 Case study

The case study used to illustrate the concepts behind the presented strategy addresses a SC design problem comparing different technologies for maleic anhydride (MA) production. MA is an important raw material used in the manufacture of phthalic-type and unsaturated polyester resins, co-polymers, surface

Figure 8.1: Supplier, production/distribution and market nodes location

coatings, plasticizers and lubricant additives (USEPA, 1980). Two main technologies are available for its manufacturing by catalytic oxidation of different hydrocarbons, benzene or butane (Chen & Shonnard, 2004). Main process reactions are as follows:

$$\text{Butane Route: } C_4H_8 + 3O_2 \rightarrow C_4H_2O_3 + 3H_2O \tag{8.11}$$

$$\text{Benzene Route: } C_6H_6 + 4.5O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O \tag{8.12}$$

From an atom economy point of view (Domenech, Ayllon, Peral, & Rieradevall, 2002), the procedure considering the conversion of butane/butene is more environmentally friendly (see Eq. (8.11)), because all butene C atoms end up as MA, while for benzene reaction (see Eq. (8.12)), only 67% of C atoms are converted into MA. Also for the butene reaction, the oxygen efficiency is greater than in the benzene reaction (50% vs 33%); just in terms of hydrogen consumption benzene reaction renders a higher atom efficiency than butene reaction (33% vs 25%). Several factors such as advances in catalyst technology, increased regulatory pressures, and continuing cost advantages of butane over benzene have led to a rapid conversion of benzene- to butane-based plants, consequently to the conversion of the whole MA SC (Felthouse, Burnett, Horrell, Mummey, & Kuo, 2001).

Table 8.1: Raw material consumption (α_{sij}) per MA kg (Ecoinvent-V1.3, 2006)

Technology	MA Technology 1	MA Technology 2
Electricity consumption [kWh]	0.540	1.08
Propane-butane [kg]	0.000	0.99
Benzene [kg]	1.026	0.00
CO_2 direct emissions [kg]	1.800	3.87

The studied SC comprises raw material extraction facilities, processing sites, distribution centers and marketplaces, fitting a cradle to distribution center approach. Different raw material suppliers are modeled considering that each of them provides the same commodities quality, but the production is performed using different technologies. Two technologies can be implemented: (i) based on benzene (MA Technology 1) and (ii) based on butane (MA Technology 2) feedstock. Table 8.1 shows raw materials requirements for each of these technologies. The material prices or costs are in Table 8.2.

A simplified potential network is proposed and restricted to Europe (see Figure 8.1). Tarragona ($Site1$), Estarreja ($Site2$) and Drusenheim ($Site3$) are considered to be possible facilities location nodes. Benzene is supposed to be available at Bilbao ($Bz1$) and Rotterdam ($Bz2$), while n-butane can be supplied from again Rotterdam ($Bt1$) and Le Havre ($Bt2$). MA is supposed to be sold at four markets Madrid ($M1$), Paris ($M2$), Munich ($M3$) and Lisbon ($M4$).

The environmental impacts associated to MA production without consideration of raw material production, transportation and electricity consumption are found in Table 8.3. Two potential benzene suppliers are considered, benzene can be obtained from a coke plant (Benzene Supplier-Tech 1-$Bz1$), or from a 50% mixture of ethylene reforming and pyrolysis gasoline (Benzene Supplier-Tech 2-$Bz2$). For the case of butane production, two suppliers are considered, one that is a proxy model obtained from a European typical refinery (Butane Supplier-Tech 1-$Bt1$) (Butane Supplier-Tech 2-$Bt2$), and another one from a mixture of the top 20 most important organic chemicals. The values were retrieved from Ecoinvent-V1.3 (2006) using SimaPro 7.1.6 (PRe-Consultants-bv, 2008). The environmental impact for raw material production can be also found

Table 8.2: Raw material (χ_{est}) and product prices ($Price_{sft}$)

Commodities		Price/cost [$]
Electricity [kWh]	Supplier-Tech 1	0.057
	Supplier-Tech 2	0.038
Benzene [kg]	Supplier-Tech 1	0.171
	Supplier-Tech 2	0.214
Butane [kg]	Supplier-Tech 1	0.224
	Supplier-Tech 2	0.280
Maleic anhydride [kg]		1.672

Table 8.3: Environmental impact for 1 kg of product and raw materials production ($\psi_{ijff'a}$) (Ecoinvent-V1.3, 2006)

Impact category	Unit	MA Technology 1	MA Technology 2	Benzene Supplier Tech 1	Benzene Supplier Tech 2	Butane Supplier Tech 1	Butane Supplier Tech 2
Carcinogens	kg C_2H_3Cl	1.4E-09	0.0E+00	3.9E-01	2.0E-01	6.3E-03	9.1E-02
Non-Carcinogens	kg C_2H_3Cl	2.7E-04	0.0E+00	1.4E-02	8.9E-04	7.6E-03	7.5E-03
Respiratory inorganic	kg PM2.5	0.0E+00	0.0E+00	4.3E-03	1.3E-03	8.1E-04	1.5E-03
Ionizing radiation	Bq C-14	0.0E+00	0.0E+00	1.3E+01	5.9E-03	9.3E+00	2.2E+01
Ozone layer depletion	kg CFC-11	0.0E+00	0.0E+00	2.4E-07	2.9E-11	4.7E-07	1.4E-07
Respiratory organics	kg C_2H_2	7.9E-06	1.3E-05	9.2E-03	9.2E-04	8.5E-04	1.4E-03
Aquatic ecotoxicity	kg TEG water	8.8E-07	2.3E-07	1.5E+02	6.0E+01	1.5E+02	1.0E+02
Terrestrial ecotoxicity	kg TEG soil	1.7E-07	3.2E-07	3.4E+01	2.4E-02	3.1E+01	1.7E+01
Terrestrial acid/nutri	kg SO_2	0.0E+00	0.0E+00	2.5E-02	3.8E-02	1.5E-02	3.9E-02
Land occupation	m^2org-arable	0.0E+00	0.0E+00	2.0E-02	1.4E-05	3.4E-03	4.8E-03
Aquatic acidification	kg SO_2	0.0E+00	0.0E+00	6.6E-03	8.3E-03	6.3E-03	9.4E-03
Aquatic eutrophication	kg P-lim	5.4E-04	5.4E-04	1.6E-05	4.4E-06	3.5E-04	4.4E-04
Global warming	kg CO_2	1.8E+00	3.9E+00	6.4E-01	1.4E+00	5.6E-01	1.6E+00
Non-renewable energy	MJ primary	0.0E+00	0.0E+00	5.4E+01	7.1E+01	5.6E+01	6.7E+01
Mineral extraction	MJ surplus	0.0E+00	0.0E+00	3.4E-03	2.5E-04	2.6E-03	1.5E-02

Table 8.4: Environmental impact associated to transport services (ψ^T_{ija}) and electricity production ($\psi_{ijff'a}$) (Ecoinvent-V1.3, 2006)

Impact category	Unit	Transport lorry 32ton [tn·km]	Transport lorry 16ton [tn·km]	Electricity supplier 1 [kWh]	Electricity supplier 2 [kWh]
Carcinogens	kg C_2H_3Cl	1.2E-03	2.0E-03	1.6E-04	1.4E-04
Non-Carcinogens	kg C_2H_3Cl	2.4E-03	3.9E-03	1.4E-04	1.4E-04
Respiratory inorganics	kg PM2.5	2.8E-04	6.5E-04	3.7E-05	2.8E-05
Ionizing radiation	Bq C-14	1.4E+00	3.8E+00	1.1E-01	3.8E+00
Ozone layer depletion	kg CFC-11	2.3E-08	4.9E-08	5.1E-09	1.7E-09
Respiratory organics	kg C_2H_2	1.7E-04	6.7E-04	1.1E-05	4.1E-06
Aquatic ecotoxicity	kg TEG water	1.8E+01	3.2E+01	1.9E+00	1.9E+00
Terrestrial ecotoxicity	kg TEG soil	1.1E+01	1.8E+01	5.2E-01	3.4E-01
Terrestrial acid/nutri	kg SO_2	7.6E-03	1.5E-02	8.7E-04	5.0E-04
Land occupation	m^2org-arable	1.3E-03	4.7E-03	5.8E-05	7.3E-05
Aquatic acidification	kg SO_2	1.2E-03	2.4E-03	3.0E-04	1.9E-04
Aquatic eutrophication	kg P-lim	1.6E-05	3.4E-05	2.0E-06	5.3E-07
Global warming	kg CO_2	1.6E-01	3.6E-01	5.2E-02	3.6E-02
Non-renewable energy	MJ primary	2.8E+00	6.0E+00	7.4E-01	8.2E-01
Mineral extraction	MJ surplus	1.3E-03	1.9E-03	6.8E-05	9.0E-05

in Table 8.3 which does not consider impacts associated to transportation, nor facilities installation.

Two different types of transportation services are assumed to be available, lorries in two different sizes (16 and 32 ton). Benzene is a chemical that is liquid at standard conditions and therefore stored and transported as a liquid. Butane, on the other hand, is a gas at standard conditions and therefore needs to be liquefied in order to be transported and stored. In this case butane liquefaction has been considered during its production, and consequently both products are transported in liquid state, with similar environmental impacts by the same kg·km. Medium voltage electricity production from different countries grid is considered. Environmental impacts associated to transport services and electricity production are found in Table 8.4. Transportation prices were estimated from current economical trends, see Table 8.5. Return rate is assumed to be 25%.

Capital investment associated to equipment and its operating costs are based on previously published results which were obtained using process simulation (Chen & Shonnard, 2004). These figures are from a design basis of $2.27 \cdot 10^7$ kg of MA /year (see Table 8.6).

Table 8.5: Materials transportation cost ($ $10^{-5}/(kg \cdot km)$, $\rho^{tr}_{eff't}$)

Material	Cost
Benzene	2.99
MA	2.75
Butane	4.25

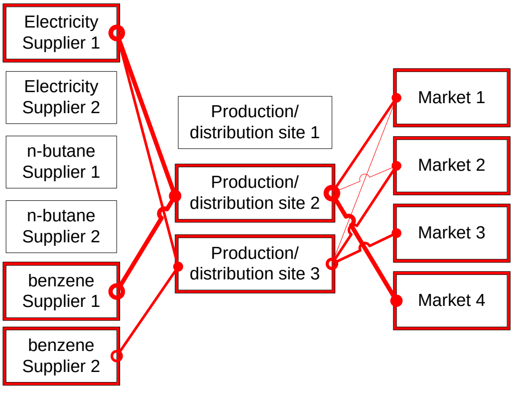
Table 8.6: Facilities capital investment ($Price^{FJ}_{jft}$) and operating cost (τ^{ut1}_{ijfe}) ($\$1 \cdot 10^7$ m.u.)

	MA Technology 1	MA Technology 2
Capital investment	1.61	1.95
Operating cost	1.42	1.30

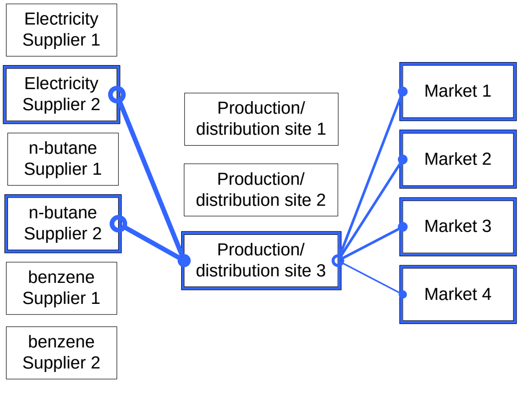
Thirty-seven monthly planning periods are considered. The implementation in GAMS (Brooke *et al.*, 1998) of the SC-LCA formulation leads to a MILP model with 15 440 equations, 137 652 continuous variables, and 1093 discrete variables. It takes 13.2 CPU s to reach a solution with a 0% integrality gap on an 2.0 GHz Intel Core 2 Duo computer using the MIP solver of CPLEX (ILOG-Optimization, 2008).

In order to evaluate comparable alternatives, the first step has consisted on determining a SC which maximizes NPV, which is used to fix a total production rate. From the supplied data, it is found that the production rate should be of 703 ton of MA. Then, since two objective functions are to be optimized, namely, NPV and environmental impact, the procedure described in Section 3.6, *Multi-objective optimization*, is followed to ensure that non-dominated solutions are computed.

Following this procedure, Figure 8.2(a) shows the obtained dominant SC that maximizes NPV. It is found that its production is based on benzene feedstock, which is bought from both available suppliers. Two facilities are built and



(a) Most profitable SC option



(b) Best environmental friendly SC option

Figure 8.2: SC configurations for extreme Pareto points

Table 8.7: Single objective optimization results

	Impact 2002+ Optimization		NPV Optimization	
	Direct value	Normalized value	Direct value	Normalized value
Human Health	6.22E+02	8.76E+04	2.49E+03	3.50E+05
Ecosystem Quality	2.79E+08	2.04E+04	2.67E+08	1.95E+04
Climate Change	3.28E+09	3.31E+05	2.27E+09	2.29E+05
Resources	4.19E+10	2.77E+05	4.93E+10	3.26E+05
Impact 2002+	7.16E+05		9.25E+05	
NPV	-1.62E+08		1.18E+08	
Raw Mat. used	n-butane		benzene	
SC structure	Fig. 8.2(b)		Fig. 8.2(a)	

MA is sold in all possible markets. Alternatively, by the minimization of the environmental impact indicator, the resulting SC (Fig. 8.2(b)) uses butane as feedstock and buys raw materials from a single supplier. This SC configuration implies a single production facility which sells MA to all four markets. Table 8.7 summarizes the most significant values corresponding to both solutions:

- In the case of minimization of environmental impact, a negative NPV is found because of the high transportation cost associated to this solution (butane suppliers locations are far from production facility locations and butane transport cost is 42% higher than benzene cost).

- Figure 8.3 shows the distribution of the environmental impacts along SC echelons for these two cases. According to Bauman and Tillman (2004), most LCA studies show that the production of materials often causes a dominant proportion of the environmental impact of a product, whereas assembly often causes a very minor proportion. If the product requires energy during its use phase, this phase often dominates the environmental profile, whereas if the product is used in a more passive way, the production phase dominates; notably the production of materials. In spite of transport being a major source of pollution in society, transportation and distribution often contribute less to the environmental impact than expected. In the presented case study, raw material production is the most important factor contributing to the overall environmental impact in both single objective optimization cases; while electricity consumption and transportation are the least impacting aspects. This clearly shows that activities to reduce environmental impact should be focused on raw material production echelon.

One alternative to reduce SC environmental impacts may be to look for new feedstock providers whose production processes are more environmental friendly. It is also important to notice that Human Health impacts are considerable high in both solutions. In the case of NPV optimization this fact is due to benzene toxic properties. It is expected that CO_2 emissions trading consid-

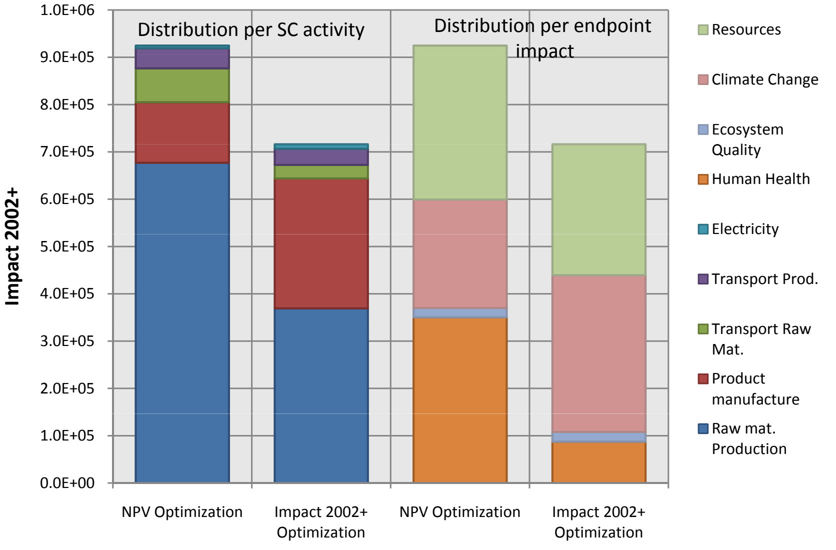


Figure 8.3: Distribution of environmental impacts for single objective optimization solutions

erations will make the butane based production more economically attractive. This aspect is analyzed in section 8.5.1.

To explicitly show the tradeoff between the NPV and environmental impact (overall factor and damage factors), a multi-objective optimization is applied (see Section 3.6). In each case NPV is optimized against one of the possible four environmental impacts (see Fig. 8.4). In this figure optimization of GWP, ecosystem quality, human health and resource depletion against NPV produces a set of dominated structures in terms of global environmental impact, as it was expected, given that each environmental damage category competes against the other ones. One can notice that best SC configurations in terms of overall environmental impact match up with the ones with minimum human health impact. It is also important to point out that the SC configuration which shows the minimum GWP produces an overall impact that is 27% greater that the minimum possible value. It is observed that the overall Impact2002+ Pareto curve portion that approximately goes from a zero to a $1.0 \cdot 10^8$ NPV value does not correspond to any damage factor optimum, SC configurations that combine butane and benzene based technologies are found there. Moreover, it is highlighted that the most environmental friendly solution in terms of overall impact highly depends on the weights and normalization factors assigned to each damage category; in this case study the most environmentally convenient solution entails high climate change impact (see change in the trend of overall impact when optimizing climate change in Fig. 8.4). The importance of optimizing each damage factor lies in the possibility of evaluating the tradeoff among them.

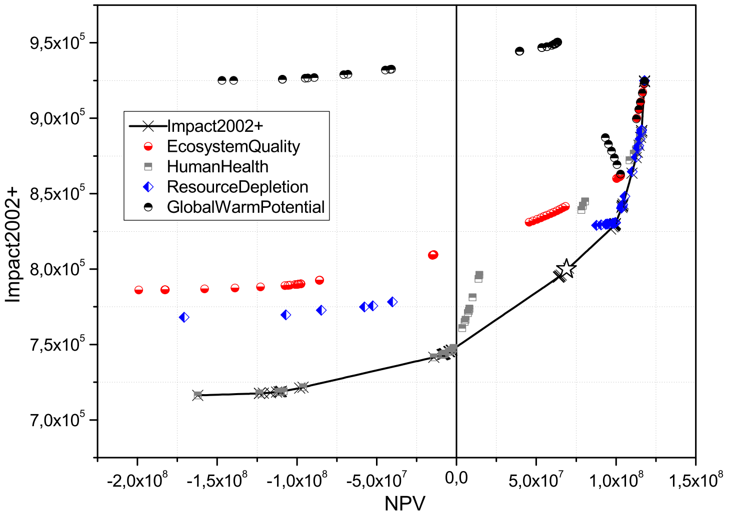


Figure 8.4: Calculated Overall impact for each end point impact optimization against NPV (✰ corresponds to the SC configuration shown in Figure 8.6)

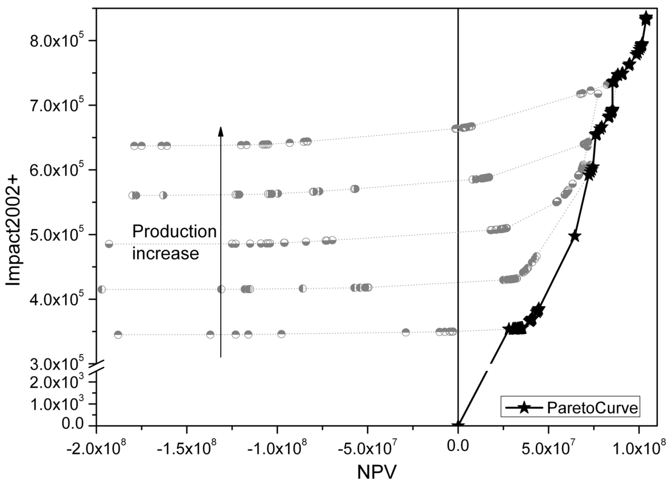


Figure 8.5: Overall environmental impact vs. NPV Pareto curve (in gray iso-production curves)

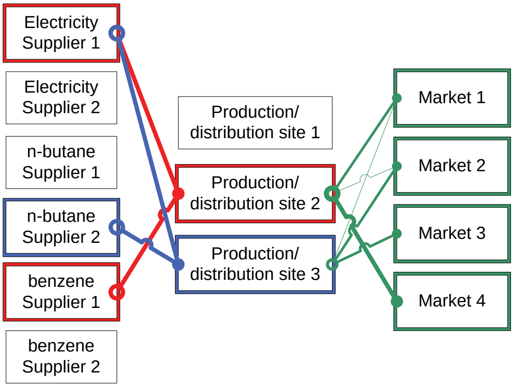


Figure 8.6: SC configuration located in the middle of the NPV vs overall environmental impact Pareto space

Furthermore, there is a SC structure dependence against its total production. Other works related to SC design and environmental issues consider that demand must be completely fulfilled. This assumption leads to an invariable total production rate and suboptimal solutions. In Fig. 8.5 iso-production curves correspond to solutions following this assumption. For these cases, minimum overall impact always leads to negative NPVs. These solutions are obviously dominated by the zero-production solution (origin). The actual Pareto curve is shown in figure 8.5 as a continuous black line which is obtained by allowing unfulfilled demand (i.e. not considering fixed produced amount). It can be seen that positive NPVs can be achieved by reducing the MA production.

It is worth noting that from the sixteen alternative SC structures only five of them are active when minimizing the total environmental impact. For example, Fig. 8.6 shows a configuration located in the middle of the Pareto space (see Figs. 8.4 and 8.5) so that a combination of benzene and n-butane based technologies may result in an optimum (nondominated) alternative. As it can be observed, the multi-objective optimization results in a set of Pareto solutions. Within this set of nondominated solutions the decision maker must select one. The stakeholder's selected solution will depend on the weights that he/she subjectively assigns to each of the objectives (i.e., NPV and Impact2002+). Several multi-attribute decision analysis (MADA) techniques are available for this purpose, for a review of these techniques the reader is referred to the work of Seppälä, Basson, and Norris (2002).

8.5.1 CO_2 emission trading considerations

In order to take into account CO_2 emissions, values for maximum free emissions caps must be available. One possible way of assessing such value is to take the best available technology (BAT) in terms of CO_2 emissions. Chen and Shonnard (2004) have studied both MA production schemes finding through simulation

Table 8.8: CO_2 emissions associated to MA kg (Ecoinvent-V1.3, 2006), and BAT data ($MaxCO2_t$, Chen and Shonnard (2004))

	MA Technology 1	MA Technology 2
BAT Tier 2 CO_2 emissions [kg]	3.41	**3.02**
Tier 1 CO_2 emissions [kg]	1.80	3.87
Tier 2 CO_2 emissions [kg]	2.05	4.38
Tier 3 CO_2 emissions [kg]	3.53	4.93

optimum flow sheets (see Table 8.8). Given that Chen and Shonnard (2004) data does not consider steam co-production, the BAT value has been increased accordingly (32%), in order to be comparable to the one reported by Ecoinvent-V1.3 (2006). According to this data, producing MA from Technology 2 has the lowest CO_2 emissions and will be used to set the free emission quota available. Tier 1, Tier 2 and Tier 3 CO_2 emissions were retrieved from Ecoinvent-V1.3 (2006).

In the economic formulation it is considered that CO_2 emissions credits are bought at the end of each year in order to cope with CO_2 emissions that exceed the maximum allowed considered using the BAT. The trading cost and price of emission rights is considered as US$23 which is a proxy of the values currently found in the trading market.

It is noteworthy that the optimal SC configuration considering the emissions trading scheme remains equal to the one obtained when optimizing NPV without this consideration (Fig. 8.2(a)) independently of the free emissions cap and the emission right price. Recall that the minimum overall environmental impact is achieved by installing butane based technologies, while the most profitable is based on benzene as feedstock. The CO_2 emission allocation along the SC is depicted in Fig. 8.7 for the maximum NPV, minimum overall impact, and minimum CO_2 emissions network configurations, optimized taking into account the CO_2 trading scheme. The least CO_2 pollutant configuration is based on benzene technology. It can be observed from this figure that the optimal overall impact configuration (butane based) is the one that emits more CO_2, most of it coming from the MA production. Under the trading scheme this configuration would be strongly penalized. As aforementioned, it was expected that regulatory pressures would lead to a conversion of benzene- to butane-based plants since benzene is considered to be more environmental harmful. Actually, benzene based SCs show greater overall impact (see Table 8.7), being human health their more impacting damage category due to benzene's carcinogenicity. However, a CO_2 trading emission scheme as the one modeled in the case study will not cause benzene based production to move towards butane; on the contrary, it can be a factor leading to change butane based into benzene based MA production.

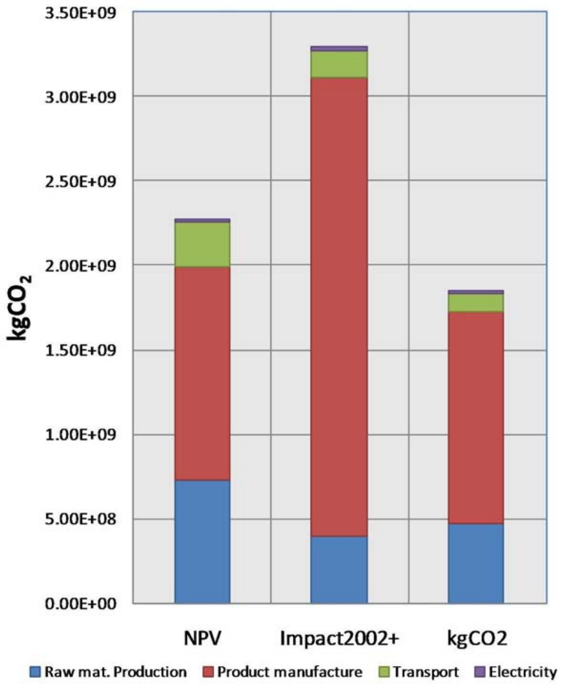


Figure 8.7: CO_2 emissions allocation along the maximum NPV configuration, minimum overall impact configuration, and minimum CO_2 emissions configuration

8.6 Final considerations

In this chapter, an approach for designing environmental friendly and profitable SC has been presented. The model consisted of a multi-period MILP that accounts for the multi-objective optimization of economics and environmental interventions. The model considered the long-term strategic decisions (e.g. installation of plants, selection of suppliers, manufacturing sites, distribution centers) with the mid-term planning for SCs. Each end-point damage categories was considered as objective function in order to avoid the subjectivity associated to their aggregation into an overall environmental impact indicator, showing the various SC possibilities obtained for each indicator. The Impact2002+ metric was adopted as a measure of overall environmental impact. Moreover, joint consideration of end point damages and trading schemes enables the proposed approach to support (i) assessment of current regulatory policies and (ii) definition of more adequate policy parameters (e.g. free emissions allowance cap for each industry, emissions trading price).

A maleic anhydride SC case study is presented where two potential technologies are available. Two problems were solved, a first approach that did not consider CO_2 trading scheme and a second one (see. subsection 8.5.1), that took it into account. It has been shown the possibility of tackling such problem with ease. A SC for MA production based on butane was found to be more environmentally friendly than one based on benzene. In this sense the current model allowed for possible selection between obtained optimal solutions. Most of works related to SC and environmental issues consider a fixed production/demand, it was demonstrated that such constraint leads to dominated solutions. By allowing unsatisfied demand, the actual Pareto curve was obtained.

Raw material production was found to be the most important contributor to overall environmental impact, while transportation and electricity consumption were the least important, this clearly shows that the current model allows for selection of improvement actions. It was found that the production process was the activity that emits most of CO_2.

It turns out that the CO_2 trading scheme will favor benzene based over butane based production. The results obtained for this specific case study question the suitability of a CO_2 trading scheme applicability to every industry sector: different regulatory schemes may be required in different industrial scenarios. Current regulations merely consider climate change damage which certainly is a very important factor but other aspects such as human health, ecosystem quality and abiotic resources usage should be also considered so that effective industrial changes regarding the environment are induced. In this sense the utilization of multiobjective optimization for each damage category shows to be helpful at discovering insights regarding how different policies will affect SC strategic and tactical decisions. One of the main achievements of this chapter is not building and solving a complex SC-environmental model, instead it is to emphasize the dangers related to deploying CO_2 emission related policies in isolation from other pollution related issues.

On the other hand, it is important to point out that environmental metrics for the interpretation of life cycle inventories involve determining aggregated measures. Usually, normalizing factors are used to determine the weight of each damage factor (climate change, human health, resources depletion, ecosystem quality) in the overall measure which may favor different solutions. When this type of analysis is performed for the selection among different design alternatives, which will be active during a long time horizon, a careful sensitivity/uncertainty analysis related to the application of these normalizing factors is required. Such analysis can be done by using a multi-criteria optimization that accounts for end-point damage categories as presented in this chapter.

8.7 Nomenclature

Indices

e	suppliers
f, f'	facility locations

i	tasks
j	equipment technology
t, t'	planning periods
a	mid point environmental impact categories
g	end point environmental impact categories

Sets

A_g	set of midpoint environmental interventions that are combined into endpoint damage factors g
I_j	set of tasks i that can be performed in technology j
$\tilde{J}_f$	technology j that can be installed at location f
J_i	technologies that can perform task i
T_L	set of periods when the emissions trading is executed
Tr	set of distribution tasks

Parameters

$Cost_t^{co_2}$	emissions right cost in period t
$distance_{ff'}$	distance from location f to locationf'
$MaxCO_{2t}$	free allowance emissions cap at period t
$NormF_g$	normalizing factor of damage category g
$Price_t^{co_2}$	emissions right price in period t
$rate$	discount rate

Greek symbols

ζ_{ag}	g end-point damage characterization factor for environmental intervention a
$\psi_{ijff'a}$	a environmental category impact CF for task i performed using technology j receiving materials from node f and delivering it at node f'
ψ_{ija}^T	a environmental category impact CF for the transportation of a mass unit of material over a length unit

Continuous Variables

$Buy_t^{co_2}$	amount of emissions extra rights bought in period t
$DamC_{gft}$	normalized endpoint damage g for location f in period t
$DamC_g^{SC}$	normalized endpoint damage g along the whole SC
$EPurch_{et}$	economic value of purchases executed in period t to supplier e
$ESales_t$	economic value of sales executed in period t
$FAsset_t$	investment on fixed assets in period t
$FCost_t$	fixed cost in period t
IC_{aft}	midpoint a environmental impact associated to site f which rises from activities in period t
$Impact_f^{2002}$	total environmental impact for site f
$Impact_{overall}^{2002}$	total environmental impact for the whole SC
$Net_t^{co_2}$	Net income due to emissions trading in period t
NPV	net present value
$P_{ijff't}$	activity magnitude of task i in equipment j in period t whose origin is location f and destination location f'

$Profit_t$	profit achieved in period t
$Sales_t^{co_2}$	amount of emissions rights sold in period t

Part IV

Treatment of Uncertainty

Chapter 9

Capturing Dynamics in Integrated SCM

9.1 Introduction

A major challenge for an enterprise to stay competitive in today's highly competitive market environment is to be able of capturing and handling the dynamics of its entire SC. This chapter incorporates uncertainty and process dynamics into enterprise wide models which also contemplate cross-functional decisions. The SC integrated solution developed includes a design-planning and a financial formulations. A model predictive control (MPC) methodology is proposed which comprises a stochastic optimization approach. A scenario based multi-stage stochastic mixed integer linear programming model is employed to address the problem. The novel control framework introduced constitutes a step-forward in closing the loop for the dynamic SC management and a supporting platform for the supervisory module handling the incidences that may arise in the SC. The potential of this approach is highlighted through a case study, where the results of the deterministic MPC and the joint control framework are compared. It is emphasized the significance of merging uncertainty treatment and control strategies to improve the SC performance.

9.2 Managing dynamics in integrated SCs

Today, for competitive customer service to be maintained the market requires environmentally friendly products, a good portfolio mix, rapid development of new products, high quality and reliability, after-sales services, etc. Furthermore, SC managers need to consider the dynamics of a rapidly changing market environment, such as variability in demand, cancellations and returns, as well as the dynamics of internal SC operations, such as processing times, production capacity pitfalls and the availability of materials. These operational SC risks and disruptions can have severe long-term effects on a firm's financial performance. An empirical analysis of the effect of SC disruptions on stock prices carried out by Hendricks and Singhal (2005) shows that companies experience 33% to 40% lower stock returns and 13.5% higher share price volatility as a result of this sort of problem.

Evidently, market dynamics and uncertainty and internal business operations make it difficult to synchronize the activities of all SC echelons; this causes significant deviation from previous objectives and plans. Therefore, for a SC to be managed efficiently it is important to systematically review variability and to take it explicitly into account in planning. These actions ensure a flexible response to changes in the business environment, increase the accuracy of decisions and improve business performance. For these reasons, research is called for into the characterization of dynamics in SCs and the application of control methodologies to improve the responsiveness of SCs (Grossmann, 2004).

In the literature, a control-oriented decision framework has been proposed for the review process. Specifically, model predictive control (MPC) is presented as a way of managing SCs in the presence of uncertainty. MPC incorporates the most recent information on the external market and internal business into the planning process. Such a framework is commonly based on deterministic predictive models. However, predictions based on deterministic models may be sub-optimal or even infeasible when a real scenario unfolds. Examples following this approach are the works of Bose and Pekny (2000); Perea-López *et al.* (2003); Perea-López *et al.* (2001); Seferlis and Giannelos (2004); and Mestan *et al.* (2006). These works have been already described in Section 2.3.3. MPC has been widely used to study the interaction among SC components by analyzing different coordination structures (i.e., centralized, semi-centralized, and decentralized SCs).

With regard to decentralized SCs, distributed/modular modeling and decision making are becoming an appealing manner to approach SC problems. This sort of analysis arises naturally because it usually corresponds to the way business systems work, and optimization methods based on distributed modeling are flexible and easy to maintain as well. A significant inconvenience of the distributed approach is that optimality cannot be guarantee in all cases. However, advances have been made in this direction by Ydstie (2004). He demonstrates that modular approach is optimal when the decisions are made in order to minimize total cost. He shows that stable and stationery solutions can be obtained for an enterprise network with fixed boundary conditions and decentralized policies. The network must satisfy that any flow of goods and services induce cost. The solution consists in the optimal values for inventories of assets and liabilities.

Another well-known approach that is presented as a robust manner of making decisions under uncertainty is to solve the planning problem using stochastic optimization (Gupta & Maranas, 2000; Tsiakis *et al.*, 2001; Ierapetritou &

Pistikopoulos, 1996; Bonfill, Espuña, & Puigjaner, 2005). A solution with the maximum expected performance is obtained by including estimated scenarios in the formulation; these estimated scenarios are generated by representing uncertain parameters as random variables (see Section 3.7).

Very recently, an ambitious platform has been built that considers an open, modular, integrated solution offering real-time supply chain optimization capabilities that are multi-objective (financial and environmental aspects are incorporated into the objective function). The technology involved uses a network of cooperative and auto-associative software agents (smart agents) that constitute a decision support system for managing the whole supply chain in a real-time environment (Puigjaner & Espuña, 2006; Puigjaner & Guillén-Gosálbez, 2007). However, incorporating low-level decisions (local scheduling, supervisory control and diagnosis, incidence handling) and the implications of incorporating these decisions for the dynamics of the entire SC (production switching between plants, dynamic product portfolios) have not yet been studied.

This chapter focuses on the strategic–tactical decision making level of the SCM problem. The (strategic) SC design problem involves identifying the combination of suppliers, producers and distributors that provides the right mix and quantity of products and services to customers in an efficient way (Talluri & Baker, 2002). (Tactical) SC planning considers a given configuration over the short to medium term, and seeks to identify how best to use the production, distribution and storage resources in the chain to respond to orders and demand forecasts in an economically efficient way (Shah, 2005).

This chapter starts from the general framework for the SC design and planning presented in Chapter 4. Recall that such a framework is based on the development of a holistic model that covers two areas of the company: process operations and finances. The model explicitly considers shareholder value as a design objective. The corporate value (CV) of the firm is calculated by means of the discounted-free-cash-flow (DFCF) method and is adopted as the objective to be maximized.

A major disadvantage of discounted cash flow methods is that they do not account for the managerial flexibility needed to be able to alter the course of an investment over time as uncertain factors unfold. Real options analysis has been proposed as an alternative valuation approach that would overcome this drawback. Traditionally, discounted cash flow methods assume a single decision pathway with fixed outcomes. In contrast, the real options approach considers multiple decision pathways as a consequence of management flexibility; thus, mid-course strategies can be corrected to deal with future uncertainty Mun (2005). Monte Carlo sampling has been coupled with real options modeling to account for different uncertain scenarios. From another standpoint, stochastic optimization models assume that decision-makers take some actions in a first stage, after which a random event occurs and affects the outcome of those first-stage decisions. Recourse decisions can then be made in the following stages to compensate for any negative effects that might have occurred as a result of the first-stage decisions. Multistage stochastic optimization models and real op-

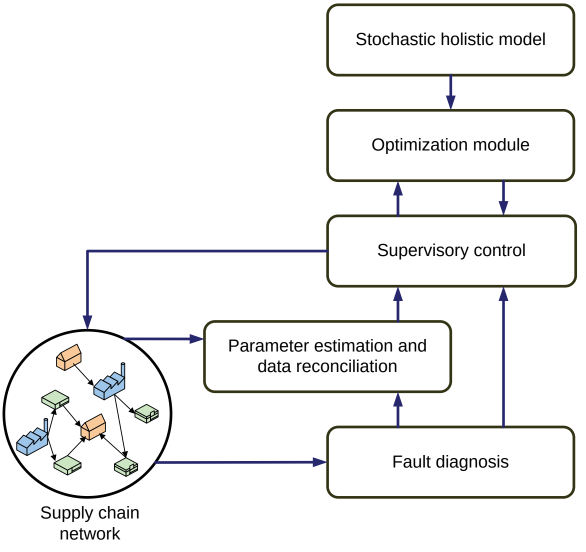


Figure 9.1: Closing the information loop for dynamic SCM.

tions analysis show significant similarities. In fact, the stochastic optimization solution consists of a map in which different decisions are proposed, depending on the scenario that arises. Consequently, a stochastic optimization model that is formulated by extending the deterministic MILP proposed in Chapter 4 will render a stochastic DFCF model with the same features as real options approaches. Furthermore, a stochastic DFCF model offers more realistic solutions, since it considers the so-called non-anticipativity conditions, whereas real options approaches typically disregard these conditions. For this reason, real options lead to "wait-and-see" solutions (i.e., complete knowledge of information is assumed during the decision-making process).

Hence, the aforementioned enterprise-wide model is extended to a stochastic program that takes demand, price and interest rates uncertainties into account. To tackle the resulting problem, scenario-based multi-stage stochastic mixed integer modeling techniques are applied. Then, the stochastic model is introduced into a model predictive controller to capture the dynamics of SC processes and their environment. The ensuing model can be used as a support tool for strategic cross-functional decision making in cases of decision under uncertainty, operational risk and disruption. This novel control framework may be a step forward in closing the loop for dynamic SCM (Fig. 9.1). This framework could take the form of a platform that is used to develop a supervisory module capable of managing the incidents that arise in the SC. Thus, visibility is broadened and the search for actions to resolve the incidents is performed at the SC level and not merely at the plant level. The main advantages of this approach are highlighted in a case study in which this strategy is compared with traditional approaches. Numerical results show that significant benefits

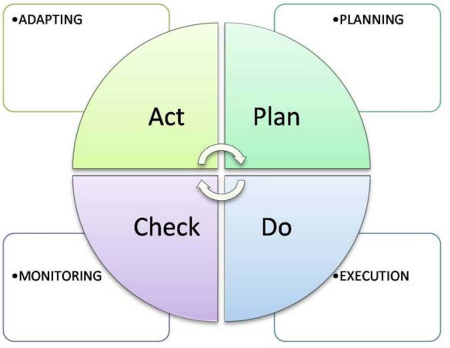


Figure 9.2: Continuous planning process.

can be obtained if an integrated stochastic formulation that accounts for the optimization of a suitable financial performance indicator is applied in an MPC framework.

9.3 Problem statement

Planning is a continuous procedure, not a one-time event. One of the cardinal factors that differentiate best-in-class companies from their competitors is their ability to create a closed-loop planning process to improve their goals. In order to continuously improve the planning process, managers should adopt a quality management philosophy that emphasizes the need for a monitoring phase so that future plans can be adapted to improve response to changes in the business environment, as shown in Figure 9.2. It has been pointed out that PSE professionals should recognize the feedback loop (monitoring) and understand how it provides adaptability, stability, and robustness properties that planning alone (static) cannot provide (Ydstie, 2004).

Here, it is suggested using MPC, a control strategy based on the explicit use of a process model to predict the process output (performance) over a long period of time (Camacho & Bordons, 1995). The model attempts to predict the control variables for a set of time periods. Predicted control variables depend on disturbance forecasts (i.e. demand, prices, and interest rates) and also on a set of given parameters that are known in the control literature as control inputs. The MPC algorithm attempts to optimize a performance criterion that is a function of the future control variables. By solving the optimizing problem all elements of the control signal are defined. However, only a portion of the control signal is applied to the system. Next, as new control input information and disturbance forecasts are collected, the whole procedure is repeated, which produces a feed-forward effect and enables the system to counteract the environment dynamics. The abovementioned facts show that an MPC strategy can be used as a suitable support tool for continuously improving SC planning.

It is worth mentioning that SC problems arising from different hierarchical levels can be addressed by using an MPC approach. Although these types of problems bring distinct time scales into play, MPC can deal with problems comprising different decision levels as long as an integrated predictive model is incorporated in the control algorithm. In this chapter, strategic and planning decisions related to network design are tackled simultaneously. As the case study shows, proactive decisions on opening and closing facilities and enlarging equipment capacity are considered. Also, reaction to incidences such as production allocation decisions when equipment breakdown occurs are taken into consideration.

In this work, the predictive model incorporated into the control algorithm is a multistage stochastic MILP. The predictive model consists in a multi-period design/planning model of a multi-echelon SC with financial considerations. The model assumes that various pieces of technological equipment are available to be installed in potential plant sites and assists in their selection. The model allows for the expansion of plant equipment capacities, not only in the first planning period but also during any other period in which managers believe there are opportunities for investing in facilities. Furthermore, the DFCF method is used in order to calculate the corporate value. The problem can be stated as follows.

The next data is assumed to be known in advance:

Process operations data

- A fixed time horizon;
- A set of products;
- A set of markets in which products are available to customers and their demand scenarios;
- A set of potential geographical sites for locating manufacturing plants and distribution centers;
- A set of potential equipment for manufacturing the different products;
- Lower and upper bounds for the capacity increment of equipment and distribution centers;
- Product recipes (mass balance coefficients and consumption of capacity);
- The suppliers limitations;
- The minimum utilization rate of capacity.

Financial data

- Direct cost parameters such as production, handling, transportation and raw material costs;
- Price scenarios for every product in each market during the time horizon;
- Coefficients for investment and sales of marketable securities;
- The relationship between capital investment and plants and distribution centers capacity;
- The relationship between indirect expenses and plants' and distribution centers' equipment capacity;
- Pledging costs;
- The tax rate and the number of depreciation time intervals;

- The interest rate on long and short-term debt;
- The salvage value;
- Shareholder risk premium data.

The goal is to determine:

- The facilities to be opened;
- The increase on plants' and distribution centers' equipment capacity in each time period;
- The assignment of manufacturing and distribution tasks to the network nodes;
- The amount of final products to be sold;
- Investments and sales of marketable securities;
- The amount of pledged receivables in each period;
- The schedule of payments to suppliers in each time period,
- The long and short term-debt acquired and repaid in each time period,

such that corporate value to be evaluated at the end of the planning horizon is maximized.

The product demands are assumed to be satisfied at the end of each period of time by means of the planning horizon. The demand and prices associated with each of these periods are regarded as random parameters and their uncertainty is represented by a set of scenarios with a given probability of occurrence. The scenario-based approach attempts to capture uncertainty by representing it in terms of a moderate number of discrete realizations of random quantities. In Section 9.5 a methodology for generating discrete scenarios is proposed. Because a network design/planning problem that is typically solved every two to five years is being addressed, the design decisions are made before the uncertain factors are unveiled. However, the operating decisions related to production and transportation flows will be recourse decisions, so they will depend on which scenario materializes.

9.4 The predictive model: a multistage stochastic approach

The stochastic SC design – planning model is presented next. This section has been divided in two parts: (i) the scenario tree representation of uncertainty and (ii) the corresponding deterministic equivalent model.

9.4.1 Scenario tree

Assume that there are $|L|$ events in which uncertainty (ξ) unfolds over the planning horizon. The value that random factors can take in event l can be identified by index h_l which belongs to set H_l. The information regarding the uncertain parameters can be represented by using a scenario tree. Figure 9.3

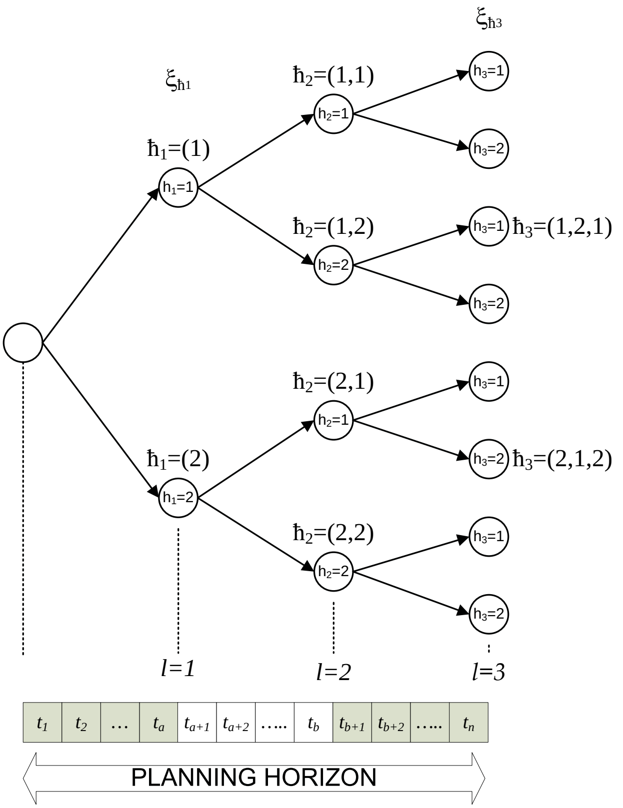


Figure 9.3: Scenario tree

shows a scenario tree in which two realizations of the uncertain parameters are considered at each of three distinct events ($|L| = 3 \wedge |H_l| = 2$).

The nodes at level l are associated to a $\hbar_l$ combination of events identified by $(h_1, h_2, \ldots, h_l)$ with $h_1 \in H_1, h_2 \in H_2, \ldots, h_l \in H_l$. Namely, $\eth_l$ is defined to be the set of l-tuples, given by $\eth_l = \{[\hbar_l = (h_1, h_2, \ldots, h_l)] | h_1 \in H_1, h_2 \in H_2, \ldots, h_l \in H_l\}$. For instance, $\eth_2 = \{(1,1), (1,2), (2,1), (2,2)\}$ corresponds to the events related to nodes at level 2 of the scenario tree. Thus, the eight scenarios ($\prod_l |H_l|$) resulting from the tree in Fig. 9.3 are related to $\eth_3$. Note that each combination of events $\hbar_l$ at level l has a single *ancestor* combination of events $\hbar_{l^*}$ at each previous level l^* which obviously accomplishes $\hbar_{l^*} \subset \hbar_l$ (i.e., from Fig. 9.3 $\{\hbar_1 = (2)\} \subset \{\hbar_2 = (2,1)\} \subset \{\hbar_3 = (2,1,2)\}$).

Additionally, it will be useful for modeling purposes to define sets T_l, L_t and $AH_{l^*\hbar_l}$. T_l is the subset of planning periods t that are associated to event l. For example, $T_1 = [t_1, t_a]$ and $T_2 = [t_{a+1}, t_b]$ in the scenario tree shown in Fig. 9.3. L_t is the reciprocal set of T_l. L_t is the event l which is related to period t. Here, $AH_{l^*\hbar_l}$ is defined to be given by $AH_{l^*\hbar_l} = \{\hbar_{l^*} | \hbar_{l^*} \subseteq \hbar_l\}$, that is $AH_{l^*\hbar_l}$ denotes the event combination related to l^* ($\hbar_{l^*}$) which is ancestor

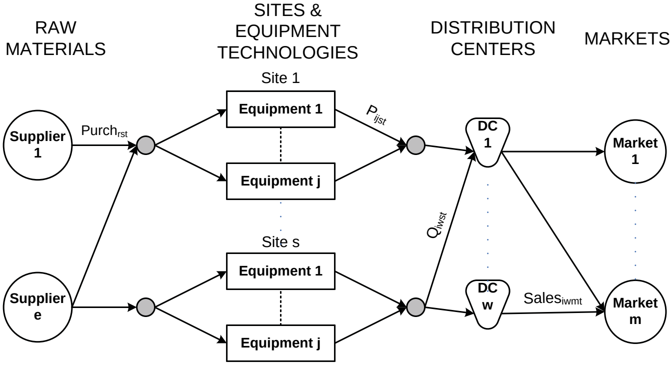


Figure 9.4: Supply chain model structure

of $\hbar_l$. As it can be observed, it is not necessary $\hbar_{l^*}$ to be a proper subset of $\hbar_l$ in order to allow the case when $l = l^*$.

9.4.2 MILP model

Next, the SC network design & planning is formulated as an $(|L| + 1)$-stage stochastic MILP, where |L| denotes the number of events that unfold throughout the planning horizon. The structure of the SC taken as reference to develop the mathematical model is illustrated in Figure 9.4. The model is the stochastic extension of the one presented in Chapter 4. The reader is referred to the aforementioned chapter for the detailed problem formulation, but for completeness and understanding, a brief description is provided here.

The information regarding the scenario tree is introduced into the model by adding two indexes to the variables: l and $\hbar_l$. As an example, variable $Y^{l^*}_{t\hbar_l}$ is associated to a decision that is made when solely the combination of events $\hbar_l$ is known, however the decision will be materialized at period t when event l^* unveils. A subscript $\hbar_l$ below a variable also indicates that is a $(l + 1)$-stage variable. For instance, a $(l + 1)$-stage variable such as $Y^l_{\hbar_l}$ would be related to a recourse decision while $Y^l_{\hbar_{l-1}}$ would be a l-stage variable related to a decision made before event l was disclosed.

In order to follow the structure of the scenario tree, when an equation requires variables associated to previous periods (i.e., $t - 1$), these variables must be related to a combination of events that is ancestor of the combination of events being evaluated by the equation ($l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}$) so as to guarantee the non-anticipativity principle. This fact will be recalled in most of the equations presented next.

The variables and constraints of the model can be classified into four groups. Process operations constraints given by the SC topology belong to the first group. The second one incorporates those constraints related to the integration of operations and finances. To the third and fourth groups pertain the constraints required for allowing cash management and evaluating the objective function (CV), respectively.

Process operations: design – planning formulation

Mass balances must be satisfied in each of the nodes that integrate the SC network. Eq. (9.1) represents the raw material balance for each manufacturing site s in every time period t and every combination of events $\hbar_l$. In this equation is just taken into account the stock of previous period ($SI^{l^*}_{rst-1\hbar_{l^*}}$) related to the combination of events that is ancestor of $\hbar_l$ ($l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}$). The mass balance for final products i in each manufacturing site s is enforced via Eq. (9.2). Eq. (9.3) expresses the mass balance for the distribution centers w. Eq. (9.4) forces the sales of product i carried out in market m during time period t to be less than or equal to the demand. Equation (9.5) imposes a minimum target for the demand satisfaction ($MinCLS$), which must be attained in all time periods t and event combinations $\hbar_l$.

$$\sum_{e \in E_r} Purch^l_{erst\hbar_l} + SI^{l^*}_{rst-1\hbar_{l^*}} = SI^l_{rst\hbar_l} + \sum_j \sum_{i \in (I_j \cap I_r)} \alpha_{rij} P^l_{ijst\hbar_l}$$
$$\forall\ r, s, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \tag{9.1}$$

$$\sum_{j \in J_i} P^l_{ijst\hbar_l} + SO^{l^*}_{ist-1\hbar_{l^*}} = SO^l_{ist\hbar_l} + \sum_w Q^l_{iwst\hbar_l}$$
$$\forall\ i, s, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \tag{9.2}$$

$$\sum_s Q^l_{iwst\hbar_l} + SW^{l^*}_{iwt-1\hbar_{l^*}} = SW^l_{iwt\hbar_l} + \sum_m Sales^l_{iwmt\hbar_l}$$
$$\forall\ i, w, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \tag{9.3}$$

$$\sum_w Sales^l_{iwmt\hbar_l} \leq Dem^l_{imt\hbar_l} \qquad \forall\ i, m, l, \hbar_l, t \in T_l \tag{9.4}$$

$$\frac{\sum_i \sum_w \sum_m Sales^l_{iwmt\hbar_l}}{\sum_i \sum_m Dem^l_{imt\hbar_l}} \geq MinCLS \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.5}$$

The capacity and facilities location constraints are following. Two different variables are defined, $FS^l_{jst\hbar_{l-1}}$ and $FWs^l_{wt\hbar_{l-1}}$, which represent the total capacity of equipment j in manufacturing sites s and distribution centres w respectively during time period t. Moreover, variables $FSE^l_{jst\hbar_{l-1}}$ and $FWE^l_{wt\hbar_{l-1}}$ denote the capacity expansion of the different network facilities during time period t. Eqns. (9.6) and (9.7) are added to control the changes in facilities capacity over time. Eqns. (9.8) and (9.9) are included to update the total capacity by the amount increased during planning period t.

$$V^{l}_{jst\hbar_{l-1}} FSE^{L}_{jst} \leq FSE^{l}_{jst\hbar_{l-1}} \leq V^{l}_{jst\hbar_{l-1}} FSE^{U}_{jst} \qquad \forall\ j,s,l,\hbar_{l-1},t \in T_l \tag{9.6}$$

$$X^{l}_{wt\hbar_{l-1}} FWE^{L}_{wt} \leq FWE^{l}_{wt\hbar_{l-1}} \leq X^{l}_{wt\hbar_{l-1}} FWE^{U}_{wt} \qquad \forall\ w,l,\hbar_{l-1},t \in T_l \tag{9.7}$$

$$FS^{l}_{jst\hbar_{l-1}} = FS^{l^*}_{jst-1\hbar_{l^*-1}} + FSE^{l}_{jst\hbar_{l-1}} \qquad \forall\ j,s,l,\hbar_{l-1},t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*-1} \in AH_{l^*-1,\hbar_{l-1}} \tag{9.8}$$

$$FW^{l}_{wt\hbar_{l-1}} = FW^{l^*}_{wt-1\hbar_{l^*-1}} + FWE^{l}_{wt\hbar_{l-1}} \qquad \forall\ w,l,\hbar_{l-1},t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*-1} \in AH_{l^*-1,\hbar_{l-1}} \tag{9.9}$$

Eqns. (9.10) and (9.11) are to calculate the planning period t when a facility (s or w) initiates its operations. SB_{st} and SW_{wt} are binary variables that take the value of 1 if the facility starts operating at period t and 0 otherwise. Thus, if the binary variable that represents the increment in the capacity of any facility in period t equals one, the summation of the new binary variable from the initial period to the current one must also equal one. Eqns. (9.10) and (9.11) are the reformulation of the previous logic condition.

$$1 - V^{l}_{jst\hbar_{l-1}} + \sum_{t'=1}^{t} \sum_{l^* \in L^*_{t'}} \sum_{h_{l^*-1} \in AH_{l^*-1,\hbar_{l-1}}} SB^{l^*}_{st'\hbar_{l^*-1}} \geq 1 \qquad \forall\ j,s,l,\hbar_{l-1},t \in T_l \tag{9.10}$$

$$1 - X^{l}_{wt\hbar_{l-1}} + \sum_{t'=1}^{t} \sum_{l^* \in L^*_{t'}} \sum_{h_{l^*-1} \in AH_{l^*-1,\hbar_{l-1}}} SW^{l^*}_{wt'\hbar_{l^*-1}} \geq 1 \qquad \forall\ w,l,\hbar_{l-1},t \in T_l \tag{9.11}$$

Eq. (9.12) forces the total production rate in each plant to be greater than a minimum desired production rate and lower than the available capacity. Eq. (9.13) is analogous to Eq. (9.12) for distributions centers w. The model assumes a maximum availability of raw materials as well. Thus, Eq. (9.14) forces the amount of raw material r purchased from supplier e to be lower than an upper bound given by supplier capacity limitations (A_{ert}). In this expression, R_e denotes the set of raw materials provided by supplier e.

$$\beta_{sj} FS^l_{jst\hbar_{l-1}} \leq \sum_{i \in I_j} \theta_{ij} P^l_{ijst\hbar_l} \leq FS^l_{jst\hbar_{l-1}} \qquad \forall\ j, s, l, \hbar_l, t \in T_l, \hbar_{l-1} \in AH_{l-1,\hbar_l} \tag{9.12}$$

$$\gamma_w FW^l_{wt\hbar_{l-1}} \leq \sum_i \upsilon_i SW^l_{iwt\hbar_l} \leq FW^l_{wt\hbar_{l-1}} \qquad \forall\ w, l, \hbar_l, t \in T_l, \hbar_{l-1} \in AH_{l-1,\hbar_l} \tag{9.13}$$

$$\sum_s Purch^l_{erst\hbar_l} \leq A_{ert} \qquad \forall\ e, r \in R_e, l, \hbar_l, t \in T_l \tag{9.14}$$

Integration between operations and finances

The integration between both formulations is carried out through the sales of products, the purchases of raw materials, transport services and utilities to final providers, the fixed cost associated with the operation of the network and the total capital investment. Thus, the accounts receivable incurred in any period t and maturing in period t' can be easily computed from the sales of products executed in period t, the fraction of these sales that will be collected in period t' and the prices of the products sold, as it is stated in equation (9.15). Here, $\delta_{mtt'}$ denotes the fraction of sales carried out in market m in period t that will be paid in period t'.

$$ASales^l_{tt'\hbar_l} = \sum_i \sum_w \sum_m Sales^l_{iwmt\hbar_l} \delta_{mtt'} Price^l_{imt\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l, t' > t \tag{9.15}$$

The external purchases from supplier e , which are computed through Eq. (9.16), include the purchases of raw materials and transport and production resources. The external purchases to supplier e ($EPurch_{et}$) can be then computed through Eq. (9.17). On the other hand, the external purchases of transport services and production utilities are determined through equations (9.18) and (9.19).

$$EPurch^l_{et\hbar_l} = Purch^{rm,l}_{et\hbar_l} + Purch^{tr,l}_{et\hbar_l} + Purch^{prod,l}_{et\hbar_l} \qquad \forall\ e, l, \hbar_l, t \in T_l \tag{9.16}$$

$$Purch^{rm,l}_{et\hbar_l} = \sum_r \sum_s Purch^l_{erst\hbar_l} \psi_{ert} \qquad \forall\ e, l, \hbar_l, t \in T_l \tag{9.17}$$

$$Purch^{tr,l}_{et\hbar_l} = \sum_i \sum_j \sum_s Q^l_{iwst\hbar_l} \rho^{tr1}_{eiws} + \sum_i \sum_w \sum_m Sales^l_{iwmt\hbar_l} \rho^{tr2}_{eiwm} \qquad \forall\ e, l, \hbar_l, t \in T_l \tag{9.18}$$

$$Purch^{prod,l}_{et\hbar_l} = \sum_i \sum_j \sum_{ijs} P^l_{ijst\hbar_l} \tau^{ut1}_{ijse} + \sum_r \sum_s SI^l_{rst\hbar_l} \tau^{ut2}_{rse} + \sum_i \sum_s SO^l_{ist\hbar_l} \tau^{ut3}_{ise} + \sum_i \sum_w SW^l_{iwt\hbar_l} \tau^{ut4}_{iwe} \qquad \forall\ e, l, \hbar_l, t \in T_l \tag{9.19}$$

The total fixed cost of operating a given SC structure can be computed by means of equation (9.20). Finally, the total investment in capital or fixed assets is computed through equation (9.21).

$$FCost^l_{t\hbar_{l-1}} = \sum_j \sum_s FCFS_{jst} FS^l_{jst\hbar_{l-1}} + \sum_w FCFW_{wt} FW^l_{wt\hbar_{l-1}} \qquad \forall\ l, \hbar_{l-1}, t \in T_l \tag{9.20}$$

$$FAsset^l_{t\hbar_l} = \sum_s \left(\sum_j Price^{FS}_{jst} FSE^{l^*}_{jst+1\hbar_{l^*-1}} + I^S_{st} SB^{l^*}_{st+1\hbar_{l^*-1}} \right) + \sum_w \left(Price^{FW}_{wt} FWE^{l^*}_{wt+1\hbar_{l^*-1}} + I^W_{wt} SW^{l^*}_{wt+1\hbar_{l^*-1}} \right) \qquad \forall\ l, \hbar_l, t \in T_l, l^* \in L_{t+1}, \hbar_{l^*-1} \in DH_{l^*-1,\hbar_l} \tag{9.21}$$

Financial formulation: cash management

As a result of the application of a stochastic finances-operations integrated model, optimal SC management and financial decisions under uncertainty should be computed simultaneously to accomplish the goal of enhancing the shareholder value under the current business circumstances. Therefore, payments to providers, short and long term borrowing, pledging decisions and the buying/selling of securities are planned in conjunction with operational decisions (SC configuration, distribution and processing tasks). The financial side of the problem is then incorporated by including the set of constraints presented next.

The cash management model also considers the same t planning periods covering the whole time horizon in the strategic SC formulation. This assumption allows an easy integration of both sets of constraints into a unique holistic model.

The cash balance for each planning period and combination of events is calculated by means of Eq. (9.22).

$$
\begin{aligned}
Cash^{l}_{t\hbar_l} &= Cash^{l^*}_{t-1\hbar_{l^*}} + ECash^{l}_{t\hbar_l} + Net^{CLine,l}_{t\hbar_l} - \sum_{e}\sum_{t'=1}^{t} Pay^{l}_{et't\hbar_l} \\
&- FCost^{l}_{t\hbar_{l-1}} + Net^{MS,l}_{t\hbar_l} - FAsset^{l}_{t\hbar_l} + Capital^{l}_{t\hbar_l} + Net^{LDebt,l}_{t\hbar_l} \\
&+ Other_t \qquad \forall\ t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*-1} \in AH_{l^*-1,\hbar_l}
\end{aligned} \tag{9.22}
$$

The cash at each period t ($Cash^{l}_{t\hbar_l}$) is a function of the available cash at period $t-1(l^*{}_{t-1\hbar_{l^*}})$, the exogenous cash from the sales of products or, in general, from any other inflow of cash ($ECash^{l}_{t\hbar_l}$), the amount borrowed or repaid to the short-term credit line ($Net^{CLine,l}$), the raw materials, production and transport payments on accounts payable incurred in any previous or actual period t ($Pay^{l}_{et't\hbar_l}$), the payments of the fixed cost ($FCost^{l}_{t\hbar_{l-1}}$), the sales and purchases of marketable securities ($Net^{MS,l}_{t\hbar_l}$), the amount invested on facilities ($FAsset^{l}_{t\hbar_l}$), the capital supported by the shareholders of the company ($Capital^{l}_{t\hbar_l}$), the amount borrowed or repaid to the long-term credit line ($Net^{LDebt,l}_{t\hbar_l}$) and finally other expected outflows or inflows of cash ($Other_t$).

A certain proportion of the accounts receivable may be pledged at the beginning of a period. It can be assumed that a certain proportion of the receivables outstanding at the beginning of a period is received during that period through pledge, as stated by Eq. (9.23). In this equation the variable $Pled^{l}_{tt'\hbar_l}$ represents the amount pledged within period t' on accounts receivable maturing in period t, while $ASales^{l}_{t't\hbar_l}$ represents the accounts receivable associated with the sales of products executed in period t' and maturing in t. Here, the parameter d^{max}_{M} denotes the maximum maturing period at the markets (Eq. (9.24)).

$$
\begin{aligned}
&\sum_{t''=t-d^{max}_{M}}^{t'} \sum_{l^* \in L_{t''}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} Pled^{l^*}_{tt''\hbar^*_l} \leq \\
&\sum_{t''=t-d^{max}_{M}}^{t'} \sum_{l^* \in L_{t''}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} ASales^{l^*}_{t''t\hbar_{l^*}} \\
&\qquad \forall\ l, \hbar_l, t \in T_l, t' \in [t-d^{max}_{M}, t]
\end{aligned} \tag{9.23}
$$

$$
d^{max}_{M} = \max_{m} \{d_m\} \tag{9.24}
$$

The exogenous cash is computed by means of Eq. (9.25) as the difference between the amount of accounts receivable maturing in period t and that incurred in previous periods t' minus the amount of receivables pledged in previous periods on accounts receivable maturing in period t plus the amount pledged in the actual period on accounts receivable maturing in future periods. In this expression, $\phi_{t't}$ represents the face value of the receivables being pledged.

$$
\begin{aligned}
ECash^{l}_{t\hbar_l} = & \sum_{t'=t-d^{max}_{M}}^{t} \sum_{l^*\in L_{t'}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} ASales^{l^*}_{t't\hbar_{l^*}} - \\
& \sum_{t'=t-d^{max}_{M}}^{t-1} \sum_{l^*\in L_{t'}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} Pled^{l^*}_{tt'\hbar_{l^*}} + \sum_{t'=t+1}^{t+d^{max}_{M}} \phi_{t't} Pled^{l}_{t't\hbar_l} \\
& \forall\ l, \hbar_l, t \in T_l
\end{aligned}
\tag{9.25}
$$

A short-term financing source is represented by an open line of credit with a maximum limit imposed by the bank (Eq. (9.26)). Eqns. (9.27) and (9.28) make a balance on borrowings, considering for each period the updated debt from the previous periods, the balance between borrows and repayments and the interest of the credit line. Moreover, the bank regularly requires a repayment greater than or equal to the interests accumulated in previous periods, as it is stated by Eq. (9.29).

$$
CLine^{l}_{t\hbar_l} \leq CLine^{max} \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.26}
$$

$$
\begin{aligned}
& CLine^{l}_{t\hbar_l} = CLine^{l^*}_{t-1,\hbar_{l^*}}(1 + ir^{SD,l}_{t\hbar_l}) + Borrow^{l}_{t\hbar_l} - Repay^{l}_{t\hbar_l} \\
& \quad \forall\ l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}
\end{aligned}
\tag{9.27}
$$

$$
Net^{CLine,l}_{t\hbar_l} = Borrow^{l}_{t\hbar_l} - Repay^{l}_{t\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.28}
$$

$$
\begin{aligned}
& Repay^{l}_{t\hbar_l} \geq ir^{SD}_{t\hbar_l} CLine^{l^*}_{t-1,\hbar_{l^*}} \\
& \forall\ l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}
\end{aligned}
\tag{9.29}
$$

With regard to the accounts payable, Eq. (9.30) forces the payments executed in period t' on accounts payable to supplier e incurred in period t to equal the total amount due. The payment constraints belonging to the last periods of time are formulated as inequalities (Eq. (9.31)), as it is not reasonable to require that total accounts payable be zero at the end of the planning period.

$$
\begin{aligned}
& \sum_{t'=t-d_e}^{t} \sum_{l^*\in L_{t'}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} Pay^{l^*}_{ett'\hbar_{l^*}} Coef_{ett'} = \\
& \qquad \sum_{l^*\in L_{t-d_e}} \sum_{\hbar^*_l \in AH_{l^*\hbar_l}} EPurch^{l^*}_{e,t-d_e,\hbar_{l^*}} \\
& \qquad \forall\ e, t \in [d_e, |T|], l \in L_t, \hbar_l
\end{aligned}
\tag{9.30}
$$

$$\sum_{t'=t}^{T} \sum_{l^* \in L_{t'}} \sum_{\hbar_l^* \in AH_{l^* \hbar_L}} Pay_{ett'\hbar_{l^*}}^{l^*} Coef_{ett'} \leq \sum_{l^* \in L_t} \sum_{\hbar_l^* \in AH_{l^* \hbar_L}} EPurch_{et\hbar_{l^*}}^{l^*} \qquad \forall\ e, \hbar_L, t > (|T| - d_e) \tag{9.31}$$

Eq. (9.32) makes a balance for marketable securities. It is assumed that all marketable securities can be sold prior to maturity at a discount or loss for the firm, as stated by Eq. (9.32). Eq. (9.33) is applied to constraint in each period the total amount of marketable securities sold prior to maturity to be lower than the available ones (those belonging to the initial portfolio plus the ones purchased in previous periods minus those sold before).

$$\begin{aligned} Net_{t\hbar_l}^{MS,l} = S_t^{MS} - \sum_{t'=t+1}^{T} Y_{t't\hbar_l}^{MS,l} + \sum_{t'=t+1}^{T} Z_{t't\hbar_l}^{MS,l} + \\ \sum_{t'=1}^{t-1} \sum_{l^* \in L_{t'}} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} \left(1 + D_{tt'}^{MS}\right) Y_{tt'\hbar_{l^*}}^{MS,l^*} \\ - \sum_{t'=1}^{t-1} \sum_{l^* \in L_{t'}} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} \left(1 + E_{tt'}^{MS}\right) Z_{tt'\hbar_{l^*}}^{MS,l^*} \qquad \forall\ l, \hbar_l, t \in T_l \end{aligned} \tag{9.32}$$

$$\begin{aligned} \sum_{t''=1}^{t'} \sum_{l^* \in L_{t''}} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} Z_{tt''\hbar_{l^*}}^{MS,l^*} \left(1 + E_{tt''}^{MS}\right) \leq S_t^{MS} + \\ \sum_{t''=1}^{t'-1} \sum_{l^* \in L_{t''}} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} \left(1 + D_{tt''}^{MS}\right) Y_{tt''\hbar_{l^*}}^{MS,l^*} \qquad \forall\ l, \hbar_l, t \in T_l, t' < t \end{aligned} \tag{9.33}$$

Eq. (9.34) balances the investment with the capital supported by shareholders ($Capital_{t\hbar_l}^l$) and the amount borrowed to banks as long term debt ($LBorrow_{t\hbar_l}^l$) at each time period t and combination of events $\hbar_l$.

$$FAsset_{t\hbar_l}^l = LBorrow_{t\hbar_l}^l + Capital_{t\hbar_l}^l \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.34}$$

Eqns. (9.35) to (9.37) reflect the payment conditions associated with the long term debt. These constraints are similar to those associated with the short term credit line, but the amount repaid in each period of time $LRepay_{t\hbar_l}^l$ remains usually constant in every planning period.

$$\begin{aligned} LDebt_{t\hbar_l}^l = LDebt_{t-1\hbar_l^*}^{l^*} (1 + ir_{t\hbar_l}^{LD,l}) + LBorrow_{t\hbar_l}^l - LRepay_{t\hbar_l}^l \\ \forall\ l, \hbar_l, t \in T_l, l^* \in L_{t-1}^*, \hbar_{l^*} \in AH_{l^* \hbar_l} \end{aligned} \tag{9.35}$$

$$Net^{LDebt,l}_{t\hbar_l} = LBorrow^{l}_{t\hbar_l} - LRepay^{l}_{t\hbar} \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.36}$$

$$\begin{gathered} LRepay^{l}_{t\hbar_l} \geq ir^{LD,l}_{t\hbar_l}\, LDebt^{l^*}_{t-1\hbar_{l^*}} \\ \forall\ l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \end{gathered} \tag{9.37}$$

Eq. (9.38) limits the cash in each period ($Cash^{l}_{t\hbar}$) to be larger than a minimum value ($MinCash$). A minimum cash is usually required to handle uncertain events.

$$Cash^{l}_{t\hbar_l} \geq MinCash \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.38}$$

Objective function: a stochastic DFCF method

The strategy presented in this paper applies the discounted free cash flow (DFCF) method to assess the decisions undertaken by a firm. The DFCF method calculates the enterprise value by determining the present value of its future cash flows and discounting them taking into account the appropriate capital cost during the time horizon for which it is defined (Grant, 2003).

$$E[CV] = \sum_{\hbar_L} P^{L}_{\hbar_L} CV^{L}_{\hbar_L} \tag{9.39}$$

Eq. (9.39) computes the expected corporate value ($E[CV]$) as the weighted average of the corporate value calculated for each combination of events at the end of the time horizon. Here, $P^{L}_{\hbar_L}$ represents the probability of occurrence of each combination of events.

$$CV^{L}_{\hbar_L} = DFCF^{L}_{\hbar_L} - NetDebt_0 \qquad \forall\ \hbar_L \tag{9.40}$$

$$NetDebt_0 = CLine_0 + LDebt_0 - Cash_0 \tag{9.41}$$

According to financial theory, enterprise market value of a firm is given by the difference between the discounted stream of future cash flows during the planning horizon and the net total debt at the beginning of the time horizon($NetDebt_0$), as it is stated by equation (9.40). The final total debt includes both, the short and the long term debt and also the cash (Eq. (9.41)).

$$\begin{aligned} DFCF^{L}_{T\hbar_L} = & \left(\sum_t \sum_{l \in L_t} \sum_{\hbar_l \in AD_{l\hbar_L}} \frac{FCF^{l}_{t\hbar_l}}{(1 + WACC^{l}_{t\hbar_l})^t} \right) + \\ & \frac{SV^{L}_{\hbar_L}}{(1 + WACC^{L}_{T\hbar_L})^T} \qquad \forall\ \hbar_L \end{aligned} \tag{9.42}$$

In the calculation of the DFCF, one must discount the free cash flows of each period t and the salvage value (SV) at a rate equivalent to the capital cost (Eq. (9.42)). The salvage value could be calculated as a percentage of the total investment or by any other applicable method.

The capital cost can be determined through the weighted average method (Eq. (9.43)). In this expression, λ_t denotes the proportion of equity over the total capital investment. To compute the expected return on equity, which is denoted by $E(ROE)$, it is applied equation (9.44).

$$WACC^l_{t\hbar_l} = \lambda_t E(ROE)^l_{t\hbar_l} + ir^l_{t\hbar_l}(1-\lambda_t)(1-trate) \qquad \forall\ t \tag{9.43}$$

$$E(ROE)^l_{t\hbar_l} = r^{0,l}_{t\hbar_l} + \varphi Re \tag{9.44}$$

Free cash flows at every period t (FCF_t) are given by the profit after taxes, net change in investments and change in net working capital. Specifically, the free cash flows are the difference between the net operating profit after taxes (NOPAT) and the increase in capital invested. From this definition it follows that there will be value creation if the incoming value ($Profit^l_{t\hbar_l}(1-trate)$) is greater than the consumed value ($\Delta NWC^l_{t\hbar_l}$) as shown in equation (9.45). Eq. (9.46) is applied to compute the profit at each period t and combination of events $\hbar_l$.

$$FCF^l_{t\hbar_l} = Profit^l_{t\hbar_l}(1-trate) - NetInvest^l_{t\hbar_l} - \Delta NWC^l_{t\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.45}$$

$$Profit^l_{t\hbar_l} = ESales^l_{t\hbar_l} - \left(\sum_e EPurch^l_{et\hbar_l} + FCost^l_{t\hbar_{l-1}} - \Delta Inv^l_{t\hbar_l} \right) \qquad \forall\ l, \hbar_l, t \in T_l, \hbar_{l-1} \in AH_{l-1,\hbar_l} \tag{9.46}$$

The net investment at each period t represents the monetary value of the fixed assets acquired in that period minus the depreciation. (Eq. 9.47)

$$NetInvest^l_{t\hbar_l} = FAsset^l_{t\hbar_l} - Dep^l_{t\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.47}$$

The change in net working capital associated with period t and combination of events $\hbar_l$ (NWC_t) is computed from the change in accounts receivables, plus the change in inventory, minus the change in accounts payable, plus any other financial expenses or incomes ($FEx^l_{t\hbar_l}$), as stated by equation (9.48).

$$\Delta NWC^l_{t\hbar_l} = \left(\Delta ARec^l_{t\hbar_l} + \Delta Inv^l_{t\hbar_l} - \Delta APay^l_{t\hbar_l} + FEx^l_{t\hbar_l}\right) \qquad \forall\ l, \hbar_l, t \in T_l \tag{9.48}$$

Equation (9.49) computes the accounts receivable corresponding to period t and combination of events $\hbar_l$. Equation (9.50) determines the change in accounts receivable. Eq. (9.51) to (9.52) express the calculation of inventory value and change and inventory, respectively. The accounts payable are determined by equation (9.53). The change in accounts payable is represented by Eq. (9.54). Finally, equation (9.55) computes other financial expenses and incomes ($FEx^l_{t\hbar_l}$) associated with the SC operation.

$$\begin{aligned} ARec^l_{t\hbar_l} = & \sum_{t'=t-d_s^{\max}+1}^{t} \sum_{t''=t+1}^{t'+d_s^{\max}} \sum_{l^*\in L_{t'}} \sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} ASales^{l^*}_{t't''\hbar_{l^*}} \\ & - \sum_{t'=t+1}^{t+d_s^{\max}} \sum_{t''=t'-d_s^{\max}}^{t} \sum_{l^*\in L_{t''}} \sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} Pled^{l^*}_{t't''\hbar_{l^*}} \qquad \forall\, l, \hbar_l, t \in T_l \end{aligned} \tag{9.49}$$

$$\begin{aligned} \Delta ARec^l_{t\hbar_l} = ARec^l_{t\hbar_l} - ARec^{l^*}_{t-1\hbar_l*} \\ \forall\, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \end{aligned} \tag{9.50}$$

$$\begin{aligned} & Inv^l_{t\hbar_l} = \sum_r \sum_s Iu^{RM}_{rt} SI^l_{rst\hbar_l} + \\ & \sum_i Iu^{FP}_{it} \left[\sum_s SO^l_{ist\hbar_l} + \sum_w SW^l_{iwt\hbar_l} \right] \qquad \forall\, l, \hbar_l, t \in T_l \end{aligned} \tag{9.51}$$

$$\begin{aligned} \Delta Inv^l_{t\hbar_l} = Inv^l_{t\hbar_l} - Inv^{l^*}_{t-1\hbar_l*} \\ \forall\, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \end{aligned} \tag{9.52}$$

$$\begin{aligned} & APay_t = \sum_e \sum_{t'=1}^{t} \sum_{l^*\in L_{t'}} \sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} EPurch^{l^*}_{et'\hbar_{l^*}} - \\ & \sum_e \sum_{t''=1}^{t} \sum_{t'=t''}^{t} \sum_{l^*\in L_{t'}} \sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} Coef_{et''t'} Pay^{l^*}_{et''t'\hbar_{l^*}} \qquad \forall\, l, \hbar_l, t \in T_l \end{aligned} \tag{9.53}$$

$$\begin{aligned} \Delta APay^l_{t\hbar_l} = APay^l_{t\hbar_l} - APay^{l^*}_{t-1\hbar_l*} \\ \forall\, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l} \end{aligned} \tag{9.54}$$

$$
\begin{aligned}
FEx^{l}_{t\hbar_l} = & \sum_{t'=t+1}^{t+d_s^{\max}} (1-\phi_{t't}) Pled^{l}_{t't\hbar_l} - \\
& \sum_{e}\sum_{t'=1}^{t} Pay^{l}_{et't\hbar_l}\,(Coef_{et't}-1) + \sum_{t'=1}^{t-1}\sum_{l^*\in L_{t'}}\sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} E^{MS}_{tt'} Z^{MS,l^*}_{tt'\hbar_{l^*}} - \\
& \sum_{t'=1}^{t-1}\sum_{l^*\in L_{t'}}\sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} D^{MS}_{tt'} Y^{MS,l^*}_{tt'\hbar_{l^*}} \qquad \forall l,\hbar_l, t\in T_l
\end{aligned} \tag{9.55}
$$

The stochastic problem can be thus mathematically posed as follows:

$$
\begin{gathered}
\underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\, E[CV] \\
\text{subject to} \\
\text{Eqns. (9.1) to (9.55)} \\
\mathscr{X} \in \{0,1\}; \mathscr{Y} \in \mathbb{R}
\end{gathered}
$$

Here $\mathscr{X}$ denotes the model binary variables set, while $\mathscr{Y}$ represents the model continuous variable set.

9.5 Scenario generation: the forecasting module

Stochastic models assume that probability distributions governing the uncertain factors are known or can be estimated. The aforementioned fact and the computational effort required to obtain solutions are the main drawbacks of this approach. In this section, a methodology based on forecasting techniques which can be utilized for scenario generation is presented.

The parameters that the proposed methodology requires from a forecasting module are the mean forecast ($\overline{\xi_t}$) and the forecast error distribution for each uncertain parameter that is considered in the predictive model.

Future uncertain parameters in period t (ξ_t) can be expressed as depicted in equation (9.56), where the uncertain parameter for scenario $\hbar_l$ ($\xi^{l}_{t\hbar_l}$) is computed as the mean value forecasted for the uncertain parameter at period t ($\overline{\xi_t}$) plus an error estimation ($\epsilon^{l}_{t\hbar_l}$).

$$
\xi^{l}_{t\hbar_l} = \overline{\xi_t} + \epsilon^{l}_{t\hbar_l} \tag{9.56}
$$

The forecast errors distributions depend on previous errors (ϵ_t) and how many periods ahead the forecast is being done. If the correct forecasting model has been chosen, and if the statistical procedure used to estimate parameters in the model yields unbiased estimates, then the expected forecast error will be zero. When the forecasting error (ϵ) is assumed to be normally distributed ($N(0,\epsilon)$), σ_ϵ of the single-period ahead forecasting error can be calculated by

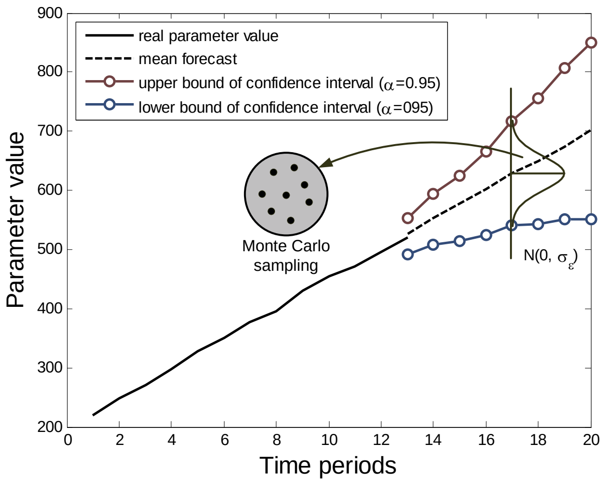


Figure 9.5: Forecasting and Monte Carlo sampling

means of equation (9.57). This approximation holds well even for non-normal errors. For more details about forecast errors estimation please refer to Montgomery, Johnson, and Gardiner (1990).

$$\sigma_{\epsilon_t} \approx 1.25 \left(\frac{\sum_t \epsilon_t}{N} \right) \tag{9.57}$$

Therefore, a Monte Carlo sampling to generate ($\epsilon^{l}_{t\hbar_l}$) assuming that this parameter is governed by a $N(0, \sigma_{\epsilon t})$ probability distribution and equation (9.56) can be utilized to create the scenarios required in stochastic mathematical models, as shown in Figure 9.5.

9.6 Control strategy: a joint framework

A general schematic of the joint control framework proposed to capture the dynamics involved in the integrated SCM is depicted in Figure 9.6. As aforementioned, the strategy consists of including a multi-stage stochastic MILP model within the control algorithm of an MPC, allowing this way to combine the *robustness* provided by stochastic programs and the *monitoring* and *adaptive* capabilities rendered by MPC. The Stochastic Model Predictive Control (SMPC) strategy introduced in this chapter can be described as follows:

1. The SC process is disturbed by all those external changes in the marketplace (i.e., demand, prices, cancellations, returns, interest rates, materials availability and costs) and also by the dynamics of internal SC operations (i.e., processing times, equipment breakdown, material consumption). The information regarding these disturbances as well as the

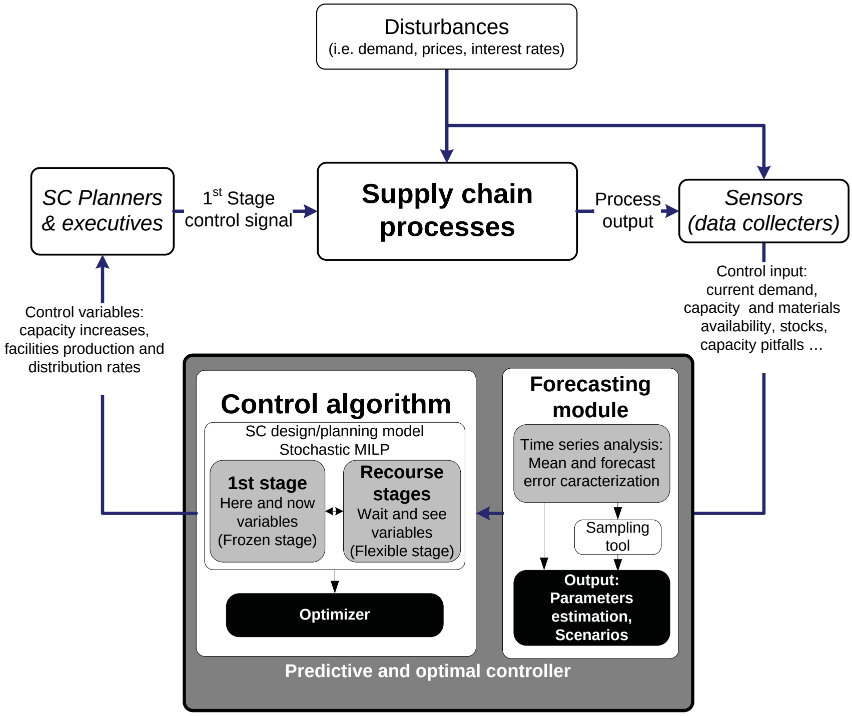


Figure 9.6: Proposed SMPC strategy

information required to describe the current SC state (i.e., stocks, capacity availability, loans, sales, accounts receivables and payables, etc.) are captured and sent as input to the controller.

2. The controller is composed by a forecasting module and a control algorithm. Using collected disturbances data, estimations of parameters in future periods are produced by the forecasting module. For those parameters which are considered random variables within the control algorithm, scenarios can be generated by utilizing the methodology presented in Section 9.5.

3. Once parameters estimations and scenarios are calculated by the forecasting module, the SC predictive model is updated (instantiated) with this new information. The set of future control variables is calculated by optimizing the updated stochastic predictive model.

4. The output of the optimizer can be classified into two types of variables: first stage and recourse variables. The first-stage variables of a stochastic program, also known as "here and now" variables, are determined prior to the resolution of any of the future underlying uncertainties. As aforementioned, in the model presented in section 9.4.2 a first stage variable

can be identified because of possessing a superscript l and a subscript $\hbar_{l-1}$. On the other hand, recourse variables are determined in the face of the uncertainty that unfolds in the period when its associated decision is implemented (i.e. sales, pledging decisions). As indicated in Fig. 9.6, the sent and implemented control signal only comprises the first stage variables resulting from the stochastic optimization problem which evidently are associated to the following period.

5. The whole strategy is repeated continuously every period. As new information is available, it is collected and handled by the forecasting module, the predictive module is updated and the horizon advances one period-step. Repeating each time the sequence described in this section.

9.7 Motivating example

The capabilities of the proposed framework are demonstrated by solving a retrofitting– planning problem of a SC comprising multiple manufacturing sites, distribution centers and markets located in different geographical locations. A set of potential equipment technologies are assumed to be available in the manufacturing sites. Furthermore, several potential locations for the manufacturing sites and the distribution centers, from which the products should be transported to the final markets, are also considered. The plants ($S1$, $S2$ and $S3$) can manufacture three different products ($P1$, $P2$ and $P3$) with three different equipments (TA to TC). These final products must be transported to the distribution centers ($W1$ to $W3$) prior to being sent to the final markets ($M1$ to $M3$), where they become available to customers. It is assumed an existing installed capacity of TA in $S1$ of 10,000 c.u. The investment cost associated with the establishment of a manufacturing site is 10 000 000 m.u. Distribution center $W1$ has already an installed capacity of 1000 m^3. The investment needed to open a distribution center amounts to 3 500 000 m.u.

The initial inventories are supposed to be equal to zero for all products and raw materials. The upper bound of equipment increase at each manufacturing site is set to 350,000 c.u and the lower bound is 50,000 c.u. The upper and lower bounds of the distribution centers capacity increase are 1,000 and 10,000 m^3. Facilities capacity can only be increased once a year. The salvage value is considered negligible at the end of the planning horizon. The availability of utilities is assumed to be unlimited.

With regard to the financial aspects, it is assumed that the firm has at the beginning of the planning horizon an initial portfolio of marketable securities. Specifically, the firm owns 25,000 m.u. in marketable securities maturing in period 2 and 70,000 m.u. maturing at period 3. The initial cash is assumed to be equal to the minimum cash allowed, which is 125,000 m.u. Under an agreement with a bank, the firm has an open line of short term credit at a 15% annual interest at the beginning of the planning horizon with a maximum debt allowed of 2,000,000 m.u. The initial debt is assumed to be equal to zero. The

Table 9.1: Computational results of motivating example

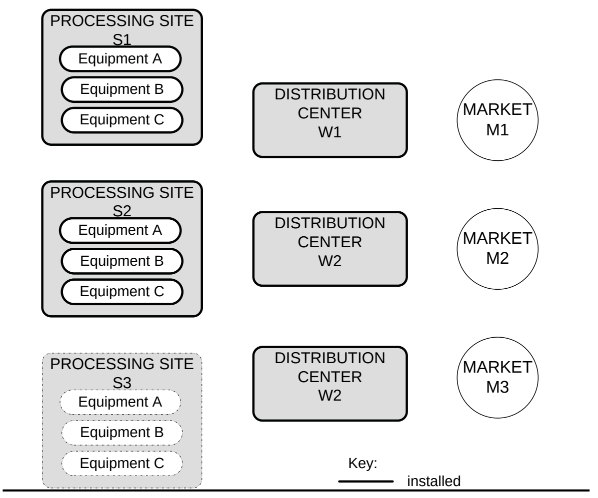
Model	Equations	Continuous variables	Discrete variables	CPU time (s)
Deterministic	6,766	7,231	306	28.34
SHT	175,588	177,293	9,792	1,584.33

prices of the materials kept as inventories are assumed to be a 85% of their market prices for final products and a 100% for raw materials.

The SC under study has three external suppliers, the first one providing raw materials, the second one transportation services and the third one labour utilities. Liabilities incurred with the raw materials supplier must be repaid within one month according to the terms of the credit (2 percent-same period, net-28 days for the raw materials supplier). The payments associated with the transport services and labor tasks cannot be stretched and must be fulfilled at the time of purchase. The technical coefficients associated with the set of marketable securities that the firm has agreed to purchase and sale have been computed by considering a 2.8% annual interest for anticipated sales and a 3.5% for maturing sales. It is considered an outflow of cash equal to 50 000 m.u. at the end of first year due to incentives payback. It is also assumed that the ratio between the long term debt and the equity must be always kept equal to 0.41. With regard to the long term debt, notice that the firm can have access to a long term credit at a 10% annual interest at the beginning of the planning horizon. Shareholders initial ROE expectation is assumed to be 30%. The taxes rate is assumed to be 30%. Depreciation is calculated by means of the straight line method applied over a time horizon of ten years. The rest of this case study data is found in Appendix D.

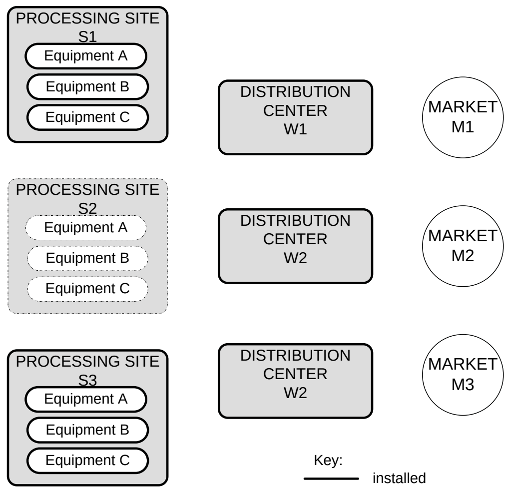
Five years are considered which are composed of twelve monthly planning periods. In this example, market demand, prices of final products and interest rates are regarded as uncertain factors which unfold every year. It is considered that uncertain factors may unveil into two different events leading to a scenario tree which contains 32 leaf nodes (scenarios). The values in which it is assumed uncertainty unveils in the first year are also shown in Appendix D. These values where chosen randomly. The forecasted parameters are calculated by using simple exponential smoothing techniques. The return rates such as $E[ROE]$ and credit line interest rates are assumed to vary in the amount that risk free rate(r_t^0) changes over the planning horizon. The two stage shrinking horizon (SHT) approximation approach presented in the work of Balasubramanian and Grossmann (2004) was used to solve the multistage stochastic problem. In the first step of the control strategy, a design-planning problem is disclosed. The computational effort required for implementing in GAMS the stochastic and deterministic formulation appears in Table 9.1. The resulting MILP models were optimized using the MIP solver of CPLEX (10.0) with a 5% integrality gap on a AMD Athlon 3000 computer.

The SC network configurations obtained by the stochastic and deterministic



Expected corporate value ($E[CV]$)				122,399,907 m.u.
		Equipment technology j		
		TA	TB	TC
Manufacturing sites				
s	t	Capacity increment (c.u.)		
$S1$	0	10,000.0	0.0	0.0
	1	350,000.0	77242.0	297351.0
$S2$	0	0.0	0.0	0.0
	1	350,000.0	61,119.0	162,944.0
$S3$	0	0.0	0.0	0.0
	1	0.0	0.0	0.0
Distribution centers		$W1$	$W2$	$W3$
	t	Capacity increment (m^3)		
	0	1,000	0.0	0.0
	1	1,000	1,000	1,000

Figure 9.7: Deterministic network design



Expected corporate value ($E[CV]$)				136,883,592 m.u.
		Equipment technology j		
		TA	TB	TC
Manufacturing sites				
s	t	Capacity increment (c.u.)		
$S1$	0	10,000.0	0.0	0.0
	1	350,000.0	50,000.0	252,599.0
$S2$	0	0.0	0.0	0.0
	1	0.0	0.0	0.0
$S3$	0	0.0	0.0	0.0
	1	350,000.0	92,023.0	350,000.0
Distribution centers		$W1$	$W2$	$W3$
	t	Capacity increment (m^3)		
	0	1,000	0.0	0.0
	1	1,000	1,000	1,000

Figure 9.8: Stochastic network design

formulation are summarized in Figures 9.7 and 9.8. Numerical results show that the solution computed by the stochastic formulation has higher performance than the optimal deterministic solution in terms of expected corporate value. Certainly, the optimal expected corporate value from the stochastic solution is 12% greater than the one computed by utilizing the deterministic approach.

Moreover, the network design accomplished by using the stochastic approach also shows an enhancement in terms of financial risks. As it can be observed in Figure 9.9, the stochastic solution accumulates more scenarios which present high corporate value. The deterministic solution could result in a corporate value approximately greater than or equal to 2.0×10^8 m.u. in five scenarios, while the stochastic solution could show a similar performance when operating under twelve scenarios. The risk curves for both formulations are shown

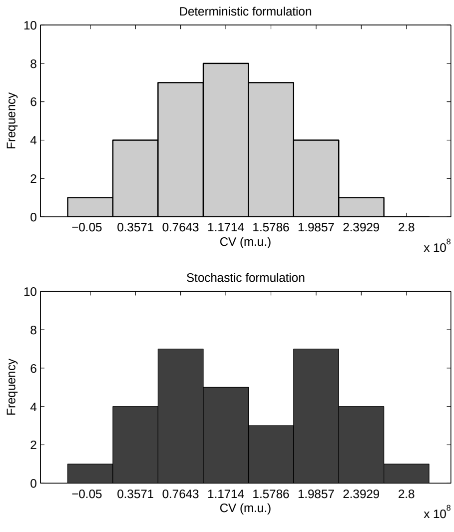


Figure 9.9: Histogram of scenario frequencies

in Figure 9.10. Here, the "wait and see" solution (WSS) is also included for comparison purposes with the stochastic solution carried out by means of the SHT approximation strategy. In fact, the expected CV of the WSS (1.48×10^8 m.u.) is just 8% higher than the one computed by the SHT strategy. As shown in Figure 9.10, the stochastic solution significantly decreases the probability of low CVs. For instance, there is a 62% probability of CVs bellow 1.3×10^8 m.u. in the deterministic solution, while such a probability is reduced to 40% in the stochastic one. It is important to notice that the cumulative curves of the SHT strategy and WSS are very similar in the scenarios with high CV. However, the behavior of the stochastic solution under scenarios with low demand, low prices and high interest rates is very similar to the one of the deterministic solution. This fact is due to the "consumption of value" experienced for covering the fixed and financial costs (long-term debt interests) associated to network idle capacity.

To demonstrate the benefits of using the proposed SMPC strategy, the algorithm has been repeated also during ten planning periods representing one month each of them. Here, the uncertainty is assumed to unveil every month. In order to model the SC process for this case, the production rates ($P^l_{ijst\hbar_{l-1}}$) and raw materials acquisition (i.e., raw materials ($Purch^{rm,l}_{et\hbar_{l-1}}$)) become first stage variables. To evaluate the advantages of the presented strategy, the deterministic MPC is carried out as well. In Figure 9.11 (a) it is compared how value is accumulated in both strategies. Figures 9.11 (b) and (c) exhibit the value creation and consumption of each strategy. By using the joint framework, the SC system yields an accumulated value equal to 2,718,368.18 m.u., whereas an accumulated value equal to 540,181.56 m.u. is accomplished at the end of the tenth period by using the deterministic MPC approach. It should be noticed that most of firms register a critical interval following investment execution afterwards the free cash flows stabilize. Hence, it is illustrated that a significant performance improvement could be obtained by merging the advantages of MPC and stochastic programming on an integrated approach. Furthermore, a breakdown at second planning period in equipment TA in site $S3$ is assumed which means a capacity reduction of 75,000 c.u (21.4%). Figures 9.12 and 9.13 illustrate the plans and capacity utilization of equipment in each site before and after the breakdown, respectively. It can be seen in spite of capacity availability of equipment TC in site $S3$ in which $P1$ can be manufactured, part of previous production assignment of TA in site $S3$ is transfered to site $S1$. This fact demonstrates that when the proposed strategy is applied, namely SC transparency is gained, the decision making process to resolve the incidents is performed at the SC level and not merely at the plant level, and also the algorithm allows to select the best choice in terms of value creation.

Moreover, one important phenomenon to be analyzed in SCs is the so-called bullwhip effect. The bullwhip effect is the magnification of demand fluctuations as one moves up the SC; from markets to suppliers. The basic phenomenon is not new and has been known to scientists for some time. Forrester (1961) illustrates the effect in a series of case studies, and points out that it is a consequence of industrial dynamics or time varying behaviors of industrial organizations. Here, the variation of the quotient given in Eq. 9.58 is proposed as a measure of the bullwhip effect. R_{it}^{bwe} is the quotient of the production generated and the real demand received by the SC for product i. In the ideal case in which information is certain, amount of production would perfectly match demand resulting in a value of R_{it}^{bwe} equal to zero. Similar measures can be found in the works of Fransoo and Wouters (2000), and Mestan *et al.* (2006). As shown in Figure 9.14, the SMPC approach has a better performance, in terms of bullwhip effect, in comparison with the classical deterministic MPC strategy. A

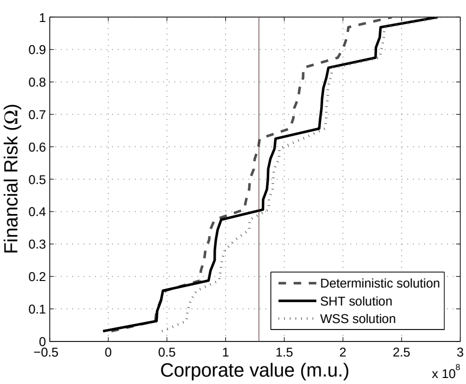


Figure 9.10: Risk curves considering uncertainty in demand, prices and interest rates

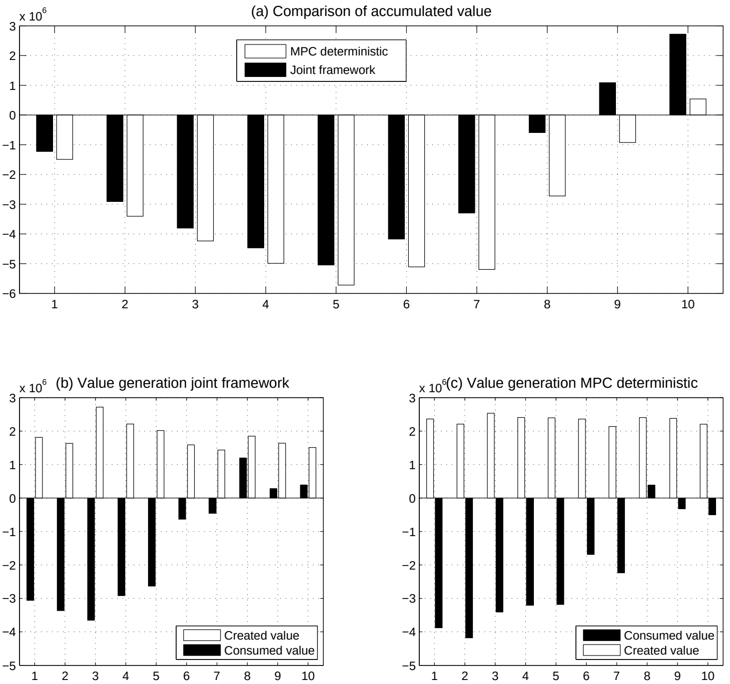


Figure 9.11: Comparison of value behavior of both approaches

significant reduction of R_{it}^{bwe} variation can be observed for product $P1$ and $P2$ when applying the proposed approach; 75.65% and 45.19% respectively (see Table 9.2).

$$R_{it}^{bwe} = \left| \frac{\sum_{s} \sum_{j} P_{ijst\hbar_{l-1}}^{l}}{\sum_{m} Dem_{imt}^{real}} - 1 \right| \tag{9.58}$$

It should be evident from this illustrative example that the proposed control strategy has a great potential to preserve and improve the firms value when addressing challenges of designing, *"re-planning"*, and solving incidences of SCs. In Chapter 11, the re-scheduling problem will be addressed. Besides,

Table 9.2: Standard deviation of R_{it}^{bwe} (adim.)

	Product		
	$P1$	$P2$	$P3$
Classical MPC	0.193	0.104	0.066
SMPC	0.047	0.057	0.052

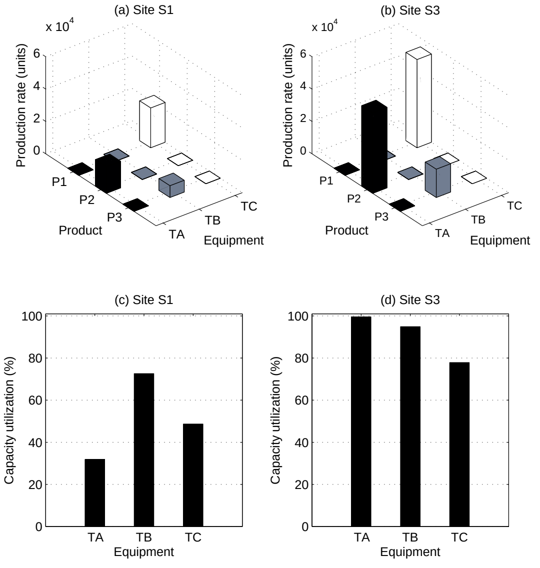


Figure 9.12: Second period production plan before equipment breakdown

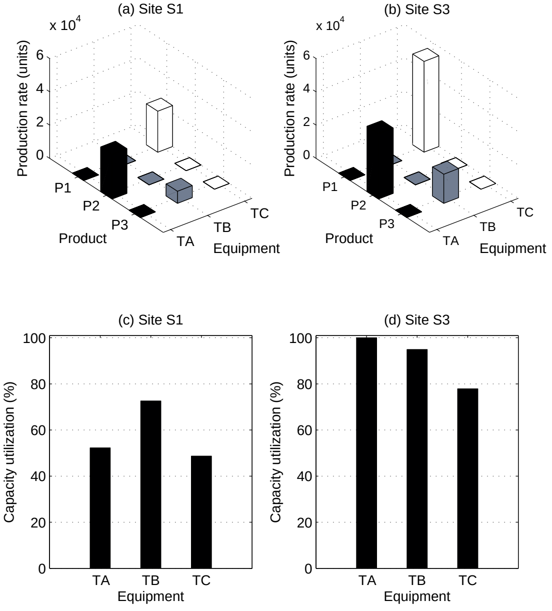


Figure 9.13: Second period production plan after equipment breakdown

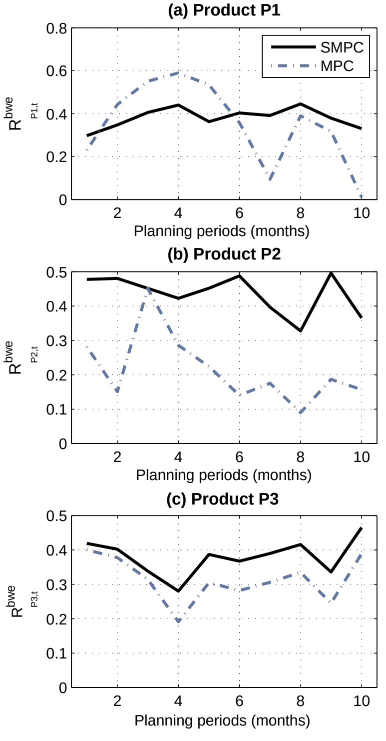


Figure 9.14: Variation of R_{it}^{bwe} for every product

that chapter will show how low level supervisory modules allow timely updating the equipment capacity data included in scheduling formulations.

9.8 Final considerations

This chapter has addressed the dynamics management of SCs by using integrated solutions. The proposed approach utilizes a SC design and planning model that incorporates financial concerns. Process operations decisions with finances considerations are optimized in tandem by using mathematical mixed integer modeling techniques. The solution framework integrates a MPC strategy and a holistic stochastic model for SCM whose objective function computes the corporate value via the DFCF method. It is important to emphasized that a drawback of DFCF methods is that they, in their deterministic version, do not considered the managerial flexibility required to alter the course of decisions depending on the scenario that unfolds. By extending a DFCF method to a stochastic formulation, this drawback is overcome since the optimization of a stochastic program actually results in a map of the decisions to be made according to the uncertainty realization. In addition, another disadvantage of discounted cash flow methods is that they do not account for uncertainties in commercial returns. In this work, to address this problem interest rates are regarded as random factors which have a direct effect upon cost of capital.

The main advantage of this joint control approach have been highlighted through a motivating case study, in which a comparison with the traditional deterministic MPC is carried out. The presented control strategy allows to handle uncertainty and incidences by combining reactive and preventive approaches. A pro-active treatment of uncertainty is included by means of stochastic programming. The review and update process that is required to tackle incidences and changes in random factors is performed by introducing the SC stochastic holistic model into an MPC. The novel control framework developed may help to close the information loop for dynamic SCM by taking the form of a supervisory module.

What is more, it has been pointed that business managers progressively become more driven by the goal of enhancing shareholder value. Numerical results show that the holistic financial-operational model embedded into the control algorithm permits decisions from different hierarchical levels (i.e. network design, production assignment, capacity pitfalls) to be all driven by firms value preservation. In addition, it has been illustrated that better transparency and broader visibility of SC is obtained when resolving incidences with the proposed strategy since a model of the whole SC is included into the control algorithm. It was also illustrated that the SMPC leads to bullwhip effect reduction.

In Chapter 11, an overall control strategy which comprises the three hierarchical levels (strategic, tactical and operational) is devised. Scheduling decisions and incidences should be also driven by value creation.

9.9 Nomenclature

Indices

e	suppliers
i	products
j	plant equipment
l	events in which uncertainty unfolds
m	markets
r	raw materials
s	manufacturing sites
t	planning periods
w	distribution centers
$\hbar_l$	combination of events at level l in scenario tree

Sets

$AH_{l\hbar_l}$	set of events combination that belong to level l and are ancestors of $\hbar_l$
E_r	set of suppliers e that provide raw material r

I_j	products that can be processed in plant equipment j
I_r	products that consumed raw material r
J_i	equipment that can process product i
L_t	level related to period t
R_e	set of raw materials provided by supplier e
T_l	set of periods associated to event l
τ	planning periods in which investments on facilities are allowed

Parameters

A_{ert}	maximum availability of raw material r in period t associated with supplier e
$CLine^{max}$	upper bound of short term credit line
$Coef_{ett'}$	technical discount coefficient for payments to external supplier e executed in period t' on accounts incurred in period t
d_e	maximum delay on payments of supplier e
d_m	maximum delay in receivables at market m
d_M^{max}	maximum delay in receivables at all markets
$D_{tt'}^{MS}$	technical coefficient for investments in marketable securities
$Dem_{imt\hbar_l}^{l}$	demand of product i at market m in period t associated with combination of events $\hbar_l$
$E_{tt'}^{MS}$	technical coefficient for sales of marketable securities
$E[ROE]_{\hbar_l}$	expected return on equity associated with combination of events $\hbar_l$
$FCFS_{jst}$	fixed cost per unit of capacity of plant equipment j at site s in period t
$FCFW_{wt}$	fixed cost per unit of capacity of distribution center w in period t
g_{ert}	cost of raw material r provided by supplier e in period t
$ir_{t\hbar_l}^{LD}$	interest rate of long term debt associated with combination of events $\hbar_l$
$ir_{t\hbar_l}^{SD}$	interest rate of short term debt associated with combination of events $\hbar_l$
I_{st}^{S}	investment required to open site s in period t
I_{wt}^{W}	investment required to open distribution center w in period t
Iu_{rt}^{RM}	value of inventory of raw material r in period t
Iu_{it}^{FP}	value of inventory of product i in period t
$MinCash$	lower bound of cash
$MinCSL$	lower bound of customer service level
$Other_t$	other expected outflows or inflows of cash in period t
$Price_{imt\hbar_l}^{l}$	price of product i at market m in period t associated with combination of events $\hbar_l$
$Price_{jst}^{FS}$	investment required per unit of capacity of equipment j increased at site s in period t
$Price_{wt}^{FW}$	investment required per unit of capacity of distribution center w increased in period t
$r_{t\hbar_l}^{0,l}$	risk free rate of return in period t related to combination of events $\hbar_l$
rp	risk premium rate
S_t^{MS}	marketable securities of the initial portfolio maturing in period t
$trate$	tax rate

$|T|$ length of planning horizon

Binary Variables

$SB^l_{st\hbar_{l-1}}$ 1 if site s is opened in period t for combination of events $\hbar_{l-1}$, 0 otherwise

$V^l_{jst\hbar_{l-1}}$ 1 if the capacity of equipment j is increased at site s in period t for combination of events $\hbar_{l-1}$, 0 otherwise

$WB^l_{wt\hbar_{l-1}}$ 1 if distribution center w is opened in period t for combination of events $\hbar_{l-1}$, 0 otherwise

$X^l_{wt\hbar_{l-1}}$ 1 if the capacity of distribution center w is increased in period t for combination of events $\hbar_{l-1}$, 0 otherwise

Continuous Variables

$APay^l_{t\hbar_l}$ amount of accounts payable in period t for combination of events $\hbar_l$

$ARec^l_{t\hbar_l}$ amount of accounts receivable in period t for combination of events $\hbar_l$

$ASales^l_{tt'\hbar_l}$ sales executed in period t and receivable in period t' for combination of events $\hbar_l$

$Borrow^l_{t\hbar_l}$ total amount borrowed from the short-term credit line in period t for combination of events $\hbar_l$

$Capital^l_{t\hbar_l}$ capital supported by shareholders in period t for combination of events $\hbar_l$

$Cash_{t\hbar_l}$ cash in period t for combination of events $\hbar_l$

$CLine^l_{t\hbar_l}$ short term debt in period t for combination of events $\hbar_l$

$CV^L_{\hbar_L}$ corporate value at the end of the planning horizon for combination of events $\hbar_L$

$Dep^l_{t\hbar_l}$ depreciation in period t for combination of events $\hbar_l$

$DFCF^L_{\hbar_L}$ sum of discounted free cash flows at the end of the planning horizon for combination of events $\hbar_L$

$ECash^l_{t\hbar_l}$ exogenous cash in period t for combination of events $\hbar_l$

$EPurch^l_{et\hbar_l}$ economic value of purchases executed in period t to supplier e for combination of events $\hbar_l$

$ESales^l_{t\hbar_l}$ economic value of sales carried out in period t for combination of events $\hbar_l$

$E[CV]$ expected corporate value

$FAsset^l_{t\hbar_l}$ increment in fixed assets in period t for combination of events $\hbar_l$

$FCF^l_{t\hbar_l}$ free cash flows in period t for combination of events $\hbar_l$

$FCost^l_{t\hbar_{l-1}}$ fixed cost in period t for combination of events $\hbar_{l-1}$

$FEx^l_{t\hbar_l}$ other financial expenses and incomes in period t for combination of events $\hbar_l$

$FS^l_{jst\hbar_{l-1}}$ total capacity of plant equipment j during period t at site s for combination of events $\hbar_{l-1}$

$FSE^l_{jst\hbar_{l-1}}$ capacity increment of plant equipment j during period t at site s for combination of events $\hbar_{l-1}$

$FW^l_{jst\hbar_{l-1}}$ total capacity at distribution center w during period t for combination of events $\hbar_{l-1}$

$FWE^l_{jst\hbar_{l-1}}$ capacity increment at distribution center w during period t for combination of events $\hbar_{l-1}$

$LBorrow^{l}_{t\hbar_l}$	total amount of money borrowed from the long term credit line in period t for combination of events $\hbar_l$
$LDebt^{l}_{t\hbar_l}$	long term debt in period t for combination of events $\hbar_l$
$LRepay^{l}_{t\hbar_l}$	total amount repaid to the long-term credit line in period t for combination of events $\hbar_l$
$Net^{CLine,l}_{t\hbar_l}$	total amount of money borrowed or repaid to the short term credit line for combination of events $\hbar_l$ in period t
$Net^{LDebt,l}_{t\hbar_l}$	total amount of money borrowed or repaid to the long term credit line in period t for combination of events $\hbar_l$
$Net^{MS,l}_{t\hbar_l}$	total amount received or paid in securities transactions in period t for combination of events $\hbar_l$
$NetDebt_0$	net total debt at the beginning of planning horizon
$NetInvest^{l}_{t\hbar_l}$	net investment in period t for combination of events $\hbar_l$
$P^{l}_{ijst\hbar_l}$	production rate of product i in equipment j at site s in period t for combination of events $\hbar_l$
$Pay^{l}_{tt'\hbar_l}$	payments to external supplier e executed in period t' on accounts payable incurred in period t for combination of events $\hbar_l$
$Pled^{l}_{tt'\hbar_l}$	amount pledged within period t' on accounts receivable maturing in period t for combination of events $\hbar_l$
$Profit^{l}_{t\hbar_l}$	profit achieved in period t for combination of events $\hbar_l$
$Purch^{rm,l}_{et\hbar_l}$	amount of money payable to supplier e in period t for combination of events $\hbar_l$ associated with consumption of raw materials
$Purch^{tr}_{et}$	amount of money payable to supplier e in period t for combination of events $\hbar_l$ associated with consumption of transport services
$Purch^{pr,l}_{et\hbar_l}$	amount of money payable to supplier e in period t associated with consumption of production utilities for combination of events $\hbar_l$
$Purch^{l}_{erst\hbar_l}$	amount of raw material r purchased to supplier e at site s in period t for combination of events $\hbar_l$
$Purch^{rm,l}_{et\hbar_l}$	amount of raw material r purchased in period t for combination of events $\hbar_l$
$Q^{l}_{iwst\hbar_l}$	amount of product i sent from site s to distribution center w in period t for combination of events $\hbar_l$
R^{bwe}_{it}	bullwhip effect quotient for product i in period t
$Repay^{l}_{t\hbar_l}$	total amount repaid to the short-term credit line in period t for combination of events $\hbar_l$
$Sales^{l}_{iwmt\hbar_l}$	amount of product i sold from distribution center w in market m in period t for combination of events $\hbar_l$
$SI^{l}_{rst\hbar_l}$	amount of stock of raw material r at site s in period t for combination of events $\hbar_l$
$SO^{l}_{ist\hbar_l}$	amount of stock of product i at site s in period t for combination of events $\hbar_l$
$SV^{L}_{\hbar_L}$	salvage value of facilities at the end of planning horizon for combination of events $\hbar_L$
$SW^{l}_{iwt\hbar_l}$	amount of stock of product i at distribution center w in period t for combination of events $\hbar_l$
$WACC^{l}_{t\hbar_l}$	weighted average cost of capital in period t for combination of events $\hbar_l$

$Y^{MS}_{tt'\hbar_l}$	cash invested in period t' in marketable securities maturing in period t for combination of events $\hbar_l$
$Z^{MS,l}_{tt'\hbar_l}$	security sold in period t' maturing in period t for combination of events $\hbar_l$
$\Delta APay^{l}_{t\hbar_l}$	change in amount of accounts payable in period t for combination of events $\hbar_l$
$\Delta ARec^{l}_{t\hbar_l}$	change in amount of accounts receivable in period t for combination of events $\hbar_l$
$\Delta Inv^{l}_{t\hbar_l}$	change in inventory value in period t for combination of events $\hbar_l$
$\Delta NWC^{l}_{t\hbar_l}$	change in net working capital in period t

Greek symbols

α_{rij}	fixed coefficient for consumption of raw material r by product i
β_{sj}	minimum utilization of plant equipment j capacity allowed at site s
γ_w	minimum utilization of distribution center w capacity allowed
$\delta_{mtt'}$	fraction of sales carried out in period t that are receivable in period t' in market m
θ_{ij}	capacity utilization of plant equipment j by product i
λ_t	proportion of equity over total capital investment in period t
ρ^{tr1}_{eiws}	unitary transport costs of product i from plant s to warehouse w payable to external supplier e
ρ^{tr2}_{eiwm}	unitary transport costs of product i from warehouse w to market m
τ^{ut1}_{ijse}	cost of the utilities associated with product i manufactured with equipment j in site s and payable to external supplier e
τ^{ut2}_{rse}	cost associated with handling the inventory of raw material r in site s and payable to external supplier e
τ^{ut3}_{ise}	cost associated with handling the inventory of final product i in site s and payable to external supplier e
τ^{ut3}_{iwe}	cost associated with handling the inventory of final product i in warehouse w and payable to external supplier e
υ_i	specific volume of product i
$\phi_{tt'}$	face value of accounts maturing in period t pledged in period t'
ψ_{ert}	price of raw material r offered by external supplier e in period t

Superscripts

L	lower bound
U	upper bound

Chapter 10

Using S-graph to Address Scheduling Under Exogenous Uncertainty

10.1 Introduction

Processes and markets uncertainties make batch plants a complex environment to manage production activities. Uncertainties may cause deviations and infeasibilities in predefined schedules; this may result in poor planning and inefficient utilization of materials. Consequently, the relevance of explicitly incorporating variability in the scheduling formulation in order to offer more efficient plans and robust decisions to changes has become recognized. Even more, significant improvement of SC performance can be obtained by encompassing low level decisions within the supply chain management. Also, such a integration results in a better treatment of supply chain dynamics. However, the inclusion of scheduling models lead to large scale problems. Therefore, one challenge in this field is the reduction of the computational burden required to solve this kind of problems. This chapter addresses the batch plants scheduling under exogenous uncertainty. The most widely utilized approach to tackle this problem is stochastic programming; however its solution results in high computational expense. From another standpoint S-graph, a graph-theoretic approach, has proved to be very efficient to deal with deterministic scheduling. In this work, the S-graph framework is enhanced so that stochastic scheduling problems can be handled. For this purpose, an LP model that is used as performance evaluator has been coupled with the S-graph framework. One of the main advantages of the proposed approach is that the search space does not exponentially increase according to the number of scenarios considered in the problem. Finally, the potential of the proposed framework is highlighted through two illustrative examples.

10.2 Scheduling under uncertainty

It is evident that uncertainties in batch operations may arise from different sources (i.e., external demand, prices of raw and final products, processing times and equipment availability) causing previous schedules to become non-optimal and in some cases infeasible. Despite the uncertain nature of scheduling problems, research efforts over last decades have primarily focused on deterministic formulations which assume all parameters to be precisely known in advance.

One of the first contributions to this field is the work of Kondili *et al.* (1993). They developed the State-Task-Network (STN) representation in order to formulate the problem of production scheduling in multipurpose plants as an MILP. Later on, Pantelides (1994) presented the Resource-Task-Network (RTN) representation which employs a uniform treatment for all available resources. Hence, RTN reduces the number of binary variables and equations when compared with the STN. Both, the STN and RTN formulation used a discrete time representation. Pinto and Grossmann (1995) extend the STN formulation to a continuous time representation. For this purpose, they proposed to use a set of global time slots with unknown duration for allocating units to tasks. Similarly, Castro, Barbosa-Póvoa, and Matos (2001) extend the RTN framework to a continuous time formulation. Lin and Floudas (2002) used the concept of event points. The global time point representation is relaxed by allowing different tasks to start at different moments in different units for the same event point. The State Sequence Network (SSN) formulation developed by Majozi and Zhu (2001) consists in a continuous formulation which eliminates the use of task and unit, thus reducing the number of binary variables compared to other continuous formulations. Finally, Cerda and co-workers (Cerdá, Henning, & Grossmann, 1997; Méndez & Cerdá, 2002) developed precedence based models which are suitable for cases where sequence-dependent changeovers are to be considered.

Scheduling problems are highly complex problems. Due to the discrete decisions involved (e.g., equipment assignment, task allocation over time) these problems are inherently combinatorial in nature, and hence very challenging from the computational complexity point of view (Pekny & Reklaitis, 1998). Therefore, a modest growth in problem size can lead to a significant increase in the computational requirements (Lin & Floudas, 2004). Furthermore, stochastic programs become deterministic equivalent programs with the utilization of scenarios or scenario tree. The size of the deterministic scheduling formulation can easily grow out of hand for a large number of scenarios, which renders the direct solution approaches numerically intractable and thus necessitates special methods, such as decomposition and aggregation (Cheng, Subrahmanian, & Westerberg, 2003). Hence, it turns out that one of the major challenges in the area of scheduling under uncertainty is to reduce the computational cost required to solve this kind of problems (NP complete problems which are complicated by the consideration of uncertainty). It is noteworthy that solution procedures based on knowledge of the specific problem have been recognized to exhibit a good potential in providing advances in this direction (Li & Ierapetritou, 2007).

S-graph is a scheduling approach that has proven to significantly reduce the computational effort compared to mathematical programming techniques. S-graph is a representation that takes into consideration the specific characteristics of chemical processes in scheduling. It allows for the formulation of scheduling problems using similar graph representations as those used to solve the job-shop problem but contemplating the higher complexity of the chemical multipurpose batch scheduling (Sanmartí *et al.*, 2002). Moreover, one of its important capabilities is that it offers a strictly continuous time formulation. Initially, this approach was only applied to problems in which the objective was to minimize makespan. The problem was solved using a Branch & Bound and an efficient graph algorithm to evaluate the makespan. Recently, S-graph has been extended to be an effective search algorithm for determining schedules that optimize throughput, revenue, or profit over a predefined time horizon in multipurpose batch plants (Majozi & Friedler, 2006). The approach presented in this chapter starts from the abovementioned latest framework. A new extension of S-graph that allows tackling scheduling problems under external uncertainty (demand and prices) is shown. The resulting schedule is equivalent to the one that can be obtained using two-stage stochastic programming techniques. It is demonstrated the capabilities of the proposed approach in addressing stochastic scheduling problems by solving two illustrative examples.

Frameworks that reduce the computational complexity of scheduling problems are crucial for the eventual integration of SC hierarchical decision levels. As mentioned before, that integration permits to find more realistic and feasible solutions for the SC design and planning. What is more, its consideration may improve the resolution of SC incidences and SC visibility. These topics will be further discussed in Chapter 11, *Detailed Scheduling Considerations into the Design of Supply Chains.*

10.3 Problem statement

In last decade many authors have recognized that it is unlikely to apply deterministic schedules in real scenarios without decreasing considerably their performance, and have made efforts to extend deterministic approaches to situations with some type of uncertainty, so as to obtain better results when their solutions are deployed in real scenarios. Here, the S-graph deterministic framework is extended for solving scheduling problems under uncertainty in demand.

Generally speaking, the scheduling problem seeks the best way of allocating and timing the different production tasks to the available resources. In this chapter, the scheduling problem aims at maximizing the business profit. The problem input data can be classified into three groups: (i) resources related data, (ii) process related data and (iii) economic data.

The first group describes all the enterprise available equipment such as processing and storage units. Data regarding its maximum capacity and minimum working capacity are usually required. Moreover, maximum availability of raw materials may be relevant depending on the problem scope. The process related data describes the different recipes that may be followed in order to obtain the final products. Here, the different tasks required to produce an intermediate or final product are determined. The input and output materials for each task are stipulated as well as their respective mass proportions and processing times. Additionally, the equipment that is suitable to perform each task is identified. Other relevant data may be the energy, vapor or any other utility consumption for each task.

Finally, the last group is concerning all the data required to quantify the expected net benefits due to production operations. On the outcome side, raw materials and operation costs are included. The revenues are generated by selling the final products to the target marketplace, thus two important input parameters to define are the market price and demand of each product. It is important to point out that given the exogenous stochastic nature of the problem tackled in this chapter, demand is considered as uncertain. Commonly, random parameters are described by using a probability distribution function. Instead, the scenario approach is adopted in this chapter so that the stochastic scheduling problem can be formulated using a deterministic equivalent approach. In case that demand probability distribution functions are available, a Monte Carlo sampling can be executed in order to obtain satisfactory equally probable scenarios of demand.

The proposed stochastic S-graph framework is intended to support plant managers on the decision making about the timing of tasks to be performed in each processing unit, the amount of material being processed at each time in each unit, and the amount of final products to be sold in each demand scenario. These decisions will be taken such that the expected profit evaluated at the end of a predefined planning horizon is maximized.

10.4 A brief introduction to S-graph

A detailed description of the S-graph framework has been presented in the works of Sanmartí *et al.* (2002) and Romero, Puigjaner, Holczinger, and Friedler (2004). Additionally, the reader is referred to the web site www.s-graph.com for further information. For comprehensiveness a short description is given here.

10.4.1 Graph representation of scheduling problems

The S-graph framework consists of a sophisticated graph theoretic model developed to address the deterministic scheduling problem in multipurpose batch plants. S-graph was originally designed for makespan minimization problems

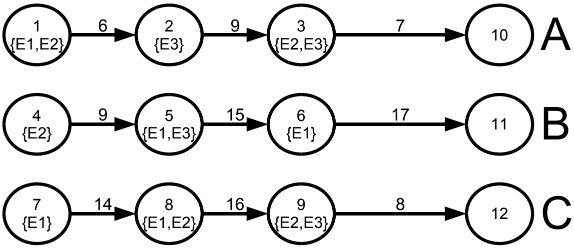


Figure 10.1: A recipe graph

assuming Non Intermediate Storage (NIS) policy. Later works have extended the framework so that other operational policies (common intermediate storage, fixed intermediate storage, zero wait) can be considered.

In an S-graph, the nodes correspond to production tasks except terminal nodes which are to denote the final products. The S-graph arcs are classified into two classes; the so-called recipe arcs and schedule arcs. It is noteworthy that recipe arcs are an input to the scheduling problem, while schedule arcs result from the S-graph algorithm solution.

Recipe arcs represent the preceding relationship among tasks. If a recipe arc leads from task k_1 to task k_2 means that task k_2 execution must start at least $c(k_1, k_2)$ time units later than task k_1 execution. Here, $c(k_1, k_2)$ is the weight of the recipe arc (k_1, k_2). In case of problem initialization and more than one equipment is suitable to perform a recipe arc (k_1, k_2) (i.e., execution of task represented by the origin node k_1), the arc weight is the minimum processing time for task k_1 among the suitable equipment units.

On the other hand, schedule-arcs denote the sequencing of tasks assigned to the same equipment unit. Assume that according to the scheduling, task k_1 and k_2 are assigned to equipment unit E_1 and additionally, these tasks will be performed in the sequence $k_1 - k_2$. Then, a zero-weighted schedule arc (or an arc with the length of change over time if appropriate) is added from all immediately subsequent tasks of k_1 in the recipe to task k_2. A graph without any schedule-arc is called recipe-graph, otherwise it is termed schedule-graph. When all tasks have been sequenced for all units, a complete schedule-graph have been generated. Note that one schedule graph exists for each feasible schedule. Therefore, an S-graph is given in the mathematical form $G(N, A_1, A_2)$, where N, A_1 and A_2 denote the sets of nodes, recipe arcs, and schedule arcs, respectively. In Figure 10.1 is shown a recipe-graph, while Figure 10.2 depicts a complete schedule-graph.

One of the special features of S-graph is that feasible schedules can be straightly identified. Loops must not appear in a S-graph corresponding to a feasible schedule. Following an appropriate Branch & Bound search strategy, the S-graph of the global optimal schedule can be efficaciously found. Please refer to Sanmartí *et al.* (2002) for details regarding the search strategy.

10.4.2 Throughput maximization using S-graph

Majozi and Friedler (2006) had recently extended the S-graph framework so that problems that involve economic performance indicators can be tackled. Specifically, they addressed the throughput maximization problem during a fixed time horizon, but their approach can be certainly extended to consider other indicators such as cost and profit.

The optimization strategy they proposed can be understood as comprised of two components: an optimality search algorithm and a feasibility test.

Feasibility test

Bearing in mind that a node ($\mathbb{P}_i$) in the search space corresponds to a discrete combination of batches of products, the feasibility test of a node basically consists in: (i) finding the minimum makespan schedule graph for the specific combination of batches of products and (ii) a comparison between the minimum makespan obtained and the fixed time horizon. Clearly, the schedule graph is feasible if the minimum makespan obtained is less or equal than the time horizon length.

Next, the optimality search algorithm is briefly explained. The algorithm roughly consists in rules that allow reducing the search space without losing optimality. Given a set of products p, the product p number of batches associated with node i is represented by N_p. Using the feasibility test, it can be found the maximum batches number of each of the products that can be processed over the time horizon of interest (N_p^u). Once the infeasibility of a node $\mathbb{P}_i$ belonging to this new reduced search region has been proved, any other node $\mathbb{P}_{i'}$ that accomplished that $N_p' \geq N_p$ for all products p is infeasible as well. Here, N_p' is the product p number of batches at node $\mathbb{P}_{i'}$ and N_p is the product p number of batches at node $\mathbb{P}_i$. Fig. 10.3 shows an example for two products, $p = \{A, B\}$. It can be noticed that the search efficiency results from the elimination of redundancy since at each search point, a node with a unique combination of batches of products is explored. Furthermore, regions with no opportunity for optimality are identified and eliminated a priori from the search algorithm.

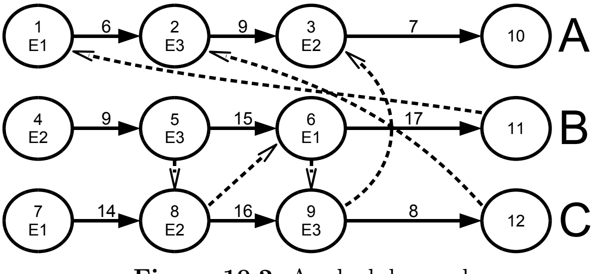


Figure 10.2: A schedule graph

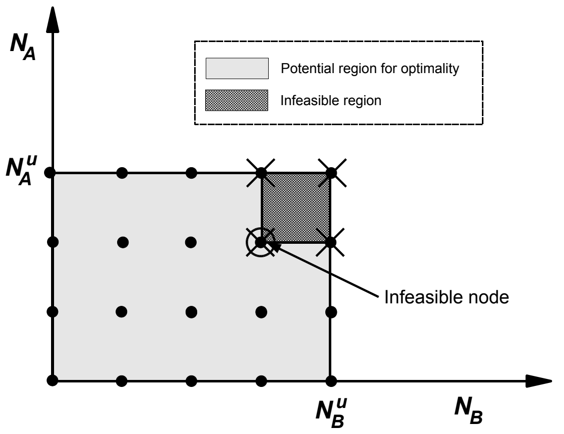


Figure 10.3: Procedure to reduce search region when it is found an infeasible node

10.5 Enhancing S-graph framework to address scheduling under uncertainty

In this section the framework proposed for solving stochastic scheduling problems is described. It basically consists in a systematic search strategy based on: the schedule generator (S-graph) and the expected performance evaluator (LP Model). The algorithm flowsheet is presented in Fig. 10.4.

The first step of the algorithm is to define the search space. This consists in the set of nodes corresponding to different combination of production routes for each final product. Routes are those different realistic ways to process a product or combination of products. Then, a node **N** could be described by an $|\mathcal{R}||\mathcal{P}|$ dimensional integer matrix, where each component $N_{p,r}$ represents the product p number of batches to produce from route r. The procedure followed to define the search space is the same described in section 10.4.2. In general, this procedure finds the maximum product p number of batches that each route r can process over the time horizon of interest ($N^u_{p,r}$) (see section 10.4.2). Here, **toTest** is defined as the set of nodes that have not been tested yet but still have an opportunity to result in a higher expected profit. The initial search space is used to initialize **toTest**.

The schedule resulting with the higher expected profit is selected from the nodes found during the definition of the search space ($N^u_{p,r}$). Such schedule is used to initialize **cb_value** and **cb_schedule** which represent the best expected profit currently found and its corresponding schedule, respectively.

The iterative part of the algorithm is explained next. While **toTest** is not empty, a node is chosen and saved in **cnode**. That node is then deleted from **toTest**. It is noteworthy that the algorithm may be accelerated by defining properly a strategy for choosing this node. Afterwards, the expected profit is computed for **cnode**. This is possible by solving the LP problem described in subsection 10.5.1. If **cnode** expected profit is less than the current best

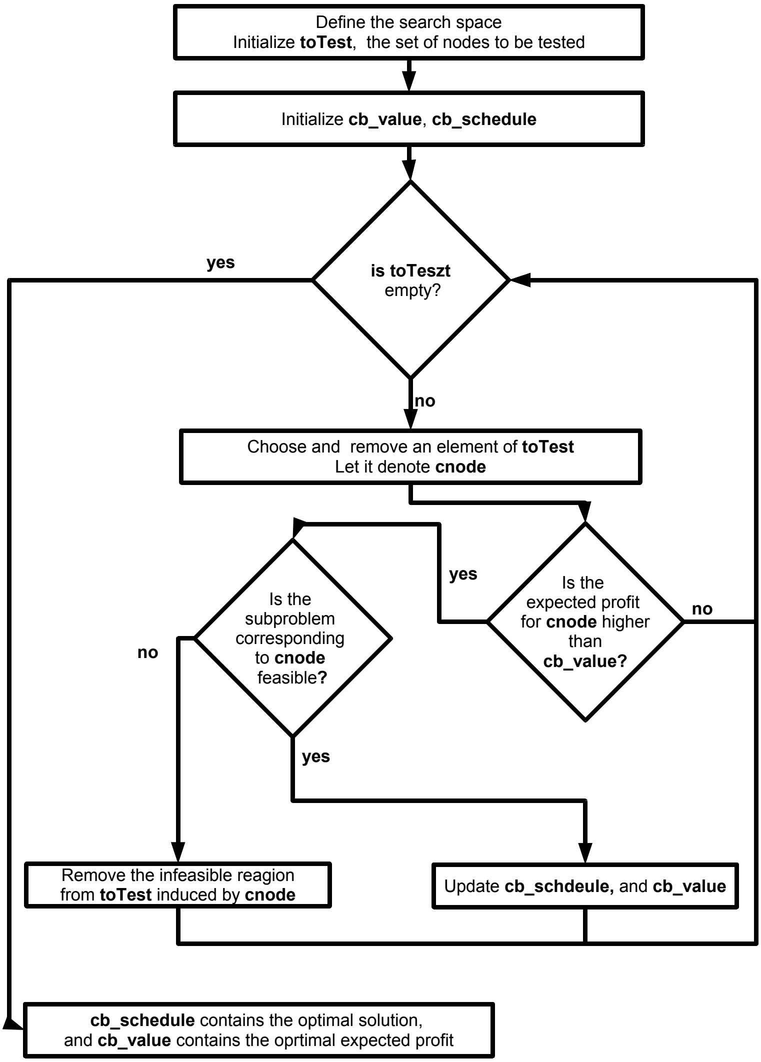


Figure 10.4: Flowsheet of the proposed algorithm

expected profit (**cb_value**), then this node is not the optimal and it is not tested for feasibility. Otherwise, **cnode** is tested for feasibility; if it has a feasible schedule within the time horizon, such schedule will be the new value for **cb_schedule**, and its corresponding expected profit will be the new value for **cb_value**. In case **cnode** is infeasible, any other node **N'** that accomplishes that $N'_{p,r} \geq N^{cnode}_{p,r}$ for all routes r and products p is infeasible as well, so it should be also removed from **toTest** as described in section 10.4.2.

If **toTest** is empty, **cb_value** is the expected profit corresponding to the optimal solution stored in **cb_schedule**. Otherwise, the iterative part of the algorithm is repeated as above described.

10.5.1 Expected performance evaluator: An LP

In this section the Linear Program for node expected profit evaluation is described. Each node corresponds to a given number of batches for each product-route. Since overproduction has as penalty the carrying inventory cost, it is not always worthy to work at full capacity. The LP model allows determining the batch sizes for each route that maximizes the expected profit at each evaluated node. The formal mathematical description is stated as follows.

Given:

- Market related inputs

  $\mathcal{P}$ set of products.

  $price_p$ product price ($p \in \mathcal{P}$)

  $Cost^{over}_p$ overproduction cost for each product ($p \in \mathcal{P}$)

  $Cost^{under}_p$ underproduction cost for each product ($p \in \mathcal{P}$)

- Recipe related inputs

  $\mathcal{R}$ set of routes

  $B^{max}_{p,r}$ the maximum batch size for product $p(\in \mathcal{P})$ that route $r(\in \mathcal{R})$ can produce

  $SF^{min}_{p,r}$ the minimum batch size for product p allowed at route r expressed as a proportion of the maximum batch size

- Scenario related inputs

  $\mathcal{S}$ set of scenarios

  p_s scenario probability ($s \in \mathcal{S}$)

  $dem_{s,p}$ the product demand p for scenario s

- Node data

  $N_{p,r}$ number of batches of product p produced using route r for the node being evaluated

The goal is to determine:

$x_{p,r}$ product p batch size as a proportion of the maximum batch size ($B_{r,p}^{max}$)

$u_{p,s}$ underproduction of product p in scenario s

$o_{p,s}$ overproduction of product p in scenario s

such that the expected profit is maximized.

The linear problem equations can be classified in three groups, namely (i) batch size equations, (ii) demand satisfaction, and (iii) the objective function.

Batch size equations

Eq. (10.1) states that product p batch size for each route ($x_{p,r}$) is bounded in the range of $[SF_{p,r}^{min}, 1]$ which represents the interval where it must fall.

$$SF_{p,r}^{min} \leq x_{p,r} \leq 1 \qquad \forall r \in R, p \in P_r \tag{10.1}$$

To avoid overlapping among search regions, $x_{p,r}$ is forced to be greater or equal than $\frac{N_{p,r}-1}{N_{p,r}}$ if $N_{p,r}$ is not equal to zero. The following constraint expresses this requirement:

$$N_{p,r} - 1 \leq N_{p,r} x_{p,r} \qquad \forall p \in R, p \in P_r \tag{10.2}$$

Demand satisfaction

Eq. (10.3) expresses that market sales must be less than or equal to demand ($dem_{p,s}$). Here, $u_{p,s}$ and $o_{p,s}$ represent the shortage and excess of product p over its corresponding demand in scenario s, respectively. This equation states that the total product demand must be equal to the amount of product p processed by this node ($\sum_{r \in R_p} x_{p,r} B_{p,r}^{max} N_{p,r}$) plus the shortage, minus the overproduction. Since demand depends on the disclosed scenario, $|\mathcal{P}||\mathcal{S}|$ equations appear.

$$\sum_{r \in R_p} x_{p,r} B_{p,r}^{max} N_{p,r} + u_{p,s} - o_{p,s} = dem_{p,s} \qquad \forall p \in \mathcal{P}, s \in \mathcal{S} \tag{10.3}$$

Objective function: expected profit

Eq. (10.4) is to calculate the profit associated to each scenario s. The objective function summarizes the revenues associated to sales and the costs of not exactly meeting the demand (shortages and overproduction). As Eq. (10.4) states, product p market sales is equal to the amount produced ($\sum_{r \in R_p} x_{p,r} B_{p,r}^{max} N_{p,r} + u_{p,s}$) minus the overproduced amount ($o_{p,s}$). Here, it is noteworthy that overproduction is equivalent to the product inventory held at the end of the scheduling horizon. Hence, the unitary overproduction cost ($Cost_p^{over}$) can represent the carrying cost of inventory associated with a specific product p. On the other hand, underproduction cost is related to those costs incurred when an item is out of stock (i.e., shortage or backorders). Businesses usually quantify these costs including the lost contribution margin on sales plus the lost customer good will.

$$\begin{aligned} profit_s = price_p \sum_{p \in \mathcal{P}} \left(\sum_{r \in R_p} x_{p,r} B_{p,r}^{max} N_{p,r} - o_{p,s} \right) \\ - \left(Cost_p^{over} o_{p,s} + Cost_p^{under} u_{p,s} \right) \qquad \forall s \in \mathcal{S} \end{aligned} \tag{10.4}$$

Once the scheduling decisions have been assessed in each possible scenario by Eq. (4.52), Equation (10.5) calculates the expected profit by considering the scenarios probability of occurrence (p_s). The expected profit is the LP objective function under the assumption that the decision maker is neutral about risk.

$$E[profit] = \sum_{s \in \mathcal{S}} p_s profit_s \tag{10.5}$$

The LP problem for evaluating the expected profit can be then mathematically posed as follows:

$$\begin{gathered} \underset{x_{p,r}, o_{p,s}, u_{p,s}}{Max} \quad E[profit] \\ \text{subject to} \\ \text{Eqns. (10.1) to (10.5)} \\ x_{p,r}, o_{p,s}, u_{p,s} \in \mathbb{R}^+ \end{gathered}$$

Extension to other uncertain parameters Market uncertainty usually escalates not merely on product demands, but also on product prices. In the strict mathematical formulation that means, that instead of just having $dem_{p,s}$ as uncertain parameter; the input for the algorithm would consider $price_{p,s}$ as random parameter as well. However, it is important to notice that such extension does not cause any alteration on the LP model. The exploration of the search space, the feasibility testing, the variables, and constraints in the LP remain the same. The profit equation is the unique change required in order to generalize the problem in this manner:

$$\begin{aligned} profit_s = price_{p,s} \sum_{p \in \mathcal{P}} \left(\sum_{r \in R_p} x_{p,r} B_{p,r}^{max} N_{p,r} - o_{p,s} \right) \\ - \left(Cost_{p,s}^{over} o_{p,s} + Cost_{p,s}^{under} u_{p,s} \right) \qquad \forall s \in \mathcal{S} \end{aligned} \tag{10.6}$$

Since the proposed algorithm is based on the Throughput Maximization method published by Majozi and Friedler (2006), it renders the advantages of

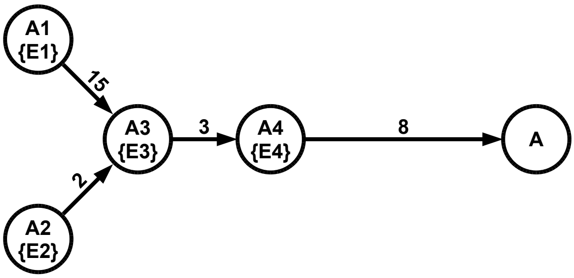


Figure 10.5: Route product A for example 1

that algorithm and the S-graph framework. Examples of those advantages are (i) globally optimal solutions are obtained, (ii) no infeasible solutions are found in terms of cross-transfers (Ferrer-Nadal, Capón-Garcia, Méndez, & Puigjaner, 2008), (iii) search space significant reduction, and (iv) it consists in a continuous formulation without the necessity of determining the so-called time points.

Usually, stochastic MILP models are very sensitive to the number of considered scenarios. Indeed, MILP model size increases dramatically by increasing the number of scenarios and accordingly the needed computational effort. By using the this algorithm, the computational time for the expected profit calculation will be increased; nevertheless the search space does not grow by increasing the number of scenarios. Notice that the search space size merely depends on route combinations. As a result, the computational burden required to solve industrial stochastic scheduling problems can be reduced by using the proposed framework.

10.6 Literature examples

The capabilities of the proposed framework are illustrated by solving the next two illustrative examples.

10.6.1 Example 1

Consider the following example introduced by Majozi and Friedler (2006) in which two products (A and B) are to be produced, according to the recipes given in Figures 10.5 and 10.6. Five different equipment units are available. The suitability of equipment units are shown in the recipe figures. Each unit of product A has a market price of 30 m.u, whereas product B has a price of 10 m.u. It is assumed that overproduction and under-production cost are equal to 15% and 25% of the market price, respectively. Three scenarios are considered for this example. The data related to product demands in each scenario is presented in Table 10.1. In this case the objective is to maximize expected profit over a time horizon of 60 h. under Non Intermediate Storage (NIS) policy.

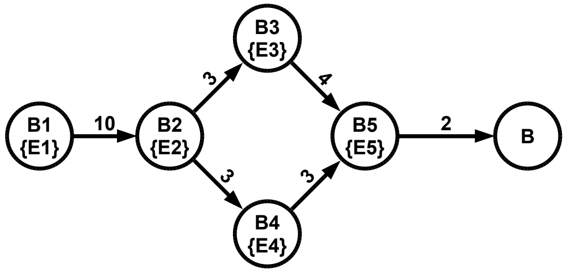


Figure 10.6: Route product B for example 1

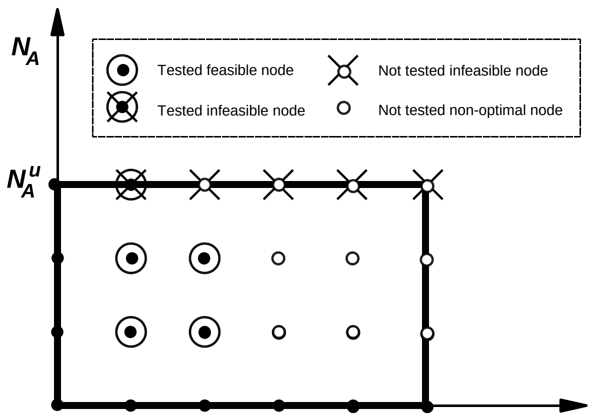


Figure 10.7: Search space for example 1

Recalling the algorithm of section 10.5, the search region contains 15 nodes. The search region is illustrated in Figure 10.7. As shown in this figure, 5 nodes are tested for feasibility. The optimal solution is found in node (2,2) which exhibits a expected profit of 3,165.20 m.u. The optimal solution comprises 2 batches of product A as well as 2 batches of product B. The corresponding batch sizes are shown in Table 10.2. In Figure 10.8 the optimal schedule obtained for this example is depicted.

Table 10.1: Scenario data for illustrative example 1

Scenario	Demand (kg)		Probability
	P1	P2	
I	58	64	0.30
II	100	92	0.40
III	148	62	0.30

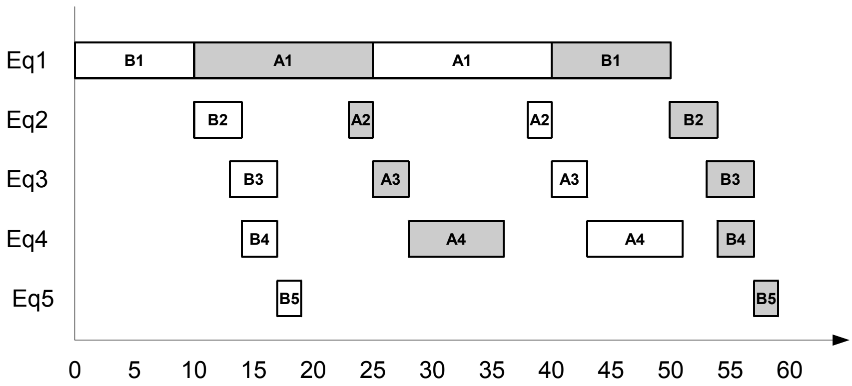


Figure 10.8: Optimal schedule for example 1

Table 10.2: Optimal batch quantity and sizes for illustrative example 1

Route	Quantity	Batch size proportion
A	2	1.00
B	2	0.92

10.6.2 Example 2

This example was first presented by Kondili *et al.* (1993). Two products are produced from three feeds according to the State-Task Network (STN) shown in Fig. 10.9. The STN utilizes five tasks which can be performed in four different units. The corresponding operational data for the example including units, tasks, and materials is given in Tables 10.3, 10.4, and 10.5. Six scenarios are considered in this problem. Table 10.6 shows scenario product demands and the probability corresponding to each of them. The objective is to maximize the expected profit within a time horizon of 18 h. following NIS policy.

For this example six different routes to produce final products exist which are depicted in Figures 10.10 to 10.15. The aforementioned fact leads to a six-dimension search region that includes 6,400 nodes. Before finding the optimal solution 318 nodes need to be tested for feasibility. The optimal solution has a expected profit of 2,475.31 m.u. The optimal schedule is shown in Figure 10.16 and the corresponding batch sizes are given in Table 10.7.

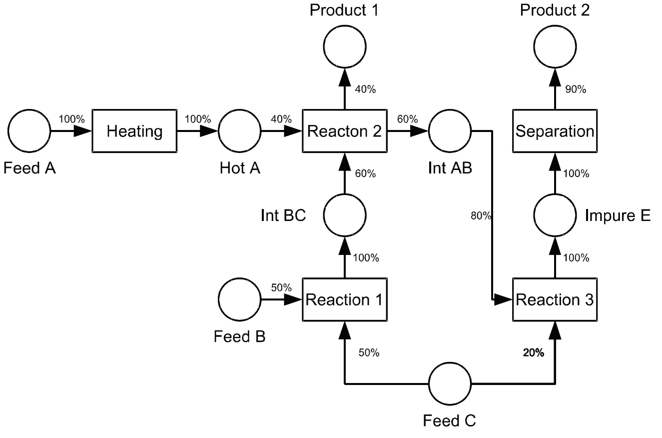


Figure 10.9: State-task network of example 2

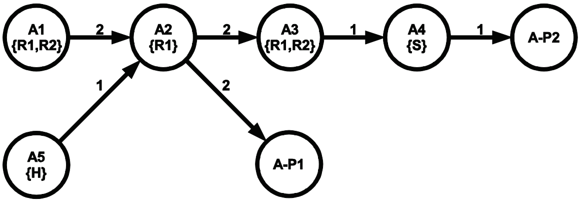


Figure 10.10: Route A for example 2

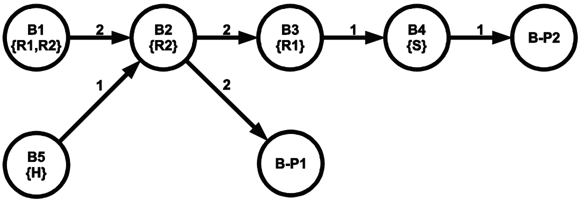


Figure 10.11: Route B for example 2

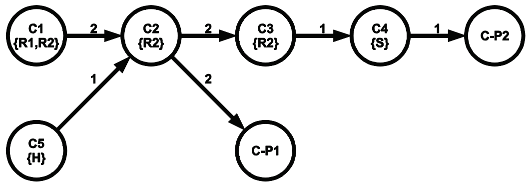


Figure 10.12: Route C for example 2

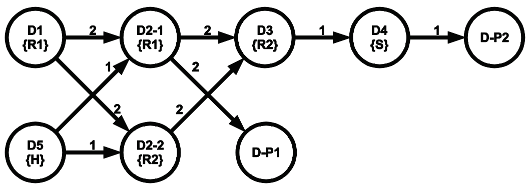


Figure 10.13: Route D for example 2

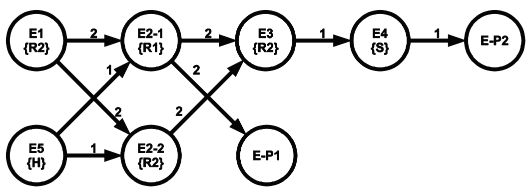


Figure 10.14: Route E for example 2

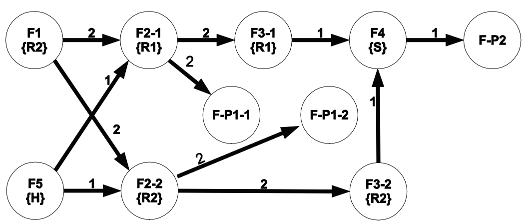


Figure 10.15: Route F for example 2

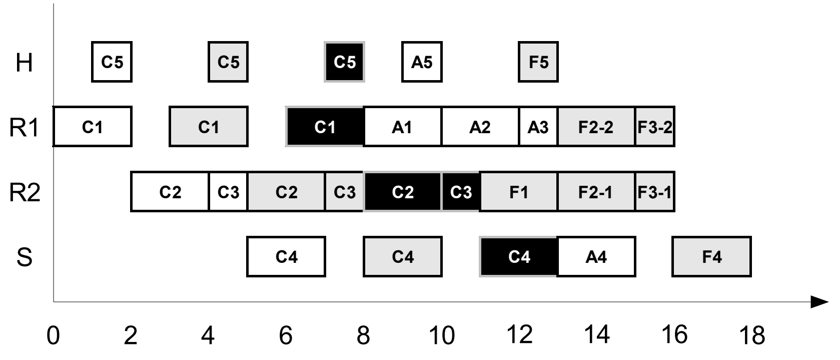


Figure 10.16: Optimal schedule for example 2

Table 10.3: Unit data for illustrative example 2

Unit	Maximum capacity (kg)	Suitable for task
Heater	100	Heating
Reactor 1	50	Reaction 1, 2, 3
Reactor 2	80	Reaction 1, 2, 3
Separator	200	Separation

Table 10.4: Task data for illustrative example 2

Task	Processing time (h)
Heating	1.0
Reaction 1	2.0
Reaction 2	2.0
Reaction 3	1.0
Separation	2.0

Table 10.5: Material data for illustrative example 2

States	Storage capacity (kg)	Market price (c.u.)	Overproduction cost (c.u.)	Underproduction cost (c.u.)
Feed A	Unlimited	0.00	0.00	0.00
Feed B	Unlimited	0.00	0.00	0.00
Feed C	Unlimited	0.00	0.00	0.00
Hot A	0.00	0.00	0.00	0.00
IntAB	0.00	0.00	0.00	0.00
IntBC	0.00	0.00	0.00	0.00
Impure E	0.00	0.00	0.00	0.00
Product 1	Unlimited	10.00	2.50	1.50
Product 2	Unlimited	10.00	2.50	1.50

Table 10.6: Scenario data for illustrative example 2

Scenario	Demand (kg)		Probability
	P1	P2	
I	102.3	174.8	0.167
II	148.8	344.2	0.167
III	158.6	128.2	0.167
IV	0.0	225.1	0.167
V	72.0	109.1	0.167
VI	54.6	268.8	0.167

Table 10.7: Optimal batch quantity and sizes for illustrative example 2

Route	Quantity	Batch size proportion
A	1	1.00
B	0	0.00
C	3	0.91
D	0	0.00
E	0	0.00
F	1	1.00

10.7 Final considerations

A new approach for solving scheduling problems under exogenous uncertainty is presented. The approach is based on the S-graph framework which has proven to be a rigorous and efficient tool for solving deterministic scheduling problems.

The proposed framework does not only inherit the advantages of S-graph, but it also has an advantage against stochastic programming techniques; namely the computational effort needed to solve the problem does not increase by increasing the number of scenarios. Such convenience relies on the fact that the search space size is independent on the number of considered scenarios. The size is uniquely dependent on the product batches combination. As the number of scenarios increases a larger LP is to be solved but still due to its nature the computational times are very small. Therefore, the presented framework has a great potential to solve industrial scale problems of scheduling under uncertainty.

Finally, note that this approach for scheduling under uncertainty can be integrated with the control strategy proposed in Chapter 11. Nevertheless, further work is needed so that other kind of objective function can be considered.

Part V

Hierarchical Decision Levels Integration

Chapter 11

Detailed Scheduling considerations into SCs Design

11.1 Introduction

One of the key components of enterprise-wide optimization is decision-making coordination and integration at all decision levels. In this chapter, a SC design-planning model, which translates a recipe representation to the supply chain environment, is coupled with a scheduling formulation so that decision levels integration is achieved. This approach enabled to assess the impact of considering scheduling aspects of process operations in the design of a SC network. A comparison of the proposed scheme and the traditional hierarchical approach shows the significance of such integration. Moreover, the scheduling details enable the dynamics of the SC to be better tracked. It is shown the degree to which a holistic decision-making model within a model predictive control framework is able to react to incidents occurring in the SC components, including disturbances arising from local monitoring, control and diagnosis of incidents in real time. Finally, a decomposition technique is applied to reduce the computational burden associated with the monolithic model solution. Validation of the proposed approach and the resulting potential benefits are highlighted by a case study.

11.2 Business decisions integration

The trend towards globalization has significantly increased the scale and complexity of current businesses. Businesses have become global networks that are made up of a number of business units and functions. Operational functions include R&D, production networks (continuous, discontinuous and discrete) and supply networks. These functions are buttressed by financial planning and marketing strategy functions. Businesses are subject to internal and external uncertainties. Examples of internal uncertainties include the success rate of R&D projects, given the technological risks involved, and disruptions to production, such as production failures and unforeseen stoppages. External uncertainties include those related to the cost of raw materials and products (unless they are subject to monopoly conditions), fluctuations in the exchange rate, and uncertainties in market size and demand, due to competition and macroeconomic factors. Businesses control their operations through the decisions they take about their capital expenditure, the financing of the company, growth strategies and operations. Strategic decisions about capital expenditure and planning include the technology used, the choice of R&D projects and decisions about infrastructure and SCM. Financial decisions are made by identifying the assets and liabilities required from the working capital for larger projects and operations, and by assessing and protecting the company from the risk of change. Examples of tactical production decisions include the following: planning activities in plants that are run on a discontinuous basis, to respond to anticipated demand; making decisions about the sources of energy used, in accordance with market prices; and increasing the production capacity in response to the pressures of demand. Current studies and solutions in the field of PSE and Operations Research tend only to consider subsets of such decisions, even though a business must act as a cohesive body in which its various functions are to a certain extent coordinated. Therefore, from a company's viewpoint, overall performance will be below optimum if strategic and tactical decisions are taken separately, as has been the practice to date. However, it is significantly more complex for a company to make decisions that involve its overall interests than to make decisions about specific functions. This explains why integral modeling that reflects the overall running of companies has been virtually unheard of to date.

The PSE community faces an increasing number of challenges, while enterprise and SCM remain subjects of major interest that offer multiple opportunities. Further progress in this area is thought to bring with it a unique opportunity to demonstrate the potential of the PSE approach to enhance a company's value. As previously mentioned, one of the key components of integrated SCM is decision-making coordination and integration at all levels. Most of the recent contributions offer models that separately address problems arising in the three, standard supply chain (SC) hierarchical decision levels (i.e., strategic, tactical aggregate planning and short-term scheduling).

As stated by Grossmann (2004), the major pending research problem is the integration of planning, scheduling and control, whether at plant or SC level. The nature of the SC planning problem is quite similar to the production scheduling problem. Both problems usually seek answers to the questions of in what amount, when and where to produce each of the products comprising the business portfolio so as to obtain financial returns. However, planning brings into play a broader, aggregated view of the problem. The time periods used in planning problems are usually longer than task processing times; thus, the sequencing/timing decisions in a scheduling problem are transformed into rough capacity decisions in a tactical planning problem. In fact, equipment capacity modeling is a highly sensitive aspect that must be taken into account in order to assure consistency and feasibility when problems are being integrated across SC hierarchical decision levels. Furthermore, at the strategic level, designing an SC network does not just involve selecting the type and size of the equipment, but also allocating this equipment to the different potential SC echelons. Therefore, we require an SC modeling approach that: (i) considers equipment capacity similarly at strategic and operational levels, so that this capacity can be aggregated and disaggregated in a straightforward and transparent manner; (ii) is able to handle strategic decisions associated with processes/equipment allocation to sites and not merely site locations; and (iii) easily represents the transport material and financial flows among SC sites at the scheduling level.

The external and internal dynamics of real businesses have not been totally represented by current models in a way that achieves desired consumer satisfaction levels and acceptable financial returns. Fluctuating demand patterns, increasing customer expectations and competitive markets, coupled with internal disturbances, mean that today's supply networks are not reliable in such an environment unless their external and internal dynamics are appropriately incorporated into the SC model. The ability to capture the dynamics of the SC has become a matter of survivability. The more survivable a network is, the more reliable it will be. As a result, another challenge is to characterize the dynamics in SCs to improve responsiveness. As indicated in Chapter 9, robust formulations have been proposed using stochastic optimization techniques (Tsiakis *et al.*, 2001; Gupta & Maranas, 2003; Guillén-Gosálbez *et al.*, 2005b). Such modeling approaches explicitly incorporate uncertainty into the model. Alternatively, predictive control technologies have been used to deal with uncertainties in SCs (Bose & Pekny, 2000; Vargas-Villamil & Rivera, 2000; Perea-López *et al.*, 2001; Seferlis & Giannelos, 2004). Particularly, some studies have developed approaches that focus on limiting a phenomenon known as the "bullwhip effect", which is the increase in fluctuation of demand upstream in the SC (Perea-López *et al.*, 2003; Mestan *et al.*, 2006). However, incorporating low-level decisions (local scheduling, supervisory control and diagnosis, incident handling) and the implications of incorporating these decisions for the dynamics of the entire SC (production switching between plants, dynamic product portfolios) have not yet been fully studied.

In general terms, the satisfactory management of a company's business matters requires the direct appraisal of the results of the decisions taken at various levels. This requires significant integration of a problem's multiple planning facets in non-conventional manufacturing networks and in multi-site systems. Financial matters are typically disregarded when SC operational decisions are addressed.

The aim of this chapter is to demonstrate that the integration of decision-making in businesses leads to significant added value. This chapter continues and extends the control strategy presented in Chapter 9 to more realistic and complex situations, which again demonstrate its ability to handle incidents that arise in the SC with visibility at both SC and plant levels in an integrated formulation that accounts for the optimization of a suitable financial performance indicator.

Here, it is presented a stochastic model in which it is possible to integrate the three classical SC hierarchical decision levels. For this purpose, the SC design-planning model proposed in Chapter 7 is used. This model translates a recipe representation to the SC context, thus facilitating the integration of scheduling decisions during SC design. Here, expected CV is the objective function to be maximized using a stochastic DFCF formulation. As stated in Chapter 9, such an approach is more effective than real options analysis. Moreover, the challenge of solving large multi-scale optimization problems becomes evident when decision level integration is considered. Therefore, a decomposition technique is applied to reduce the computational burden associated with the model solution. Finally, the scheduling details about production equipment enable the dynamics of SC to be tracked. By considering information from the equipment supervisory module, which we can incorporate into the scheduling formulation, it is possible to handle the incidents that may arise in the SC in low-level decisions. The main advantages of the integrated approach are highlighted by a case study in which the proposed strategy is compared with the traditional sequential, hierarchical approach.

11.3 SCM as a control strategy

It is noteworthy that SC planning is a dynamic activity. Firms are in the need of a closed-loop planning approach in order to preserve competitiveness. Such approach should be capable of revising planned activities, updating uncertain parameters (e.g., lead times, market demand and interest rates) and considering the effects of incidences; so that future plans are adapted to enhance SC performance under the current highly dynamic business environment. A Model Predictive Control (MPC) framework can be used as an appropriate approach to continuously improve the SC planning (see Chapter 9). Indeed, SCM can be conceived as an “onion-shell” comprised of different control loops, each corresponding to one hierarchical level. At the top level, the strategic decision making may integrate the mid-term planning, then midterm planning may incorporate short-term decision making. Decisions regarding each hierarchical level should be revised at different intervals depending on the nature of the problem being addressed so that the most recent information about SC state and uncertainties is taken into account. The strategic decisions of capacity expansion could be analyzed every year; while planning is usually revised every month or week. What is more, information from low level equipment control and supervisory modules can be used to feed the SC planning and scheduling decision making process. Such information can be utilized to account for equip-

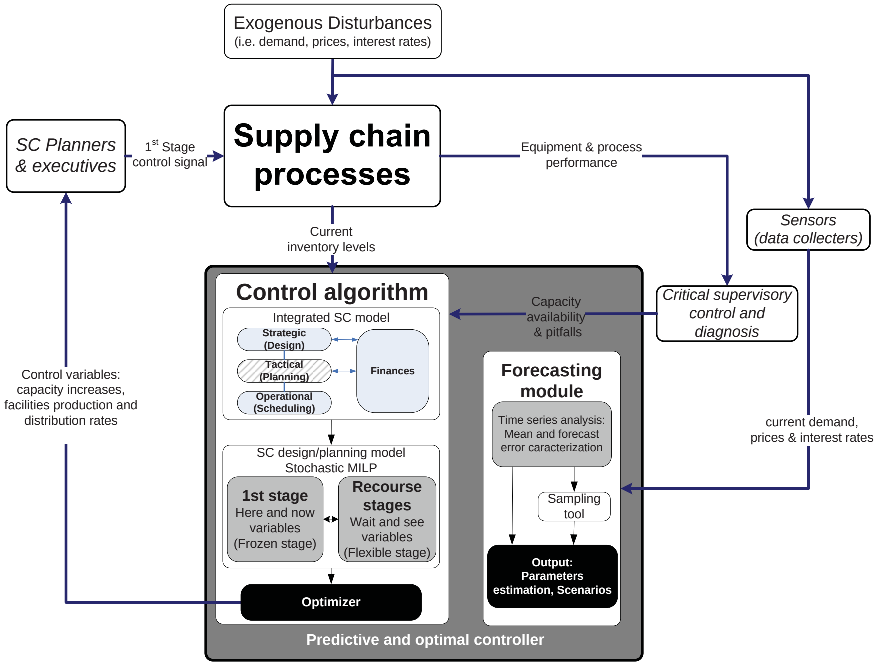


Figure 11.1: Control strategy for SCM

ment pitfalls and breakdowns, so that actual capacity availability is considered when planning-scheduling SC operations.

Briefly, an MPC framework attempts to optimize a performance criterion that is a function of the future control variables. By solving the optimization problem associated to the control algorithm all elements of the control signal are defined. However, only a portion of the control signal is applied to the system. Next, as new control input information and disturbance forecasts are collected, the whole procedure is repeated, which produces a feed-forward effect and enables the SC system to follow-up the process dynamics.

In Fig. 11.1, a general schematic of the proposed MPC framework for SCM is shown. Note that the strategy presented in Chapter 9 is enhanced in order to include scheduling decisions and information from supervisory systems as well. It follows a brief description of the control strategy. When the SC process is disturbed, data required to describe the current SC state are captured and sent to the controller. This information include the actual SC state (e.g., current inventory levels, new historic demand data, capacity availability). The information related to capacity can be collected by a supervisory system. Such system may be able to collect information about the critical equipment capacity which is then given as input data to the SC control algorithm. On the other hand, information about those external parameters regarded as uncertain in the mathematical model is sent to the forecasting model. That module computes the mean value and does the forecast error characterization for each uncertain parameter so as to define the different scenarios to be considered in the predictive model. This consist in a multistage stochastic mathematical model. The variables associated to first stage decisions are the control signal that is implemented in the SC processes. In fact, first stage variables are associated to next period decisions which are made prior to uncertainty realization.

Notice that for the actual period the proposed algorithm is considering the detailed scheduling, therefore disturbances can be contemplated as frequent as the time bucket considered by the scheduling formulation. It is also important to point out that we are integrating the three standard hierarchical decision levels; however more decision levels may exist in an organization. The disturbances can be considered as frequent as the time bucket of the lower decision level allows when using discrete time SC formulations. Continuous time SC formulations should overcome this drawback.

It is important to point out that the proposed control strategy allows to handle uncertainty and incidences by combining reactive and preventive approaches. A pro-active treatment of uncertainty is included by means of stochastic programming. The review and update process that is required to tackle incidences and changes in random factors is performed by introducing the SC stochastic holistic model into a MPC framework.

As shown in Fig. 11.1, the predictive controller entails a stochastic multiperiod design/ planning/ scheduling MILP model of a multi-echelon SC with financial considerations. The model assumes that different technological equipment is available to be installed in potential sites and assists in their selection. Regarding the financial area, again the mathematical program endeavors to evaluate the CV by using a DFCF method.

11.4 The predictive model

The stochastic SC design – planning – scheduling model is presented next. This section has been divided in three parts: (i) the scenario tree representation of uncertainty and (ii) the operations model.

11.4.1 Scenario tree

Here, it is followed the notation introduced in Chapter 9. The reader is referred to Section 9.4.1 for more details. It will be useful to recall sets T_l, L_t and $AH_{l^*\hbar_l}$. Here, it is also assumed that there are $|L|$ events in which uncertainty (ξ) unfolds over the planning horizon. The value that random factors can take in event l can be identified by index h_l which belongs to set H_l. Then, $\hbar_l$ is the combination of event realizations identified by $(h_1, h_2, \dots, h_l)$. T_l is the subset of planning periods t that are associated to uncertain event l. L_t is the reciprocal set of T_l. L_t is the event l which is related to period t. Finally, $AH_{l^*\hbar_l}$ is defined to be given by $AH_{l^*\hbar_l} = \{\hbar_{l^*} | \hbar_{l^*} \subseteq \hbar_l\}$, that is $AH_{l^*\hbar_l}$ denotes the event combination related to l^* ($\hbar_{l^*}$) which is ancestor of $\hbar_l$. Notice that it is not necessary $\hbar_{l^*}$ to be a proper subset of $\hbar_l$ in order to allow the case when $l = l^*$.

11.4.2 Operations model

Here, the SC operations model presented in Chapter 7 is extended to a stochastic version. That chapter proposes a flexible SC design-planning formulation whose distinctive features are that (i) considers all feasible links and material flows among the potential SC components inherently and (ii) does not need any pre-established process network superstructure so that the sub-trains (if any) in which production process is decoupled and their location are determined by the model. Consequently, the model does merely require as input the SC production process recipe representation. Furthermore, a more appropriate description of manufacturing processes at the SC level is achieved by translating a recipe representation to the SC environment. Finally, it is worth mentioning given that the SC model is a translation of a classical multipurpose plant scheduling formulation it facilitates the consideration/integration of scheduling decisions while designing a SC.

The SC operations model can be divided in four parts: mass balance equations, constraints related to design and capacity modeling, market and suppliers limitations, and those equations that allow integrating scheduling implications within strategic-tactical SC decision making.

Mass Balances

Mass balances must be satisfied for each material in every facility that integrates the SC network. Equation (11.1) represents the material balance for each facility f and state s in every period t and every combination of events $\hbar_l$. In this equation, it is taken into account the inventory of previous period ($S^{l^*}_{sft-1\hbar_{l^*}}$) related to the combination of events that is ancestor of $\hbar_l$ ($l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}$). Change in inventory ($S^l_{sft\hbar_l} - S^{l^*}_{sft-1\hbar_{l^*}}$) must be equal to the difference between the material produced/transported by tasks whose destination is facility f ($P^l_{ijf'ft\hbar_l}$) and material consumed by tasks whose origin is facility f ($P^l_{ijff't\hbar_l}$). Here, α_{sij} and $\bar{\alpha}_{sij}$ represent the mass fraction coefficient of material s for task i performed in equipment j.

$$St^l_{sft\hbar_l} - St^{l^*}_{sft-1\hbar_{l^*}} = \sum_{f'} \sum_{i \in T_s} \sum_{j \in (J_i \cap \hat{J}_{f'})} \alpha_{sij} P^l_{ijf'ft\hbar_l} - \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (J_i \cap \hat{J}_f)} \bar{\alpha}_{sij} P^l_{ijff't\hbar_l} \quad (11.1)$$
$$\forall\ s, f \notin (Sup \cup M), \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*\hbar_l}$$

Design and capacity constraints

Equation (11.2) is to control the changes in the facilities capacity over time. These constraints include binary variables $V_{jft\hbar_{l-1}}$, which take a value of 1 if the facility being represented is expanded in capacity, otherwise is set to zero. The capacity increments are bounded in the range $[FJE^L_{jft}, FJE^U_{jft}]$, which represents the realistic interval where they must fall. Equation (11.3) is added to update the total capacity ($F_{jftjft\hbar_l}$) by the amount increased during planning period t ($FE_{jft\hbar_l}$).

Equation (11.4) forces the total production/distribution rate in each facility to be greater than a minimum desired capacity utilization and lower than the available capacity. In this equation, $\theta_{ijff'}$ represents the capacity utilization rate of equipment j by task i. Here, β_{jf} expresses the minimum percentage of utilization of equipment j at site f. Recall that the model considers that task i is to be performed in equipment that is installed on the facility of "origin".

$$\begin{gathered} V^l_{jft\hbar_{l-1}} FE^L_{jft} \leq FE^l_{jft\hbar_{l-1}} \leq V^l_{jft\hbar_{l-1}} FE^U_{jft} \\ \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, l, \hbar_{l-1}, t \in T_l \end{gathered} \tag{11.2}$$

$$\begin{aligned} F^l_{jft\hbar_l} &= F^{l^*}_{jft-1\hbar_{l^*}} + FE^l_{jft\hbar_{l-1}} \\ \forall\ f \notin (Sup \cup M), j &\in \hat{J}_f, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \\ \hbar_{l^*} &\in AH_{l^*,\hbar_l}, \hbar_{l-1} \in AH_{l-1,\hbar_l} \end{aligned} \tag{11.3}$$

$$\begin{gathered} \beta_{jf} F^l_{jft\hbar_l} \leq \sum_{f'} \sum_{i \in I_j} \theta_{ijff'} P^l_{ijff't\hbar_l} \leq F^l_{jft\hbar_l} \\ \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, j \notin JStor, l, \hbar_l, t \in T_l \end{gathered} \tag{11.4}$$

In the same way, total inventory in facility f is constrained to be equal to or lower than the available capacity ($F^l_{jft\hbar_l}$) in each period t and combination of events $\hbar_l$ (Eq. (11.5)). In this equation, υ_s holds for specific volume of material s.

$$\begin{gathered} \sum_s \upsilon_s St^l_{sft\hbar_l} \leq F^l_{jft\hbar_l} \\ \forall\ f \notin (Sup \cup M), j \in \hat{J}_f, j \in JStor, l, \hbar_l, t \in T_l \end{gathered} \tag{11.5}$$

Markets and suppliers

Eq. (11.6) is to compute the sales of state s executed at each market. Eq. (11.7) forces the sales of state s carried out in markets during time period t to be less than or equal to the demand. While, equation (11.8) imposes a minimum target for the demand satisfaction ($MinCLS$), which must be attained in all periods t and event combinations $\hbar_l$.

$$\sum_{f' \notin M} \sum_{i \in (T_s \cap Tr)} \sum_{j \in (J_i \cap \hat{J}_f)} \alpha_{sij} P^l_{ijf'ft\hbar_l} = Sales^l_{sft\hbar_l} \qquad \forall\ s \in FP, f \in M, l, \hbar_l, t \in T_l \tag{11.6}$$

$$Sales^l_{sft\hbar_l} \leq Dem^l_{sft\hbar_l} \qquad \forall\ s \in FP, f \in M, l, \hbar_l, t \in T_l \tag{11.7}$$

$$\frac{\sum\limits_{f \in M} Sales^l_{sft\hbar_l}}{\sum\limits_{f \in M} Dem^l_{sft\hbar_l}} \geq MinCLS \qquad \forall\ s \in FP, l, \hbar_l, t \in T_l \tag{11.8}$$

The model assumes a maximum availability of raw materials. Therefore, Eq. (11.9) forces the amount of raw material, $s \in RM$, purchased from location $f \in Sup$ at each period t to be lower than an upper bound A_{sft}. In this expression, R_f denotes the set of raw materials that can be obtained from location f.

$$\sum_{f' \notin Sup} \sum_{i \in (\bar{T}_s \cap Tr)} \sum_{j \in J_i} \bar{\alpha}_{sij} P^l_{ijff't\hbar_l} \leq A_{sft} \qquad \forall\ f \in Sup, s \in R_f, l, \hbar_l, t \in T_l \tag{11.9}$$

Integration of SC scheduling

The scheduling formulation is an extension of STN representation (Kondili *et al.*, 1993). Here, the formulation permits scheduling in multiple facilities. The proposed model divides the planning horizon into H periods of length $H1$ where aggregated production is planned by using the previous model. Time buckets at this level are represented by index t. The first planning period ($t = 1$) of the time horizon is divided into time intervals of lower length $H2$ where detailed scheduling is executed as depicted in Fig. 11.2. Time buckets at the scheduling level are represented by index t_k. When the proposed control strategy is applied, the model is to be rerun every planning period t as new information regarding disturbances and SC state are updated (i.e., the model is to be applied following a rolling horizon approach).

The equations concerning the short term decision level can be classified into two groups; namely, the detailed scheduling constraints and the integrating equations. The expressions that account for the mass balance, the assignment and the batch sizes restrictions are gathered into the set of detailed scheduling equations. The latter group includes those equations that assure the consistency between planning and scheduling models.

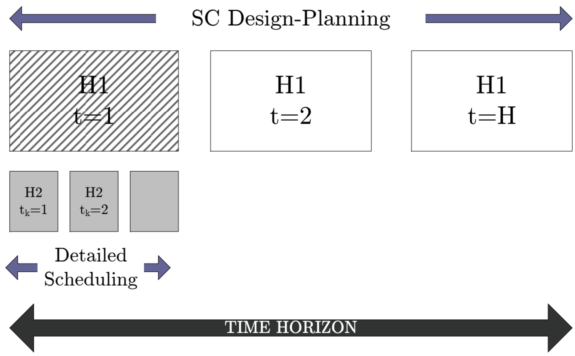


Figure 11.2: Rolling horizon strategy

Detailed scheduling equations Eq. (11.10) is the mass balance applied at each time interval (t_k). It can be noticed that this equation is very similar to the mass balance in the planning formulation (Eq. (11.1)). The basic assignment constraint is stated by Eq. (11.11).

$$\begin{aligned} Ssched^l_{sft_k\hbar_l} - Ssched^l_{sft_k-1\hbar_l} &= \sum_{i\in T_s} \sum_{j\in(J_i\cap\hat{J}_f)} \alpha_{sij} B^l_{ijft_k-pt_i\hbar_l} \\ &- \sum_{i\in\bar{T}_s} \sum_{j\in(J_i\cap\hat{J}_f)} \bar{\alpha}_{sij} B^l_{ijft_k\hbar_l} + RawM^l_{sft_k\hbar_l} \\ &\forall\ s, f \notin (M\cup Sup), t_k \in L_{t_k}, \hbar_l \end{aligned} \tag{11.10}$$

$$\sum_{i\in J_i} \sum_{t'_k=t_k}^{t'_k=t_k-pt_i+1} W^l_{ijft'_s\hbar_l} \leq 1 \qquad \forall\ f \notin (M\cup Sup), j\in(J_{batch}\cap\hat{J}_f), t_k, l\in L_{t_k}, \hbar_l \tag{11.11}$$

The capacity limits for equipment can be approximated as follows:

$$B^l_{ijft_k\hbar_l} \leq \left(\frac{pt_i}{\theta_{ijff}}\right) W^l_{ijt_k\hbar_l} \quad \forall\ i, j, f \notin (Sup\cup M), t_k, l\in L_{t_k}, \hbar_l \tag{11.12}$$

Notice that the supervisory control is providing to the mathematical model updated information about installed capacity. Once a equipment failure is diagnosed, its implications on capacity availability are passed to the model. Specifically, the batch sizes ($B^l_{ijft_k\hbar_l}$) associated to activities to be performed in a failed equipment j are restricted to be equal to zero while the failure is repaired. Then, one can observe that capacity turns out to be the essential factor integrating the different hierarchical levels; even more the supervisory and control module is linked to the predictive model by means of capacity.

Integrating equations The integration between design-planning and scheduling models is carried out through Eqns. (11.13) – (11.15). Eq. (11.13) states that production allocated in equipment j is identical in both hierarchical levels. In Eq. (11.14) the availability of raw material is computed from received materials according to the planning formulation. Raw material availability ($RM^l_{sft_k\hbar_l}$) is then included into the scheduling mass balance (Eq. (11.10)). Scheduling equations may be applied in more than one planning period. The appropriate equations for incorporating scheduling in first planning period ($t = 1$) are presented next.

$$P^l_{ijfft\hbar_l} = \sum_{t_k} B^l_{ijft_k\hbar_l} \qquad \forall\, f, j \in (J_{batch} \cap J_f), i \in I_j, t = 1, l \in L_t, \hbar_l \quad (11.13)$$

$$RawM^l_{sft_k\hbar_l} = \sum_{f' \neq f} \sum_{i \in \bar{T}_s} \sum_{j \in J_i} \bar{\alpha}_{sij} P^l_{ijf'ft\hbar_l} \qquad \forall\, s, f, t_k = 1, t = 1, l \in L_t, \hbar_l \quad (11.14)$$

Finally, Eq. (11.15) is included to rectify capacity availability in the planning model. This correction is done based on the scheduling model task assignment ($W^l_{ijt_k\hbar_l}$). Eq. (11.15) should be merely applied to those equipments which are production bottlenecks. Additionally, it is worth to mention that it must be checked that market demand is not actually the bottleneck process in the planning period, where scheduling is performed.

$$\sum_{i \in I_j} \theta_{ijff} P^l_{ijfft\hbar_l} \leq \sum_{i \in I_j} \sum_{t_k} W^l_{ijft_k\hbar_l} pt_i \qquad \forall\, f, j \in (J_{bottle} \cap \hat{J}_f), t > 1, l \in L_t, \hbar_l \quad (11.15)$$

As it can be noticed, Eqns. (11.10) to (11.15) can be easily unplugged from the whole operations model in case the SC manager decides not to consider scheduling issues.

11.4.3 Integration between operations and financial model

The integration between the operations and financial formulations is carried out again through: the sales of products, the purchases of raw materials, transport services and utilities to final providers, the fixed cost associated with SC network operation and the total capital investment.

Operating income

Revenue is calculated by means of net sales which are the income source related to the normal SC activities. Thus, the total income incurred in any period t

can be easily computed from the sales of products executed in period t as it is stated in Eq. (11.16).

$$ESales^{l}_{t\hbar_l} = \sum_{s\in FP}\sum_{f\in M} Sales^{l}_{sft\hbar_l} Price^{l}_{sft\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{11.16}$$

Operating cost

Indirect cost The total fixed cost of operating a given SC structure can be computed using equation (11.17). $FCFJ_{jft}$ is the fixed unitary capacity cost for production and distribution equipment.

$$FCost^{l}_{t\hbar_l} = \sum_{f\notin(Sup\cup M)}\sum_{j\in\hat{J}_f} FCFJ_{jft}F^{l}_{jft\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{11.17}$$

Direct cost The cost of purchases from supplier e, which is computed through Eq. (11.18), includes purchases of raw materials, transportation, and production resources. Let us notice that e refers to supplier entity and not to supplier location f ($f \in Sup$).

$$EPurch^{l}_{et\hbar_l} = Purch^{rm,l}_{et\hbar_l} + Purch^{tr,l}_{et\hbar_l} + Purch^{prod,l}_{et\hbar_l} \qquad \forall\ l, \hbar_l, t \in T_l \tag{11.18}$$

The purchases ($Purch^{rm,l}_{et\hbar_l}$) associated to raw materials made to supplier e can be computed through Eq. (11.19). Here, ψ_{est} is the cost associated to raw material s purchased from supplier e. Since it is assumed that several suppliers of raw materials may exists, Eq. (11.20) expresses that the total quantity of raw materials purchased in period t must be equal to the sum of the amounts purchased from each supplier e.

$$Purch^{rm,l}_{et\hbar_l} = \sum_{s\in RM_e}\sum_{f\in Sup} Purch^{l}_{esft\hbar_l}\psi_{est} \qquad \forall\ e, l, \hbar_l, t \in T_l \tag{11.19}$$

$$\sum_{f'}\sum_{i\in(\bar{T}_s\cap Tr)}\sum_{j\in J_i} \bar{\alpha}_{sij} P^{l}_{ijff't\hbar_l} = \sum_{E_s} Purch^{l}_{esft\hbar_l} \qquad \forall\ s \in RM, f \in Sup, l, \hbar_l, t \in T_l \tag{11.20}$$

Otherwise, for the sake of simplicity external transportation services as well as production resources are assumed to be "acquired" each of them from one unique supplier (i.e., $|\tilde{E}_{tr}| = |\hat{E}_{prod}| = 1$). Production and transportation costs are determined by Eqns. (11.21) and (11.22), respectively. Here, $\rho^{tr}_{eff'}$ denotes the unitary transportation cost associated with sending products from location

f to location f'; while τ^{ut1}_{ijfe} represents the unitary production cost associated to perform task i in processing equipment j, and τ^{ut2}_{sfe} represents the unitary inventory costs.

$$Purch^{tr,l}_{et\hbar_l} = \sum_{i\in Tr}\sum_{j\in J_i}\sum_{f}\sum_{f'} P^l_{ijff't\hbar_l}\rho^{tr}_{eff'} \qquad \forall\ e\in \tilde{E}_{tr}, l, \hbar_l, t\in T_l \tag{11.21}$$

$$\begin{gathered} Purch^{prod,l}_{et\hbar_l} = \sum_{f}\sum_{i\notin Tr}\sum_{j\in(J_i\cap\hat{J}_f)} P^l_{ijfft\hbar_l}\tau^{ut1}_{ijfe} + \\ \sum_{s}\sum_{f\notin(Sup\cup M)} St^l_{sft\hbar_l}\tau^{ut2}_{sfe} \qquad \forall\ e\in \hat{E}_{prod}, l, \hbar_l, t\in T_l \end{gathered} \tag{11.22}$$

Capital investment

Finally, the total investment on fixed assets is computed through Eq. (11.23). This equation includes the investment made to expand the equipment j capacity in facility site f at period t ($Price^{FJ}_{jft}FE^l_{jft\hbar_l}$), plus the investment required to open a manufacturing plant in location f, in case it is opened at period t ($I^J_{ft}JB^l_{ft\hbar_l}$), plus the investment required to set a distribution center if it is opened at period t ($I^S_{ft}SB^l_{ft\hbar_l}$). Here, $JB^l_{ft\hbar_l}$ and $SB^l_{ft\hbar_l}$ are binary variables which take value of 1 in case the facility being represented, processing site or distribution center, starts construction in period t.

$$\begin{gathered} FAsset^l_{t\hbar_l} = \sum_{f}\sum_{j} Price^{FJ}_{jft}FE^l_{jft\hbar_{l1}} + \\ \sum_{f}\left(I^S_{ft}SB_{ft\hbar_l} + I^J_{ft}JB^l_{ft\hbar_l}\right) \qquad \forall\ l, \hbar_l, t\in T_l \end{gathered} \tag{11.23}$$

Equations (11.24) and (11.25) are to force definition of variable JB_{ft}, while Eqns. (11.26) and (11.27) restrict variable SB_{ft}.

$$\begin{gathered} \sum_{j\in(J_f\cap JProd)}\left(\sum_{t'\le t}\sum_{l^*\in L_{t'}}\sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} JB^{l^*}_{ft'\hbar_{l^*}} - V^l_{jft\hbar_{l-1}}\right) \ge 0 \\ \forall\ f\notin(Sup\cup M), l, \hbar_{l-1}, t\in T_l \end{gathered} \tag{11.24}$$

$$\sum_{t}\sum_{l^*\in L_t}\sum_{\hbar_{l^*}\in AH_{l^*\hbar_l}} JB^{l^*}_{ft\hbar_{l^*}} \le 1 \qquad \forall\ f\notin(Sup\cup M), t=T, l\in L_t, \hbar_l \tag{11.25}$$

$$\sum_{j \in (J_f \cap JStor)} \left(\sum_{t' \leq t} \sum_{l^* \in L_{t'}} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} SB^{l^*}_{ft'\hbar_{l^*}} - V^{l}_{jft\hbar_{l-1}} \right) \geq 0 \qquad \forall\, f \notin (Sup \cup M), l, \hbar_{l-1}, t \in T_l \tag{11.26}$$

$$\sum_{t} \sum_{l^* \in L_t} \sum_{\hbar_{l^*} \in AH_{l^* \hbar_l}} SB^{l^*}_{ft\hbar_{l^*}} \leq 1 \qquad \forall\, f \notin (Sup \cup M), t = T, l \in L_t, \hbar_l \tag{11.27}$$

11.4.4 Financial model

The financial model aims at computing the expected corporate value ($E[CV]$) which is the objective function to be maximized. The financial model and the expressions required to compute the objective function are similar to the ones presented in Chapter 9. The reader is referred to Section 9.4.2 for details.

The stochastic problem embedded in the control algorithm can be thus mathematically posed as follows:

$$\begin{gathered} \underset{\mathscr{X},\mathscr{Y}}{\text{Maximize}}\ E[CV] \\ \text{subject to} \\ \text{Eqns } 11.1 - 11.27;\ 9.22 - 9.55 \\ \mathscr{X} \in \{0,1\};\ \mathscr{Y} \in \mathbb{R} \end{gathered}$$

Here, $\mathscr{X}$ denotes the model binary variables set, while $\mathscr{Y}$ represents the model continuous variable set. This model considers demand as uncertain parameter, however it can be easily extended to consider other parameters' uncertainty. The only change to be done is to add the indexes l and $\hbar_l$ to the new uncertain parameter. These indexes identify and locate the parameter inside the scenario tree. Problems considering prices and interest rates uncertainty have been tackled in Chapter 9.

11.5 Case study

This example was first introduced by You and Grossmann (2008). This case study, which is also utilized in Chapter 7, is motivated by a real world application concerning a polystyrene SC design. The polystyrene production process is shown in Fig. 11.3. Styrene monomers are produced from ethylene and benzene, then styrene is processed to obtain five final products: three different types of solid polystyrene (SPS) and two types of expandable polystyrene (EPS). It is assumed that only one type of reactor can be installed for each production task (i.e., I, II, III) The equipment capacity may be increased in a discrete manner which corresponds to quantity of installed reactors. Additionally, it is considered that a cleaning task must be performed when shifting to a different polystyrene production. Potential benzene suppliers are located in Texas (TX), Louisiana (LA), and Alabama (AL); while ethylene suppliers are located in Illinois (IL), TX and Mississippi (MS). Customers are aggregated into nine sale regions according to their geographical proximity. Distribution centers and processing plants may be established in eight different states which are Michigan (MI), TX, California (CA), LA, Nevada (NV), Georgia (GA), Pennsylvania (PA), and Iowa (IA). Figure 11.4 shows the SC components location.

An horizon of four years is considered. Each year is composed of twelve monthly planning periods. In this example, market demand is regarded as an uncertain factor which unfolds every year. It is considered that demand may unveil into three different events leading to a scenario tree which contains 81 scenarios. Given that the considered demand pattern does not show any trend and seasonal component, simple exponential smoothing techniques are used in the forecasting module in order to determine the mean values and the forecast error characterization. A methodology to generate scenarios from demand forecasting has been proposed in Section 9.5. Such methodology has been applied in this chapter. Basically, the forecast errors distributions depend on previous errors and how many periods ahead the forecast is being done. If the correct forecasting model has been chosen, and if the statistical procedure used to estimate parameters in the model yields unbiased estimates, then the expected forecast error will be zero and its standard deviation (σ) can be easily calculated (Montgomery *et al.*, 1990). Once the standard deviation error is calculated, a Montecarlo sampling method can be applied to the error probability distribution described by $N(0, \sigma)$ in order to obtain error scenarios. Later on, error is added to the mean demand to get their corresponding demand scenarios. To approximate the multistage stochastic problem solution, the two stage shrinking horizon (SHT) approach presented in the work of Balasubramanian and Grossmann (2004) is used.

The case study has been also solved using a sequential manner in order to emphasize the benefits that may be gained by using the proposed integrated approach. In the sequential approach, the scheduling is not considered when dealing with the design of the SC network. Under this scheme, decisions are

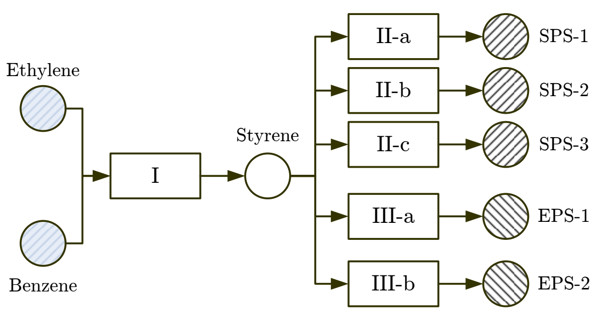


Figure 11.3: Polystyrene production process

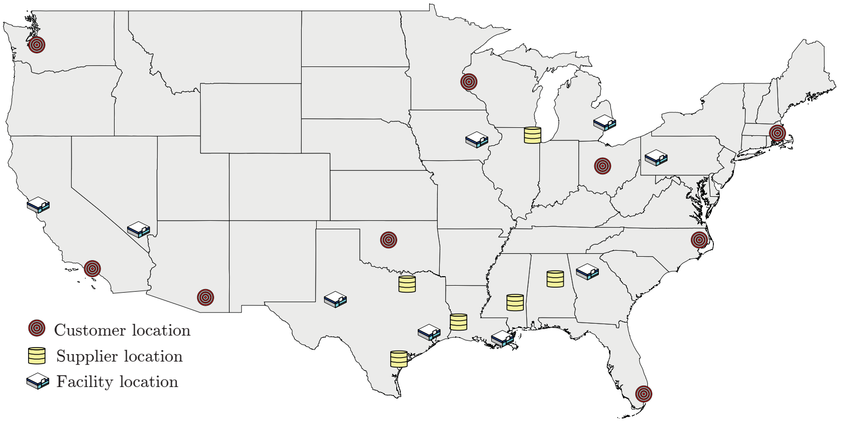


Figure 11.4: Potential SC echelons location map

made following a hierarchical decision-making process. First the SC design decisions are made in an isolated manner. Then, once the SC network configuration has been obtained, the planning and scheduling decisions are determined. Otherwise, the integrated approach considers planning and scheduling decisions when designing the SC network. The integrated approach is deployed by using the MILP previously described.

The case study results are divided in three subsections. Firstly, the SC design problem is tackled. From this first step, the optimal SC network configurations for both approaches (i.e., sequential and integrated) are obtained. Secondly, both solutions are tested using the MPC loop; so that operations are scheduled for every period following a rolling horizon procedure. Here, it is demonstrated how well SC configurations work when deployed for daily operations use (i.e, considering scheduling details). As a matter of fact, the results from this step show a more adequate performance assessment of the optimal SC network configurations. Finally, it is shown how equipment failures are resolved using the MPC algorithm.

11.5.1 The design problem

In the first step of the control strategy, a SC design problem is solved. The scheduling model is taken into consideration in the first month for the integrated approach. As shown in Figure 11.5, the $E[CV]$ and financial risk for the traditional sequential approach seem to yield better values. Here, financial risk can be defined as the probability of not meeting a certain CV level. For this case study, the integrated approach results in a solution 2.05% lower than the sequential one. However, it should be emphasized that SC performance may worsen when executing detailed scheduling for the sequential approach. Evidently, capacity aggregation considered at the design level results in higher nominal plant productivity, since idle times introduced by task sequencing and

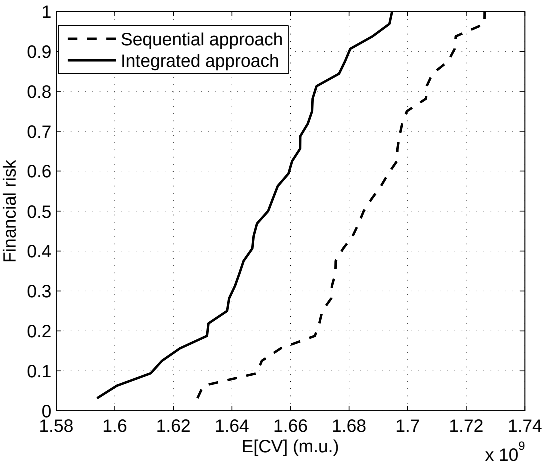


Figure 11.5: Risk curve for Corporate Value (Sequential approach: $E[CV] = 1.68\text{x}10^9$ m.u.; Integrated approach: $E[CV] = 1.65\text{x}10^9$ m.u.)

changeovers are disregarded at the strategic level. The integrated approach avoids this situation by incorporating the scheduling formulation in the design problem. Therefore, no proper comparison nor conclusions can be drawn from these preliminary results.

The optimal configuration obtained by addressing the SC design-planning problem using the sequential approach is shown in 11.6; while the optimal SC network configuration resulting from the integration of the three hierarchical decision levels is shown in 11.7. As it can be noticed, the SC network configurations proposed by each approach are quite different. The integrated approach installs equipment technology II in three additional sites, namely, LA, MI, TX (Midland); while equipment technology III is also installed in three additional sites, namely, TX (Houston), GA, IA. In those figures, it is shown that more capacity is installed for equipment technologies II and III by the integrated approach. This is a result of a more adequate capacity assessment, which is accomplished by considering scheduling issues (e.g., cleaning times, changeovers) in the SC design phase.

Lagrangian Decomposition

The Optimal Condition Decomposition (OCD), which is a particular case of the Lagrangian relaxation procedure, is applied to overcome the computational cost of solving the monolithic problem which integrates the design, planning and scheduling formulations. Further details about this decomposition strategy can be found in Section 3.8.1.

The variables which are complicating the integrated mathematical model are the first stage, design variables ($V^l_{jft\hbar_{l-1}}, FE^l_{jft\hbar_{l-1}}$). These two variables

Location	Equipment (h/period) I	Equipment (h/period) II	Equipment (h/period) III	Distribution center (c.u.)
TX (Houston)	18000.0	3600.0		1080.0
CA	1440.0	1440.0		
LA	18720.0		2880.0	832.0
MI	1440.0		1440.0	
TX (Midland)				633.1
GA				576.3
IA				287.6

Installed

Not installed

Figure 11.6: Optimal network configuration obtained by using the sequential approach

are duplicated so that one copy exists for every combination of events ($\hbar_l$). The following constraints have been added in order to do so.

$$\tilde{V}^l_{jft\hbar_l} - V^l_{jft\hbar_{l-1}} = 0$$
$$\forall\ f \notin (Sup \cup M), j \in \hat{J}_f, l, t \in T_l, \hbar_l, \hbar_{l-1} \in AH_{l-1,\hbar_l} \tag{11.28}$$

$$\tilde{FE}^l_{jft\hbar_l} - FE^l_{jft\hbar_{l-1}} = 0$$
$$\forall\ f \notin (Sup \cup M), j \in \hat{J}_f, l, t \in T_l, \hbar_l, \hbar_{l-1} \in AH_{l-1,\hbar_l} \tag{11.29}$$

Now, the affected Eqns. 11.2 and 11.3 are rewritten in terms of the proper duplicated variables.

$$\tilde{V}^l_{jft\hbar_l} FE^L_{jft} \leq \tilde{FE}^l_{jft\hbar_l} \leq \tilde{V}^l_{jft\hbar_l} FE^U_{jft}$$
$$\forall\ f \notin (Sup \cup M), j \in \hat{J}_f, l, \hbar_l, t \in T_l \tag{11.30}$$

$$F^l_{jft\hbar_l} = F^{l^*}_{jft-1\hbar_{l^*}} + \tilde{FE}^l_{jft\hbar_l}$$
$$\forall\ f \notin (Sup \cup M), j \in \hat{J}_f, l, \hbar_l, t \in T_l, l^* \in L^*_{t-1}, \hbar_{l^*} \in AH_{l^*,\hbar_l} \tag{11.31}$$

The main difference between the OCD and the classical Lagrangian decomposition is that the OCD does not dualize all the complicating constraints. Here, a subproblem is constructed for every scenario ($\hbar_L$). Let us define $\hbar_{L'}$ as the scenario that is being evaluated in each subproblem. Then, the Lagrangian decomposition is applied by dualizing those Eqns. (11.28) and (11.29) that belong

Location	Equipment (h/period) I	II	III	Distribution center (c.u.)
TX (Houston)	18000.0	2880.0	720.0	957.0
CA	720.0	1440.0		
LA	18000.0	720.0	2880.0	938.8
MI	1440.0	720.0	2160.0	536.2
TX (Midland)		720.0		501.5
GA			720.0	606.7
IA			720.0	

Installed
Not installed

Figure 11.7: Optimal network configuration obtained by using the integrated approach

to other subproblems (i.e., scenarios). Notice that the following subproblem is decomposable when the Lagrange multipliers (π^I, π^{II}) and the duplicated variables for other scenarios are fixed to a given value. Also it noteworthy that constraints (11.28) and (11.29) related to the scenario being evaluated $(\hbar_{L'})$ are left into the subproblem, so that their corresponding dual variables (i.e., π^I, π^{II}) are obtained and updated using the subproblem solution.

$$
\begin{aligned}
&\text{maximize} \quad P_{\hbar_L'}^{L'} CV_{\hbar_L'}^{L'} \\
&+ \sum_{f \notin (Sup \cup M)} \sum_{j \in \hat{J}_f} \sum_{l} \sum_{t \in T_l} \sum_{\hbar_l \notin AH_{l,\hbar_{L'}}} \sum_{\hbar_{l-1} \in AH_{l-1,\hbar_l}} \left(\pi^I_{f,j,l,t,\hbar_l,\hbar_{l-1}} \left(\tilde{V}^l_{jft\hbar_l} \right.\right. \\
&\left.\left. - V^l_{jft\hbar_{l-1}} \right) + \pi^{II}_{f,j,l,t,\hbar_l,\hbar_{l-1}} \left(\tilde{FE}^l_{jft\hbar_l} - FE^l_{jft\hbar_{l-1}} \right) \right) \qquad (11.32) \\
&\text{subject to} \\
&\text{Eqns. } 11.1;\ 11.4 - 11.31;\ 9.22 - 9.55 \qquad \forall\ \hbar_l \in AH_{l,\hbar_{L'}}
\end{aligned}
$$

The decomposition procedure is described in Algorithm 11.1. The decomposition subproblems complexity for this case study is presented in Table 11.1.

Table 11.1: Decomposition subproblems complexity

Problem	Iterations	Equations	Variables	Discrete Variables	Time (CPU sec)
Decomposed	9	80,256	780,612	14,724	49,885

As shown, this kind of problems can be solved with reasonable computational cost by using the OCD strategy. The problem were solved in an Intel 2 Core Duo- 2.0 GHz - 2 GB RAM with a 3% integrality gap.

Algorithm 11.1: Optimal Condition Decomposition algorithm

Data: Initial values for complicating variables and multipliers (π^{I}, π^{II}), gap tolerance (*tolerance*).
Result: The optimal solution $E[CV], \mathscr{X}, \mathscr{Y}$.
begin
$gap \longleftarrow \infty$;
$k^{a} \longleftarrow 0$;
while $gap > tolerance$ **do**
  forall $\hbar_{L'}$ **do**
    forall $f \notin (Sup \cup M); j \in \hat{J}_f; l; t \in T_l; \hbar_l \notin AH_{l,\hbar_{L'}}$ **do**
      $\tilde{V}^{l}_{jft\hbar_l} \longleftarrow \hat{\tilde{V}}^{l,k}_{jft\hbar_l}$;
      $\tilde{FE}^{l}_{jft\hbar_l} \longleftarrow \hat{\tilde{FE}}^{l,k}_{jft\hbar_l}$;
      forall $\hbar_{l-1} \in AH_{l-1,\hbar_l}$ **do**
        $\pi^{I}_{f,j,l,t,\hbar_l,\hbar_{l-1}} \longleftarrow \hat{\pi}^{I,k}_{f,j,l,t,\hbar_l,\hbar_{l-1}}$;
        $\pi^{II}_{f,j,l,\hbar_l,\hbar_{l-1}} \longleftarrow \hat{\pi}^{II,k}_{f,j,l,\hbar_l,\hbar_{l-1}}$;
    Solve sub-problem (11.32);
    forall $l; t \in T_l; \hbar_l \in AH_{l,\hbar_{L'}}$ **do**
      $\hat{\mathscr{X}}^{k+1} \longleftarrow \mathscr{X}^{*b}$;
      $\hat{\mathscr{Y}}^{k+1} \longleftarrow \mathscr{Y}^{*}$;
      forall $f \notin (Sup \cup M); j \in \hat{J}_f; \hbar_{l-1} \in AH_{l-1,\hbar_l}$ **do**
        $\hat{\pi}^{I,k+1}_{f,j,l,t,\hbar_l,\hbar_{l-1}} \longleftarrow \pi^{I*}_{f,j,l,t,\hbar_l,\hbar_{l-1}}$;
        $\hat{\pi}^{II,k+1}_{f,j,l,t,\hbar_l,\hbar_{l-1}} \longleftarrow \pi^{II*}_{f,j,l,t,\hbar_l,\hbar_{l-1}}$;
  $gap \longleftarrow \|[\hat{\mathscr{X}}^{k+1} - \hat{\mathscr{X}}^{k}]^{T}|[\hat{\mathscr{Y}}^{k+1} - \hat{\mathscr{Y}}^{k}]^{T}\|$;
  $k \longleftarrow k+1$;
end

[a] k refers to the iteration number
[b] An * indicates the optimal variable value

11.5.2 Testing solutions using the MPC framework

To demonstrate the benefits of using the integrated model, the algorithm has been repeated also during the 48 planning periods contemplated in the whole planning horizon. Each period represents one month. Here, the uncertainty is assumed to unveil every month. In order to model the SC process for this case, the production rates and acquisition of production resources ($P^{l}_{ijfft\hbar_l}$) become

Table 11.2: Production predicted during design vs simulated production

	Production	Integrated approach	Sequential approach
s5	Predicted (10^6 kg)	1.63	1.83
	Simulated (10^6 kg)	1.48	1.06
	Deviation (%)	-9.35	-41.99
s6	Predicted (10^6 kg)	3.87	3.98
	Simulated (10^6 kg)	3.91	3.87
	Deviation (%)	0.92	-2.60
s7	Predicted (10^6 kg)	3.80	3.73
	Simulated (10^6 kg)	3.71	2.14
	Deviation (%)	-0.02	-0.43
s8	Predicted (10^6 kg)	2.44	2.44
	Simulated (10^6 kg)	2.47	2.16
	Deviation (%)	1.16	-11.38
Total	Predicted (10^6 kg)	11.74	11.97
	Simulated (10^6 kg)	11.56	9.24
	Deviation (%)	-1.54	-22.86

first stage variables. Both SC optimal configurations (integrated and sequential) have been tested. As previously stated, the results from this step allow us to make a fair and real comparison between the integrated and sequential approach.

Fig. 11.8 shows how average corporate value behaves along the planning horizon for both approaches. The values presented in that figure are obtained by simulating production scheduling for each period using the MPC framework. The execution of the MPC loop is equivalent to applying a rolling horizon procedure. At the end of 48^th period by using the integrated approach, the SC system yields to a CV of 1.66x10^9 m.u. which is 0.79% higher than the one predicted during the design phase (1.65x10^9 m.u.). On the other hand, the sequential approach yields to a CV equal to 1.44x10^9 m.u. at the end of the planning horizon which is 14.47% lower than the one predicted during the design phase (1.69x10^9 m.u.). The production levels for final products are depicted in Figures 11.9 to 11.12. It can be seen from these figures that the sequential approach SC configuration does not have enough capacity to reach the $s5$ and $s6$ production levels that were predicted during the design phase. Table 11.2 compares the final product total production levels predicted during the SC design step and the ones obtained during the production scheduling simulation. The overall total production deviation is -1.54% for the integration approach, while -22.86% for the sequential one.

These results show that the integrated approach allows the SC manager to make more appropriate strategic decisions. The deviations observed in the SC performance, when SC network designs are deployed into real scenarios, can be reduced by using the integrated approach. What is more, the SC configuration proposed by the integrated approach clearly outperforms in terms of CV (15.47%) the one proposed by the sequential approach when they are tested using the production scheduling simulation.

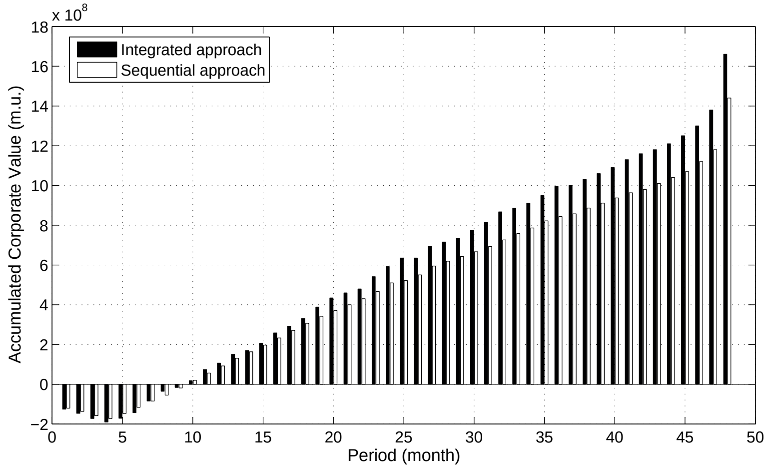


Figure 11.8: Corporate value behavior by simulating operations scheduling for both approaches

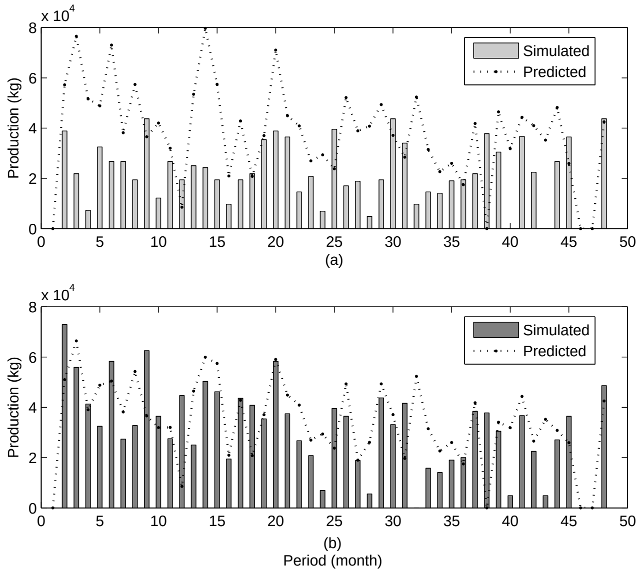


Figure 11.9: Production level obtained by the design phase vs production level obtained by simulating scheduling operations for final product $s5$ (a) sequential approach (b) integrated approach

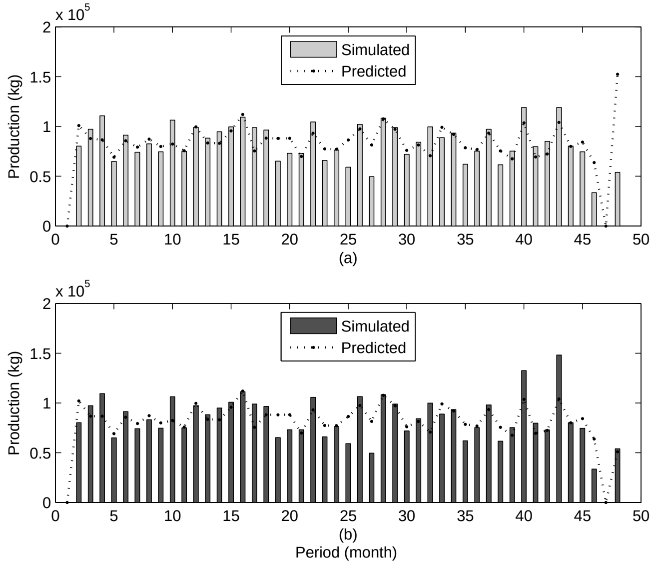


Figure 11.10: Production level obtained by the design phase vs production level obtained by simulating scheduling operations for final product $s6$ (a) sequential approach (b) integrated approach

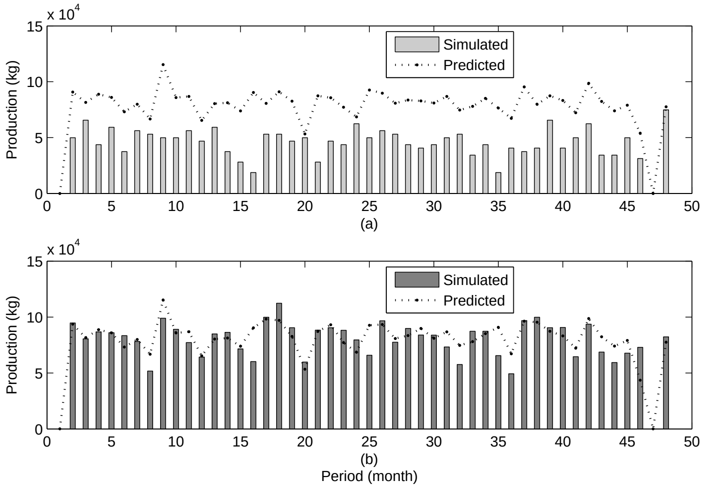


Figure 11.11: Production level obtained by the design phase vs production level obtained by simulating scheduling operations for final product $s7$ (a) sequential approach (b) integrated approach

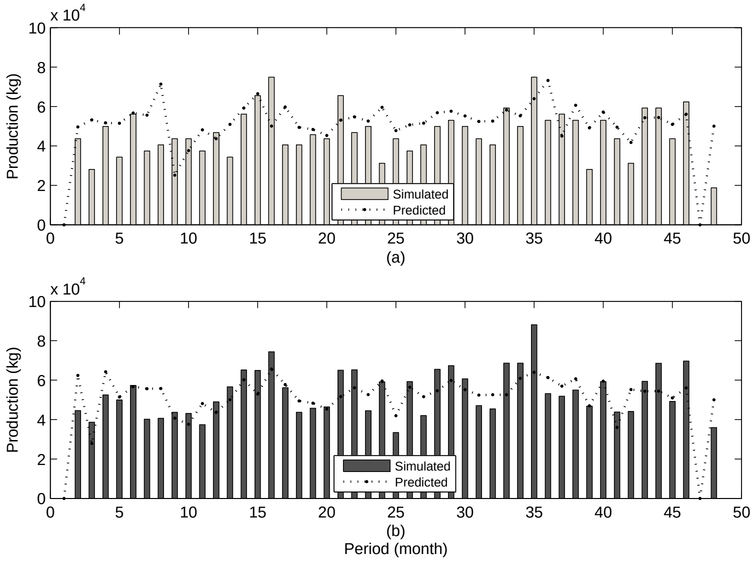


Figure 11.12: Production level obtained by the design phase vs production level obtained by simulating scheduling operations for final product $s8$ (a) sequential approach (b) integrated approach

11.5.3 Failures consideration

Regarding the control policy at the low level, a statistical process strategy is considered for the styrene reactor. A multivariate statistical process control strategy based on latent variable model is implemented for the reactor in order to monitor the polymer production. The monitoring strategy will enable to determine whether the reactor operation is or not under control. The monitoring strategy determine whether a reactor breakdown exists or not when the system is found out of control. The system is supposed to be continuously monitoring the reactor operation. Once an abnormal situation is detected and diagnosed, a decision about how to continue the operations has to be made by the SC controller shown in Fig. 11.1. For the sake of simplicity, merely the operation time and the reactor temperature are considered as control variables and their respective values are obtained by a simplified reactor simulation model. The monitoring model was developed in Matlab (The Mathworks, 2004), the connection with the SC control algorithm was carried out by using matgams (an interface created by Ferris (1999))

A breakdown in equipment technology III in plant site in LA is simulated and detected at ninth planning period. The main changes in production planning due to this failure are the following:

- Production levels for $EPS-I$ and $EPS-II$ are considerably reduced

Table 11.3: Changes in production tasks due to equipment failure

Site	Material	Production level (kg) Before failure	After failure
LA	Styrene	94437.3	90957.7
	EPS-1	43680.0	26743.9
	EPS-2	18720.0	20056.1
GA	EPS-1	9328.5	15600.0
IA	EPS-1	8489.1	15600.0

Table 11.4: Changes in distribution tasks due to equipment failure

Sites From	To	Material	Distribution level (kg) Before failure	After failure
LA	GA	Styrene	8862.1	14820.0
LA	IA	Styrene	9370.7	14820.0

in LA site. The tasks to produce these two products are performed in equipment technology III.

- The styrene production level is slightly reduced in site LA. A tactical decision at the SC level is made by the algorithm to transfer to sites GA and IA the styrene production that cannot be processed at this site.

- The production level of $EPS - I$ is increased at sites GA and IA. Both locations had idle capacity of technology III before the failure.

The production and distribution levels before and after the failure for the affected sites are shown in Tables 11.3 and 11.4. As shown in this example, styrene (an intermediate material) has been transferred from LA to GA and IA as a result of this failure. Such movement of materials is not usually considered in traditional SC planning models. Furthermore, the capacity of other sites have been contemplated in order to resolve the incidence in LA site. This example demonstrates again that when the strategy is applied, namely SC transparency is gained, the decision making process to resolve the incidents is performed at the SC level and not merely at the plant level, thus allowing to select the best plan in terms of value creation. Even more, it should be highlighted that the planning model utilized in this control strategy is able to consider movement of raw materials, intermediates and final products between the different facilities comprising the SC network. Such flexibility increases the number of alternatives available to resolve the incidences since production and its corresponding input materials can be transfered accordingly from one site to another.

11.6 Final considerations

A means of integrating the three standard SC decision levels is presented. Moreover, a SC design-planning model that permits a soft integration with scheduling models is presented. The results show that significant improvements can be gained when all of these decision levels are incorporated into a single model. It is demonstrated that decisions made solely on the SC design and disregarding the production scheduling scenario can lead to aggregated capacity overestimation and consequently to a fictitious better corporate value. Aggregated capacity overestimation can be solved by incorporating scheduling constraints into the design-planning problem. As a result, production rates are adjusted to the real working scenario and expected production profiles can be better sustained during the whole planning horizon. Additionally, the SC operations formulation included in the control strategy is able to transfer any kind of material between any pair of SC components. This is an important feature towards finding the best way of resolving SC incidences.

It is important to highlight that capacity has been utilized as the linking aspect when integrating SC design, planning and scheduling. What is more, it is demonstrated how capacity is the core factor that integrates supervisory control modules with scheduling formulations. The scheduling formulation requires details about individual equipment capacity which facilitates the exchange of information with the equipment supervisory control module. The integration of process monitoring capability allow us to take into account the effects of equipment failures and out of control operation conditions in the SC activities.

It has been shown that a Lagrangian decomposition can significantly reduce the computational burden associated to the solution of monolithic problems. In this work, the Optimal Condition Decomposition was applied. This technique facilitates updating the Lagrangian multipliers. In this way one of the most common difficulties when applying Lagrangian relaxation methods is overcome.

Even though the computational cost increases with the number of periods, this increase is not significant if it is compared to the computational cost added with the number of scenarios. For that reason, a decomposition scheme is applied to tackle medium size problems. However, the number of scenarios to consider is still limited given the complexity of the integrated model. It is envisaged that the use of a parallel computing frameworks may help to reduce the time required to the solution of this kind of problems.

11.7 Nomenclature

Indices

e	suppliers
f	facility locations
i	tasks
j	equipment

l	events in which uncertainty unfolds
s	states (materials)
t	planning periods
t_k	scheduling time buckets
$\hbar_l$	combination of events at level l in scenario tree

Sets

$AH_{l\hbar_l}$	set of combination of events that belong to level l and are ancestors of $\hbar_l$
E_s	set of suppliers e that provide raw material s
$\hat{E}_{prod}$	set of suppliers e that provide production services
$\tilde{E}_{tr}$	set of suppliers e that provide transportation services
FP	set of states s that are final products
$\hat{J}_f$	equipment j that can be installed at location f
J_i	equipment that can perform task i
$JProd$	equipment that performs production tasks
$JStor$	storage equipment
M	set of market locations
R_f	set of raw materials that can be provided from location f
RM	set of states s that are raw materials
RM_e	set of raw materials that are offered by supplier e
Sup	set of supplier locations
Tr	set of distribution tasks
T_s	set of tasks producing state s
$\bar{T}_s$	set of tasks consuming state s

Parameters

A_{sft}	maximum availability of raw material s in period t at location f
$Dem^{l}_{sft\hbar_l}$	product s demand at market f in period t for combination of events $\hbar_l$
$FCFJ_{jft}$	fixed cost per unit of capacity of plant equipment j at location f in period t
$FCFS_{ft}$	fixed cost per unit of distribution center capacity at location f in period t
I^{J}_{ft}	investment required to establish a processing facility in location f in period t
I^{S}_{ft}	investment required to establish a distribution center in location f in period t
$MinCSL$	lower bound of customer service level
$Other_t$	other expected outflows or inflows of cash in period t
pt_i	task i processing time
$Price_{sft}$	price of product s at market f in period t
$Price^{FJ}_{jft}$	investment required per unit of capacity of equipment j increased at facility f in period t
$Price^{FS}_{ft}$	investment required per unit of distribution center capacity increased at facility f in period t
$\|T\|$	length of planning horizon

Binary Variables

$JB^{l}_{ft\hbar_{l-1}}$	1 if a processing site at location f is established in period t, 0 otherwise
$SB^{l}_{ft\hbar_{l-1}}$	1 if a distribution center at location f is established in period, 0 otherwise t
$V^{l}_{jft\hbar_{l-1}}$	1 if the equipment j capacity is increased at location f in period t 0, otherwise
$\tilde{V}^{l}_{jft\hbar_{l}}$	duplicated variable for $V^{l}_{jft\hbar_{l-1}}$
$W^{l}_{ijft_k\hbar_{l}}$	1 if task i starts at scheduling time bucket t_k to be performed in equipment j at site s for combination of events $\hbar_l$

Continuous Variables

$B^{l}_{ijft_s\hbar_{l}}$	Batch size for task i performed in technology j at site f in period t for combination of events $\hbar_l$
$CV^{L}_{\hbar_{L}}$	corporate value at the end of the planning horizon for combination of events $\hbar_L$
$EPurch^{l}_{et\hbar_{l}}$	economic value of purchases executed in period t to supplier e for combination of events $\hbar_l$
$ESales^{l}_{t\hbar_{l}}$	economic value of sales carried out in period t for combination of events $\hbar_l$
$E[CV]$	expected corporate value
$FAsset^{l}_{t\hbar_{l}}$	increment in fixed assets in period t for combination of events $\hbar_l$
$FCost^{l}_{t\hbar_{l}}$	fixed cost in period t for combination of events $\hbar_l$
$F^{l}_{jft\hbar_{l}}$	plant equipment j total capacity during period t at location f for combination of events $\hbar_l$
$FE^{l}_{jft\hbar_{l}}$	plant equipment j capacity increment at location f during period t for combination of events $\hbar_l$
$\tilde{FE}^{l}_{jft\hbar_{l}}$	duplicated variable for $FE^{l}_{jft\hbar_{l}}$
$P^{l}_{ijst\hbar_{l}}$	production rate of product i in equipment j at site s in period t for combination of events $\hbar_l$
$Profit^{l}_{t\hbar_{l}}$	profit achieved in period t for combination of events $\hbar_l$
$Purch^{rm,l}_{et\hbar_{l}}$	amount of money payable to supplier e in period t for combination of events $\hbar_l$ associated with consumption of raw materials
$Purch^{tr,l}_{et\hbar_{l}}$	amount of money payable to supplier e in period t for combination of events $\hbar_l$ associated with consumption of transport services
$Purch^{pr,l}_{et\hbar_{l}}$	amount of money payable to supplier e in period t associated with consumption of production utilities for combination of events $\hbar_l$
$Purch^{l}_{esft\hbar_{l}}$	amount of raw material s purchased to supplier e at site f in period t for combination of events $\hbar_l$
$RawM^{l}_{sft_k\hbar_{l}}$	incoming of material s to facility f during time bucket t_k for combination of events $\hbar_l$
$Sales^{l}_{sff't\hbar_{l}}$	amount of product s sold from location f in market f' in period t for combination of events $\hbar_l$
$Ssched^{l}_{sft_k\hbar_{l}}$	inventory of state s at location f in time bucket t_k for combination of events $\hbar_l$
$St^{l}_{sft\hbar_{l}}$	inventory of state s at location f in period t for combination of events $\hbar_l$

Greek symbols

α_{rij}	fixed coefficient for consumption of raw material r by product i
β_{sj}	minimum utilization of plant equipment j capacity allowed at site s
θ_{ij}	capacity utilization of plant equipment j by product i
$\pi^{I}_{f,j,l,\hbar_l,\hbar_{l-1}}$	Lagrange multipliers for Eq. (11.28)
$\pi^{II}_{f,j,l,\hbar_l,\hbar_{l-1}}$	Lagrange multipliers for Eq. (11.29)
$\rho^{tr}_{eff'}$	unitary transport costs from location f to location f' payable to external supplier e
τ^{ut1}_{ijfe}	cost associated with task i manufactured in equipment j in site f and payable to external supplier e
τ^{ut2}_{sfe}	cost associated with handling the inventory of material s in site f and payable to external supplier e
ψ_{est}	price of raw material s offered by external supplier e in period t
υ_s	specific volume of material s

Superscripts

L	lower bound
U	upper bound

Part VI

Conclusions and Outlook

Chapter 12

Conclusions and Future Work

12.1 Conclusions

The advantages and contribution of the solution approaches proposed to this thesis objectives have been opportunely highlighted along this document. A summary of these contributions is outlined next.As it has been previously mentioned, the integrated SCM research challenges can be grouped as follows: better representation of production-distribution processes at the SC level, integrated modular approaches, considerations of SC uncertainty, and decomposition strategies. This thesis is an endeavor, a further step in an attempt to tackle these challenges and devise holistic support models for integrated SCM.

Part I identifies these challenges through an extensive state-of-the-art review. Although SCM has recently become the subject of intensive and extensive research, an attentive review reveals those areas where new contribution is expected for a major impact in real applications. In this part, the fundamental concepts underlying the methods used throughout the thesis are presented as well.

Part II shows some mathematical models to approach the enterprise business functionalities integration problem. Chapter 4 addresses the design and retrofit of SCs taking into account financial concerns. The proposed framework applies MILP modeling techniques to develop a mathematical model for SCM that is able to optimize the process operations decisions in conjunction with finances. The model pursues the maximization of a suitable financial key performance indicator, the corporate value of the firm at the end of the time horizon. The corporate value is computed by a discounted-free-cash-flow (DFCF) method which is introduced as part of the mathematical formulation. Most SC modeling approaches usually ignore net working capital (NWC), which represents the variable assets associated with the daily SC operations. NWC is the capital tied up within the cash conversion cycle (e.g., material inventories, accounts receivable, accounts payable), which measures how efficiently an enterprise converts its inputs into cash through final product sales. By using the DFCF method to compute the corporate value, the actual capital cost, the changes in NWC, and the liabilities and other financing funds required to support SC operations are explicitly considered when appraising SC performance. Indeed, this allows evaluating SC operations impact on financial decisions and value generation. In order to emphasize the advantages of this approach, a multi-objective optimization is carried out which also accounts for the maximization of biased key performance measures such as profit and NPV. The novel framework suggested in this chapter is thus in consonance with the new trends in PSE, which is going towards an enterprise wide optimization framework that aims to integrate various functional decisions into a global model that should optimize an overall key performance measure. This chapter proposes the corporate value as a suitable alternative to this posed requirement.

In Chapter 5, the model presented in Chapter 4 is extended to incorporate for the first time R&D pipeline management and also to deal with the endogenous nature of specific (clinical trial in the chosen example) uncertainties during the development process. To tackle this problem, a scenario based multi-stage stochastic MILP formulation is proposed. Performance comparison with the traditional sequential decision approach is also made, demonstrating the significant economic benefits of holistic approaches. Moreover, the model is able to account for financial risk restrictions that may be imposed by stockholders. It is shown that probability of low SC performance is considerable reduced by incorporating the risk management formulation. Finally, a specific type of Lagrangian decomposition technique (Optimal Condition Decomposition) has been adapted to successfully achieve substantial reduction in the computational burden associated with the solution of this kind of problems. Another extension of the model developed in Chapter 4 is presented in Chapter 6. Here, the interface between SC operations and marketing functions is addressed for the first time. A MINLP model that integrates a marketing engineering contribution, the BRANDAID model, is presented. The relevance of a correct appraisal of the trade-off existing between the demand, which can be induced by marketing expenditure and pricing decisions, and the SC capacity investments required to meet such a demand is pointed out. Furthermore, the model allows synchronizing marketing and SC strategic plans so as to maximize corporate value. Again, a performance comparison with the traditional sequential decision approach is made to demonstrate the benefits of this integrated approach.

Part III deals with strategic and tactical issues. The strategic problem of designing a SC network is addressed in Chapter 7 by translating the recipe concept to the whole SC environment. Instead of a rigid predefined network structure, the proposed approach utilizes a SC design and planning model that permits material flows of any kind (i.e., raw and intermediate materials, final products) between any kind of facilities. Even more, only potential locations are provided to the model as input data; decisions regarding the installation of a processing plant, a distribution center or both of them at a location are made during the optimization procedure. In addition, a more adequate representation of all operations and materials entailed in a production system can be achieved by using this model. It is noteworthy that a main feature of the proposed model is that it does not require any pre-established process network superstructure thus allowing to optimally define the sub-trains in which production process is decoupled and their respective locations. As a result, processing facilities outputs may be intermediate materials. This is one key feature in modeling the complex global SCs behavior. It is demonstrated that great potential to improve firm's economic performance can be gained by exploring the whole range of available alternatives when designing a SC. This model enables to do this exploration in a straightforward manner.

The model presented in Chapter 7 is extended in Chapter 8 to consider the optimization of SC planning and design accounting economical and environmental issues. This extension is suitable to collect all SC node information through a single variable, which eases the environmental formulation. A LCA approach has been selected in order to incorporate the environmental aspects of the model. To measure environmental performance, IMPACT 2002+ methodology is used which provides a feasible implementation of a combined midpoint-endpoint evaluation. The proposed approach reduces the value-subjectivity inherent to the assignment of weights in the calculation of an overall environmental impact by considering end-point damage categories as objective function. Additionally, the model performs an impact mapping along the comprising SC nodes and activities. Such mapping allows to focus financial efforts to reduce environmental burdens to the most promising subjects.

Part IV deals with approaches to manage uncertainty. A stochastic version of the model developed in Chapter 4 is presented in Chapter 9. The proposed framework integrates an MPC strategy and a holistic stochastic model for SCM. The control strategy presented in this chapter allows to handle uncertainty and incidences by combining reactive and preventive approaches. A pro-active treatment of uncertainty is included by means of stochastic programming. The review and update process that is required to tackle incidences and changes in random factors is performed by introducing the SC stochastic holistic model into an MPC. In addition, it is illustrated that better transparency and broader visibility of SC is obtained when resolving incidences with the proposed strategy since a model of the whole SC is included into the control algorithm. It is also illustrated that the proposed framework leads to reduce the so-called *bullwhip* effect. Here, it is noteworthy that a major disadvantage of discounted-cash-flow methods is that they do not account for the managerial flexibility needed to be able to alter the course of an investment over time as uncertain factors unfold. As a result, real options analysis has been proposed as an alternative valuation approach that would overcome this drawback. The stochastic DFCF model presented in this chapter renders the same features as real options approaches.

Furthermore, a stochastic DFCF model offers more realistic solutions, since it considers the so-called non-anticipativity conditions, whereas real options approaches typically disregard these conditions.

In Chapter 10, a novel alternative approach for solving scheduling problems under exogenous uncertainty is presented. The approach is based on the combination of (i) S-graph framework, which has proven to be a rigorous and efficient tool for solving deterministic scheduling problems, and (ii) an LP model that serves as evaluator of the expected objective function. S-graph is a representation that takes advantage of the specific characteristics of chemical processes in scheduling. The proposed framework does not only inherit the advantages of S-graph, but it also has an advantage against stochastic programming techniques; namely the computational effort needed to solve the problem does not increase by increasing the number of scenarios. Such convenience relies on the fact that the search space size is independent on the number of considered scenarios. The size is uniquely dependent on the product batches combination. As the number of scenarios increase a larger LP is to be solved but still due to its nature the computational times are very small. Such a feature reduces the computational cost required to solve this kind of problems which is one of the major challenges in this field, thus constituting a robust alternative to existing schedulers to become eventually the best option in integrated SCM.

Finally in Part V the hierarchical decision levels integration is attempted. Chapter 11 addresses the decision-making coordination and integration at hierarchical decision levels. In this chapter, the SC design-planning model developed in Chapter 7 is coupled with a scheduling formulation so that decision levels integration is achieved. This approach enables to assess the impact of considering scheduling aspects of process operations in the design of a SC network. Again, a comparison of the proposed scheme and the traditional hierarchical approach shows the significance of such integration. It is demonstrated that decisions made solely on the SC design and disregarding the production scheduling scenario can lead to aggregated capacity overestimation and consequently to an overly optimistic SC performance. Aggregated capacity overestimation can be solved by incorporating scheduling constraints into the design-planning problem. As a result, production rates are adjusted to the real working scenario and expected production profiles can be better sustained during the whole planning horizon. Additionally, the SC operations formulation included in this work is able to transfer any kind of material between any pair of SC components. This is an important feature towards finding the best way of resolving SC incidences. It is important to highlight that capacity has been utilized as the linking aspect when integrating SC design, planning and scheduling. Even more, it is demonstrated how capacity is the core factor that integrates supervisory control modules with scheduling formulations. The scheduling formulation requires details about individual equipment capacity which facilitates the exchange of information with the equipment supervisory control module. The integration of process monitoring capability allows taking into account the effects of equipment failures and out of control operation conditions in the SC activities. Finally, a Lagrangian decomposition technique is applied to reduce the computational burden associated with the monolithic model solution.

12.2 Future work

From Section 2.4, *Trends and challenges*, it can be seen that this thesis a number of the research challenges posed in the integrated SCM field. Integrated SCM is still and will keep offering a wide range of opportunities for future research work. Some of them which can be thought as a natural step following the work carried out in this thesis are pointed out next.

- The utilization of grid computing frameworks in order to solve SC problems that have been mathematically decomposed is an interesting task. This will eventually allow (i) finding optimal solutions for problems of larger scale, and (ii) increasing the complexity and details considered in SC optimization models.
- There is a huge amount of market data available thanks to e-commerce and bar code technology. Further research is needed to use data mining and response surface techniques to transform such data into models describing marketing activities and competitors effects on firm's market share. Then, such descriptive models may be integrated with SC management decision making.
- Further research should be focused on the consideration of uncertainty associated to environmental impacts. This is an important factor that may influence the decisions regarding emissions trading schemes. Another future research topic in this area is the analysis of how decisions related to the short-term may contribute to reduce SC environmental burdens. Also it is noteworthy to point out that the SC model used in Chapters 7 and 8 can be easily extended to address closed loop SC operations.
- Other kind of uncertainties need to be investigated. Up to date, most of SC models considering uncertainty are focused on product demand and prices variability. However, how much the uncertainty associated to suppliers performance, processes output, and financial markets affects business performance has not been studied enough.
- Advancement on the combined utilization of multi-parametric programming and mathematical decomposition techniques to tackle stochastic programming may be a promising area that deserves further investigation.
- The S-graph approach for scheduling under uncertainty presented in Chapter 10 allows to be integrated with the control strategy proposed in Chapter 11. Nevertheless, further work is needed so that other kinds of objective function can be considered. Besides, future work should also be

addressed towards converting this approach into an exact one by considering explicitly the probability distribution of product demands in the LP model and not just a discrete number of demand scenarios. Research efforts should continue developing accelerating algorithms for this stochastic S-graph framework.

- Advancement in real time monitoring and diagnosis in integrated SCM to timely provide and update the SC state information needed by the different decision-making hierarchical levels will contribute to reduce the risk of unexpected events and improve the efficiency of SC planning.

- Improved manners to include the impact of scheduling decisions into SC design may be further explored. One interesting approach to be examined is the use of attainable regions for modeling feasible aggregated production rates.

- More research efforts are required to address decentralized SCs problems. As previously mentioned, duality and separability principles may provide frameworks to achieve overall optimal solutions by interchanging among SC partners non-critical information (i.e., dual values) instead of usually confidential data (e.g., costs, prices, technology parameters). Additionally, it would be interesting to explore the use of complementarity programs for decentralized SC modeling.

Appendixes

Appendix A

Publications

This is a list of the works carried out so far within the scope of this thesis, in reversed chronological order.

A.1 Journals

A.1.1 Manuscripts published

Puigjaner, L.; Laínez, J. M.; Alvarez, C. R. Tracking the Dynamics of the Supply Chain for Enhanced Production Sustainability. *Industrial & Engineering Chemistry Research*, ISSN: 0888-5885, 48 (21): 9556 – 9570 **(2009)**.

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Financial & Financial Engineering Considerations in Supply Chain and Product Development Pipeline Management. *Computers & Chemical Engineering*, ISSN: 0098-1354, 33 (12): 1999 – 2011 (**2009**).

Bojarski, A. D.; Laínez, J. M.; Espuña, A.; Puigjaner, L. Incorporating Environmental Impacts and Regulations in a Holistic Supply Chains Modeling: An LCA Approach. *Computers & Chemical Engineering*, ISSN: 0098-1354, 33 (10): 1747 – 1759 (**2009**).

Laínez, J. M.; Kopanos, G.; Espuña, A.; Puigjaner, L. Flexible Design-Planning of Supply Chain Networks. *AIChE Journal*, ISSN: 0001-1541, 55 (7): 1736 – 1753 (**2009**).

Puigjaner, L.; Laínez, J. M. Capturing Dynamics in Integrated Supply Chain Management. *Computers & Chemical Engineering*, ISSN: 0098-1354, 32 (11): 2582 – 2605 (**2008**).

Laínez, J. M.; Guillén, G.; Badell, M.; Espuña, A.; Puigjaner, L. Enhancing Corporate Value in the Optimal Design of Chemical Supply Chains. *Industrial & Engineering Chemistry Research*, ISSN: 0888-5885, 46 (23): 7739 – 7757 (**2007**).

A.1.2 Manuscripts Accepted

Laínez, J. M.; Hegyháti, M.; Friedler, F.; Puigjaner, L. Using S-graph to Address Uncertainty in Batch Plants. *Clean Technologies and Environmental Policy Journal*, **2009**. doi: 10.1007/s10098-009-0240-5

A.2 Conference proceeding articles

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Linking Marketing and SC Models for Improved Business Strategic Decision Support. *10th International Symposium on Process Systems Engineering* (PSE'09), Salvador de Bahía, Brazil.

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Managing Financial Risk in the Coordination of Supply Chain and Product Development Decisions. *European Symposium on Computer Aided Process Engineering* (ESCAPE-19), (J. Jeżowski and J. Thullie, Eds.), 1027 – 1032, ISBN: 978-0-444-53433-0, 2009.

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Financial & Financial Engineering Considerations in Supply Chain and Product Development Pipeline Management. *Foundations of Computer-Aided Process Operations* (FOCAPO), (M. Ierapetritou, M. Bassett and S. Pistikopoulos, Eds), 530 – 541, ISBN: 0965589111, 2008.

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Enhancing Value in Supply Chains by Integrating Capacity Allocation Decisions and R&D Pipeline Management. *Foundations of Computer-Aided Process Operations* (FOCAPO), (M. Ierapetritou, M. Bassett and S. Pistikopoulos, Eds), 489 – 492, ISBN: 0965589111, 2008.

Laínez, J. M.; Kopanos, G.; Badell, M.; Espuña, A.; Puigjaner, L. Integrating Strategic, Tactical and Operational Supply Chain Decision Levels in a Model Predictive Control Framework. *European Symposium on Computer Aided Process Engineering* (ESCAPE-18), (B. Braunschweig and X. Joulia, Eds.), 477 – 482, ISBN: 978-0-444-53227-5, 2008.

Laínez, J. M.; Bojarski, A.; Espuña, A.; Puigjaner, L. Mapping Environmental Issues within Supply Chains: an LCA Based Approach. *European Symposium on Computer Aided Process Engineering* (ESCAPE-18), (B. Braunschweig and X. Joulia, Eds.), 1131 – 1136, ISBN: 978-0-444-53227-5, 2008.

Laínez, J. M.; Guillén, G.; Badell, M.; Espuña, A.; Puigjaner, L. Integrating Process Operations and Finances for the Optimal Design of Chemical Supply Chains. *European Symposium on Computer Aided Process Engineering* (ESCAPE-17) (V. Plesu and P.S. Agachi, Eds.), 715 – 721, ISBN: 978-0-444-53157-5, 2007.

Laínez, J. M.; Espuña, A.; Puigjaner, L. A Joint Control Framework for Supply Chain Planning. *European Symposium on Computer Aided Process Engineering* (ESCAPE-17) (V. Plesu and P.S. Agachi, Eds.), 722 – 726, ISBN: 978-0-444-53157-5, 2007.

A.3 Other congresses and workshops

Laínez, J. M.; Kopanos, G.; Espuña, A.; Puigjaner, L. Supply Chain Design Considering Operational Level Details. *AIChE Annual Meeting 2009*, Nashville, USA, 2009.

Kopanos, G.; Laínez, J. M.; Puigjaner, L. Short-Term Scheduling in Multi-Stage Batch Plants through Lagrangean Decomposition. *AIChE Annual Meeting 2009*, Nashville, USA, 2009.

Laínez, J. M.; Reklaitis, G. V.; Puigjaner, L. Sinchronizing New Product Development Projects and Supply Chain Retrofitting for Financial Sustainability in the Pharmaceutical Industry. *World Congress of Chemical Engineering*, Montréal, Canada, 2009. (accepted)

Kopanos, G.; Laínez, J. M.; Badell, M.; Espuña, A.; Puigjaner, L. Enhancing Supply Chain Network Design by Considering Financial Analysis Issues. *AIChE Annual Meeting 2008*, Philadelphia, USA, OMNIPRESS, pp. 575 – 576, ISBN: 978-0-8169-1050-2, 2008.

Laínez, J. M.; Kopanos, G.; Espuña, A.; Puigjaner, L. Process Operations Scheduling Conscious Design of Supply Chains. *11th Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2008.

Laínez, J. M.; Bojarski, A.; Espuña, A.; Puigjaner, L. Green Supply Chain Management – Discovering Critical Activities for Emission Reduction and Control. *11th Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2008.

Kopanos, G.; Laínez, J. M.; Puigjaner, L. Supply Chain Management Considering International Logistics - Production Issues. *11th Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2008.

Kopanos, G.; Laínez, J. M.; Pérez-Fortes, M.; Puigjaner, L. Biomass for Energy Production Supply Chain Network Design. *11th Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2008.

Laínez, J. M.; Hegyhati, M.; Puigjaner, L.; Friedler, F. Using S-graph to Address Uncertainty in Batch Plants. *11th International Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction* (PRES), Prague, Czech Republic, 2008.

Laínez, J. M.; Kopanos, G.; Espuña, A.; Puigjaner, L. A Novel MILP Model for Flexible Chemical Supply Chains Design. *11th International Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction* (PRES), Prague, Czech Republic, 2008.

Kopanos, G.; Laínez, J. M.; Espuña, A.; Puigjaner, L. Multi-Parametric Optimization into a Model Predictive Control Framework for Supply Chain Planning and Design. *11th International Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction* (PRES), Prague, Czech Republic, 2008.

Ivanov, B.; Laínez, J. M.; Vaklieva-Bancheva, N.; Minchev, K.; Shopova, E.; Puigjaner, L.; Espuña, A. "SC-MOPP"- Platform for Planning and Scheduling Multi-site Manufacturing Systems. *Computer Aided Process Engineering (CAPE) Forum*, Thessaloniki, Greece, 2008.

Laínez, J. M.; Benqliou, C.; Espuña, A.; Ivanov, B.; Vaklieva-Banchevab, N.; Puigjaner, L. Use of CAPE-OPEN Standards in the Coordinated Optimization of Plant Production Scheduling and Supply-Chain Planning. *6th European Congress of Chemical Engineering* (ECCE-6), Copenhagen, Denmark, Norhaven Books, pp. 539 – 540, 2007.

Kopanos, G.; Laínez, J. M.; Badell, M.; Espuña, A.; Puigjaner, L. Operations and Logistic Planning Considering Vendor Uncertainties to Enhance the Flexibility and Reduce the Risk of Chemical Supply Chain Networks. *6th European Congress of Chemical Engineering* (ECCE-6), Copenhagen, Denmark, Norhaven Books, pp. 483 – 484, 2007.

Badell, M.; Kopanos, G.; Laínez, J. M.; Espuña, A.; Puigjaner, L. Making Value with Order Management for Agent Based Systems. *6th European Congress of Chemical Engineering* (ECCE-6), Copenhagen, Denmark, Norha-ven Books, pp. 657 – 658, 2007.

Puigjaner, L.; Guillén, G.; Laínez, J. M. Merging Process Operations and Financial Analysis to Enhance the Supply Chain Management. *INFORMS Annual Meeting 2006*, Pittsburgh, USA, Michael Trick, pp. 293 – 293, 2006.

Laínez, J. M.; Guillén, G.; Badell, M.; Espuña, A.; Puigjaner, L. Assessment of Traditional Key Performance Indicators for Supply Chain Management in the Chemical Industry. *AIChE Annual Meeting 2006*, San Francisco, USA, OMNIPRESS, pp. 301L – 301L, 2006.

Appendix B

Data for Chapter 4 Case Study

This appendix presents the data used for the case study illustrating the integrated approach of Chapter 4, *Enhancing Corporate Value in the Design of Supply Chains*.

B.1 Operations Data

The specific volumes of products and raw materials are shown in Table B.1.

Table B.1: Specific volume of products i (υ_i (10^{-5} m^3/kg))

Product	υ_i
P1	4.3
P2	8.0
P3	5.5

The capacity coefficients for each equipment and product are shown in Table B.2.

Table B.2: Capacity utilization of plant equipment j by each product i (θ_{ij} (c.u./kg))

Product	Equipment			
	TA	TB	TC	TD
P1	8.00	7.20	8.40	7.60
P2	7.00	8.40	7.35	8.82
P3	7.00	8.40	7.35	7.70

The amount of each type of raw material required to manufacture each product depends on the specific equipment being applied in each case (see Table B.3).

Table B.3: Mass fractions for consumption of raw materials by plant equipment j (α_{rij} (adim.))

Product	Raw material					
	R1	R2	R3	R4	R5	R6
$j = TA$						
P1	0.59	0.35	0.18			
P2				0.47	0.24	0.30
$j = TB$						
P2				0.47	0.24	0.30
P3	0.24	0.71			0.30	
$j = TC$						
P1	0.59	0.30	0.18			
P2				0.53	0.24	0.30
P3	0.24	0.77			0.30	
$j = TD$						
P1	0.59	0.35	0.12			
P3	0.24	0.71			0.24	

Table B.4 gives raw materials costs and their maximum availability at each period, which is assumed to remain constant within the whole planning horizon.

Table B.4: Cost (m.u./kg) and maximum availability ($A_{ert}(10^3\text{kg})$)of raw material r at each period of time t

	Raw material					
	R1	R2	R3	R4	R5	R6
Availability	150.0	125.0	335.0	60.0	60.0	40.0
Cost	10.10	6.60	6.10	8.10	12.1	10.1

The demand data are listed in Table B.5.

Table B.5: Demand of product i at market m at each period t (Dem_{imt} (10^3kg))

Product i	t: $1-7$	$8-20$	$21-23$	$24-32$	$33-47$	$48-56$	$57-60$
$m = M1$							
P1	105.0	105.0	105.0	150.0	105.0	150.0	105.0
P2	50.8	50.8	50.8	72.5	50.8	72.5	50.8
P3	43.8	43.8	43.8	62.5	43.8	62.5	43.8
$m = M2$							
P1	105.0	600.0	105.0	150.0	105.0	150.0	105.0
P2	119.0	680.0	119.0	170.0	119.0	170.0	119.0
P3	133.0	760.0	133.0	190.0	133.0	190.0	133.0
$m = M3$							
P1	35.0	35.0	35.0	50.0	35.0	50.0	35.0
P2	220.5	220.5	220.5	315.0	220.5	315.0	220.5
P3	150.5	150.5	150.5	215.0	150.5	215.0	150.5
$m = M4$							
P1	70.0	400.0	70.0	100.0	70.0	100.0	70.0
P2	294.0	1680.0	294.0	420.0	294.0	420.0	294.0
P3	147.0	840.0	147.0	210.0	147.0	210.0	147.0
$m = M5$							
P1	140.0	140.0	140.0	200.0	140.0	200.0	140.0
P2	171.5	171.5	171.5	245.0	171.5	245.0	171.5
P3	49.0	49.0	49.0	70.0	49.0	70.0	49.0

B.2 Economic data

Table B.6 shows the fixed and investment costs associated with each equipment.

Table B.6: Equipment j fixed cost ($FCFS_{jst}$ (m.u./Mg)) and investment ($Price^{FS}_{jst}$ (m.u./kg))

	Equipment j			
	TA	TB	TC	TD
Fixed cost	25.0	37.0	50.0	45.0
Investment	3.26	3.91	2.93	4.04

The data associated with fixed cost and investments of DCs can be found in Table B.7.

Table B.7: Distribution centers fixed cost ($FCFW_{wt}$ (m.u./m^3)) and investment ($Price^{FS}_{wt}$ (m.u./m^3))

	Distribution center w			
	W1	W2	W3	W4
Fixed cost	17.5	15.0	15.0	13.75
Investment	100.0	80.0	75.0	70.0

Transportation costs are given in Tables B.8 and B.9, whereas production costs are shown in Table B.10.

Table B.8: Transportation cost of product i from site s to distribution center w (m.u./m^3)

Distribution center w	Site s		
	S1	S2	S3
$i = P1$			
W1	0.02	0.48	0.27
W2	0.48	0.02	0.18
W3	0.19	0.36	0.24
W4	0.21	0.60	0.24
$i = P2$			
W1	0.04	0.90	0.49
W2	0.90	0.04	0.34
W3	0.36	0.67	0.45
W4	0.38	1.12	0.45
$i = P3$			
W1	0.03	0.62	0.34
W2	0.62	0.03	0.23
W3	0.25	0.46	0.31
W4	0.26	0.77	0.31

Table B.9: Transportation cost of product i from distribution center w to market m (m.u./m^3)

Distribution center w	Market m				
	M1	M2	M3	M4	M5
$i = P1$					
W1	0.02	0.48	0.21	0.15	0.11
W2	0.48	0.02	0.39	0.60	0.22
W3	0.21	0.39	0.04	0.18	0.22
W4	0.21	0.60	0.17	0.02	0.22
$i = P2$					
W1	0.04	0.90	0.38	0.27	0.20
W2	0.90	0.04	0.72	1.12	0.40
W3	0.38	0.72	0.07	0.34	0.40
W4	0.38	1.12	0.32	0.04	0.40
$i = P3$					
W1	0.03	0.62	0.26	0.19	0.14
W2	0.62	0.03	0.49	0.77	0.28
W3	0.26	0.49	0.05	0.23	0.28
W4	0.26	0.77	0.22	0.03	0.28

Table B.10: Production cost of product i manufactured in plant equipment j at site s (m.u./kg)

Plant equipment j	Site s S1	S2	S3
$i = P1$			
TA	0.63	0.59	0.71
TB	0.51	0.48	0.58
TC	0.72	0.69	0.82
TD	0.77	0.73	0.88
$i = P2$			
A	0.55	0.52	0.62
B	0.59	0.56	0.67
C	0.63	0.60	0.72
D	0.90	0.85	1.02
$i = P3$			
A	0.55	0.52	0.62
B	0.59	0.56	0.67
C	0.63	0.60	0.72
D	0.78	0.74	0.89

The market prices of the final products are assumed to remain constant during the whole planning horizon and are provided in Table B.11.

Table B.11: Price of product i at each market m and period $t(Price_{imt}$ (m.u./kg))

Product P1	P2	P3
$m = M1, M3, M4, M5$		
16.15	17.51	18.39
$m = M2$		
16.43	17.81	18.71

Finally, receivables on sales in any period are paid with a delay according to the proportions given in Table B.12 and may be pledged at a 80% of their face value regardless of their maturing period.

Table B.12: Fraction of sales that are receivable n time periods after sale is executed ($\delta_{mtt'}$)

Market m	Time periods between execution and maturing period of sales ($n = t' - t$) 0	1	2	3	4	5	6
M1, M3, M5	0.05	0.10	0.25	0.60	0.00	0.00	0.00
M2	0.00	0.00	0.00	0.00	0.05	0.20	0.75
M4	0.00	0.05	0.05	0.15	0.75	0.00	0.05

Appendix C

Examples Data for Chapter 7

This appendix presents the data used for the examples presented in Chapter 7, *Flexible Design – Planning of Supply Chain Networks*.

C.1 Illustrative example 1 input data

Table C.1: Establishing investment (m.u.)

Site	Plant	Distribution Center
LA	62250	133579.6
LB	1182750	270787.5
LC	996000	115733.3
LD	933750	369765.0

Table C.3: Raw materials data

Raw Material	Purchase Price (m.u.)	Supplier Capacity (tns)
$s1$	30	2500
$s2$	24	2000

Table C.2: Sale prices (m.u.)

Product	Markets	
	$M1$	$M2$
s4	540	492
s5	720	762

Table C.4: Products demands (tns)

Market	Periods				
	$t1$	$t2$	$t3$	$t4$	$t5$
Product S=$S4$					
$M1$	2108	1784	3290	3737	3077
$M2$	727	733	765	1288	558
Product S=$S5$					
$M1$	740	791	1030	826	829
$M2$	358	595	1041	831	624

Table C.5: Distribution center data (m.u.)

Site	Installation Cost	Fixed Cost
LA	89.05	4.45
LB	180.53	9.03
LC	77.16	3.86
LD	246.51	12.33

Table C.6: Equipment technology data

	Equipment	FJE^L (tns)	FJE^U (tns)	Installation Cost (m.u.)	Fixed Cost (m.u.)
$j1$	Reactor I	25	250	4200	168
$j2$	Reactor II	25	250	8000	320
$j3$	Reactor III	25	250	16000	640

Table C.7: Transportation costs (m.u./tn)

Site	Sites				Markets	
	LA	LB	LC	LD	$M1$	$M2$
LA	0	157.6	36	191.2	68	62.4
LB	157.6	0	51.2	59.2	140	124
LC	36	51.2	0	71.2	33.6	84
LD	191.2	59.2	71.2	0	96	137.6

C.2 Illustrative example 2 input data

Table C.8: Establishing investment (m.u.)

Site	Plant	Distribution Center
LA	2387000	127050
LB	1155707	432400
LC	1222555	929605
LD	1155000	693000

Table C.9: Raw materials data

Raw Material	Purchase Price (m.u.)	Supplier Capacity (tns)
$s7$	25	2500
$s8$	20	2000
$s9$	37.5	2250

Table C.10: Sale prices (m.u.)

Product	Markets					
	$M1$	$M2$	$M3$	$M4$	$M5$	$M6$
$s1$	275.00	286.00	247.50	302.50	264.00	363.00
$s2$	240.00	248.00	220.00	244.00	268.00	211.20
$s3$	231.00	220.00	302.50	192.50	247.50	302.50

Table C.11: Products demands (tns)

Market	Periods				
	$t1$	$t2$	$t3$	$t4$	$t5$
Product S=$S1$					
$M1$	6763	8478	6895	8014	11294
$M2$	4217	3569	6581	7475	6155
$M3$	2907	2931	3057	5148	2233
$M4$	2275	3632	3661	6331	5182
$M5$	1829	1805	1400	2393	2817
$M6$	1806	2414	3572	4378	3216
Product S=$S2$					
$M1$	1666	3099	2713	3340	1608
$M2$	352	465	589	373	608
$M3$	2210	1928	1105	1794	1240
$M4$	1843	2557	2350	1925	2216
$M5$	812	1396	840	1009	1195
$M6$	594	931	630	1184	1092
Product S=$S3$					
$M1$	2542	3962	6054	5933	4477
$M2$	1149	1017	1003	1808	1936
$M3$	1783	1162	1946	2204	2868
$M4$	1333	1384	2181	1828	845
$M5$	1006	630	686	971	1176
$M6$	459	542	511	240	680

Table C.12: Equipment technology data (m.u./c.u.)

	Equipment	FJE^L	FJE^U	Unitary installation cost
$j1$	Heater (H)	50	300	220.70
$j2$	Reactor (R1)	50	300	662.20
$j3$	Reactor (R2)	50	300	882.90
$j4$	Separator (S)	50	300	1655.50

Table C.13: Transportation costs (m.u./tns)

Site	Sites				Markets					
	LA	LB	LC	LD	$M1$	$M2$	$M3$	$M4$	$M5$	$M6$
LA	0	33.6	26.4	33	54	84	1.2	84.6	75	71.4
LB	33.6	0	18	48.6	104.4	106.8	141.6	70.2	1.2	35.4
LC	26.4	18	0	30.6	65.4	69.6	36.6	106.2	126	1.2
LD	33	48.6	30.6	0	1.2	64.8	69.6	124.2	1.2	47.4

C.3 Illustrative example 3 input data

Table C.14: Establishing investment (m.u.)

Site	Plant	Distribution Center
$fc1$	18060000	2600
$fc2$	12180000	870000
$fc3$	13020000	3850
$fc4$	9240000	924000
$fc5$	5460000	1150000
$fc6$	5880000	1050000
$fc7$	5460000	2250000
$fc8$	6300000	1000000

Table C.15: Raw materials data

Raw Material	Purchase Price (m.u.)	Supplier Capacity (tns)
$s7$	30	2500
$s8$	24	2000
$s9$	45	2250

Table C.16: Sale Prices (m.u.)

Product	Markets					
	$fc12$	$fc13$	$fc14$	$fc15$	$fc16$	$fc17$
$s1$	600	624	540	660	576	720
$s2$	240	248	220	244	268	192
$s3$	168	160	220	140	180	200
$s4$	144	168	120	160	140	150

Table C.17: Products Demands (tns)

Product	Markets					
	$fc12$	$fc13$	$fc14$	$fc15$	$fc16$	$fc17$
$s1$	5701	3665	3398	2686	1342	2310
$s2$	2116	365	1468	1355	910	630
$s3$	3246	887	1369	1353	609	410
$s4$	2582	295	3016	466	556	700

Table C.18: Equipment technology data

	Equipment	FJE^L (tns)	FJE^U (tns)	Installation Cost (m.u.)	Fixed Cost (euros)
$j1$	Heater	25	250	3010	120.4
$j2$	Reactor	25	250	9030	361.2
$j3$	Reactor	25	250	12040	481.6
$j4$	Separator	25	250	4515	180.6

Table C.19: Transportation costs (m.u./tn)

Site	Sites								Markets					
	$fc1$	$fc2$	$fc3$	$fc4$	$fc5$	$fc6$	$fc7$	$fc8$	$fc12$	$fc13$	$fc14$	$fc15$	$fc16$	$fc17$
$fc1$	0	263.98	201	320.26	97.82	140.7	180.9	249.24	0	83.08	108.54	71.02	68.34	75.04
$fc2$	263.98	0	85.76	99.16	178.22	159.46	144.72	127.3	87.1	0	170.18	103.18	97.82	103.18
$fc3$	201	85.76	0	119.26	105.86	75.04	58.96	73.7	120.6	187.6	0	188.94	167.5	159.46
$fc4$	320.26	99.16	119.26	0	223.78	186.26	152.76	92.46	151.42	203.68	243.88	0	191.62	192.96
$fc5$	97.82	178.22	105.86	223.78	0	46.9	87.1	152.76	253.26	289.44	349.74	222.44	0	76.38
$fc6$	140.7	159.46	75.04	186.26	46.9	0	40.2	108.54	233.16	238.52	316.24	156.78	0	79.06
$fc7$	180.9	144.72	58.96	152.76	87.1	40.2	0	68.34	146.06	155.44	81.74	237.18	281.4	0
$fc8$	249.24	127.3	73.7	92.46	152.76	108.54	68.34	0	0	144.72	155.44	277.38	0	105.86

Appendix D

Data for Chapter 9 Case Study

This appendix presents the data used for the case study illustrating the stochastic MPC approach of Chapter 9, *Capturing Dynamics in Integrated Supply Chain Management*.

The specific volumes of the products are shown in Table D.1.

Table D.1: Specific volume of products i (υ_i (10^{-5} m^3/kg))

Product	υ_i
$P1$	1.5
$P2$	2.8
$P3$	3.6

The capacity coefficients for each equipment and product are shown in Table D.2.

Table D.2: Capacity utilization of plant equipment j by each product i (θ_{ij} (c.u./kg))

Product	Equipment		
	TA	TB	TC
$P1$	8.00	8.50	5.00
$P2$	7.00	9.00	7.50
$P3$	9.00	5.00	7.50

The amount of each type of raw material required to manufacture each product depends on the specific equipment being assigned in each case (see Table D.3).

Table D.3: Mass fractions for consumption of raw materials by plant equipment j (α_{rij} (adim.))

Product	Raw material			
	$R1$	$R2$	$R3$	$R4$
$j = TA$				
$P1$		0.45	0.35	0.20
$P2$		0.55		0.55
$j = TB$				
$P2$		0.55		0.55
$P3$	0.40	0.65		
$j = TC$				
$P1$		0.45	0.35	0.25
$P2$		0.55		0.55
$P3$	0.45	0.70		

Table D.4 gives the costs of the raw materials and their maximum availability at each period, which is assumed to remain constant within the whole planning horizon.

Table D.4: Cost (m.u./kg) and maximum availability ($A_{ert}(10^3\text{kg})$)of raw material r at each period of time t

	Raw material			
	$R1$	$R2$	$R3$	$R4$
Availability	150.0	125.0	335.0	60.0
Cost	20.00	6.00	10.00	15.00

The values in which it is assumed uncertainty unveils in the first year are shown in Tables D.5, D.6 and D.7.

Table D.5: Real demand of product i at market m at each period t (Dem_{imt} (10^3kg))

	$P1$			$P2$			$P3$		
t	$M1$	$M2$	$M3$	$M1$	$M2$	$M3$	$M1$	$M2$	$M3$
1	60203	41184	43325	49833	39798	51061	17449	15798	18707
2	40740	33535	39231	35438	66829	44958	13538	12107	16866
3	30262	42842	48123	24969	49821	52521	9573	17574	14225
4	44484	35554	52559	42091	134379	50054	8888	19032	9480
5	40676	50814	49412	54155	74767	45097	8579	11045	14585
6	29362	49562	45195	78579	30239	51343	13104	12902	13807
7	46963	39012	46190	34209	42291	47078	5632	16598	16322
8	50972	36186	42505	15590	24439	47864	9481	18505	11877
9	33740	60572	48675	31125	38980	44870	13621	13567	14423
10	30657	55727	41171	27436	48876	52537	12711	11083	12859
11	27335	48497	42255	24827	21354	40744	20079	15040	10173
12	47314	46153	43354	22251	37776	52295	15471	10584	17087

Table D.6: Real value of risk free rate in period of time t (%)

t	1	2	3	4	5	6
r_t^0	1.90	1.90	2.20	2.20	1.90	2.00
t_t	7	8	9	10	11	12
r_t^0	2.00	2.00	1.90	2.00	2.00	1.90

Table D.7: Real prices of product i at each market m and period $t(Price_{imt}$ (m.u./kg))

	$P1$			$P2$			$P3$		
t	$M1$	$M2$	$M3$	$M1$	$M2$	$M3$	$M1$	$M2$	$M3$
1	29.4	29.6	30.9	35.0	35.3	36.5	28.7	28.6	29.8
2	29.4	29.9	30.9	34.7	35.0	36.3	28.7	28.5	30.1
3	29.2	29.8	30.8	35.0	35.0	36.4	28.7	28.5	29.8
4	29.6	29.5	30.7	35.2	35.0	36.6	28.6	28.6	30.0
5	29.4	29.7	30.8	34.9	35.1	36.5	28.8	28.8	30.0
6	29.7	29.5	31.0	35.0	34.9	36.3	28.6	28.6	29.9
7	29.7	29.5	30.7	34.6	35.2	36.5	28.8	28.6	29.6
8	29.8	29.9	31.0	35.0	35.0	36.6	28.5	28.7	29.8
9	29.4	29.9	30.9	34.9	34.9	36.3	28.4	28.4	29.7
10	29.5	29.7	31.0	35.1	34.8	36.5	28.7	28.5	29.6
11	29.7	29.4	31.0	35.2	35.0	36.5	28.6	28.7	29.9
12	29.6	29.6	31.3	35.1	35.2	36.7	28.6	28.4	30.0

Table D.8 shows the investment and indirect costs associated with each technology. The same data associated with the DCs can be found in table D.9.

Table D.8: Equipment j fixed cost ($FCFS_{jst}$ (m.u./Mg)) and investment ($Price_{jst}^{FS}$ (m.u./kg))

	Equipment j		
	TA	TB	TC
Fixed cost	1.5	2.25	3.00
Investment	13.00	15.60	11.25

Table D.9: Distribution centers fixed cost ($FCFW_{wt}$ (m.u./m^3)) and investment ($Price_{wt}^{FS}$ (m.u./m^3))

	Distribution center w		
	$W1$	$W2$	$W3$
Fixed cost	17.5	15.0	15.0
Investment	400.0	320.0	300.0

Transportation costs are given in Tables D.10 and D.11, whereas production costs are shown in Table D.12.

Table D.10: Transportation cost of product i from site s to distribution center w (m.u./m^3)

Distribution centre w	Site s		
	$S1$	$S2$	$S3$
$i = P1$			
$W1$	0.05	1.05	0.79
$W2$	1.05	0.05	0.42
$W3$	0.42	0.79	0.05
$i = P2$			
$W1$	0.08	1.68	1.26
$W2$	1.68	0.08	0.67
$W3$	0.67	1.26	0.08
$i = P3$			
$W1$	0.06	1.26	0.95
$W2$	1.26	0.06	0.51
$W3$	0.51	0.95	0.06

Table D.11: Transportation cost of product i from distribution center w to market m (m.u./m^3)

Distribution center w	Market m		
	$M1$	$M2$	$M3$
$i = P1$			
$W1$	0.08	1.58	0.79
$W2$	1.58	0.08	1.42
$W3$	0.79	1.18	0.08
$i = P2$			
$W1$	0.13	2.53	1.26
$W2$	2.53	0.13	2.27
$W3$	1.26	1.90	0.13
$i = P3$			
$W1$	0.10	1.90	0.95
$W2$	1.90	0.10	1.71
$W3$	0.95	1.42	0.10

Table D.12: Production cost of product i manufactured in plant equipment j at site s (m.u./kg)

Plant equipment j	Site s		
	$S1$	$S2$	$S3$
$i = P1$			
TA	1.00	0.77	1.00
TB	0.89	0.74	0.89
TC	0.56	0.54	0.63
$i = P2$			
TA	0.88	0.67	0.88
TB	0.94	0.79	0.94
TC	0.84	0.81	0.94
$i = P3$			
TA	1.13	0.86	1.13
TB	0.52	0.44	0.52
TC	0.84	0.81	0.94

Finally, it is assumed that receivables on sales in any period are paid with a delay according to the proportions given in Table D.13 and may be pledged at a 85% of their face value if maturing in following period.

Table D.13: Fraction of sales that are receivable at n time periods after sales ($\delta_{mtt'}$)

	Time periods between execution and maturing period of sales ($n = t' - t$)					
Market m	0	1	2	3	4	5
$M1$, $M3$	0.05	0.10	0.10	0.60	0.15	0.00
$M2$	0.00	0.00	0.00	0.10	0.25	0.65

Bibliography

Acevedo, J., & E.N. Pistikopoulos. "A parametric MINLP algorithm for process synthesis problem under uncertainty." *Industrial & Engineering Chemistry Research* 35: (1996) 147–158.

———. "A Hybrid Parametric/Stochastic Programming Approach for Mixed-Integer Linear Problems under Uncertainty." *Industrial & Engineering Chemistry Research* 36: (1997) 2262–2270.

Adhitya, A., R. Srinivasan, & I.A. Karimi. "Heuristic Rescheduling of Crude Oil Operations to Manage Abnormal Supply Chain Events." *AIChE Journal* 53: (2007a) 397–422.

———. "A model-based rescheduling framework for managing abnormal supply chain events." *Computers & Chemical Engineering* 31: (2007b) 496–518.

Ahmed, S., & N.V. Sahinidis. "Robust process planning under uncertainty." *Industrial & Engineering Chemistry Research* 37: (1998) 1883–1892.

Al-Ameri, T.A., N. Shah, & L.G. Papageorgiou. "Optimization of vendor-managed inventory systems in a rolling horizon framework." *Computers & Industrial Engineering* 54: (2008) 1019–1047.

Al-Qahtani, K., & A. Elkamel. "Multisite Refinery and Petrochemical Network Design: Optimal Integration and Coordination." *Industrial & Engineering Chemistry Research* 48: (2009) 814–826.

Al-Qahtani, K., A. Elkamel, & K. Ponnambalam. "Robust Optimization for Petrochemical Network Design under Uncertainty." *Industrial & Engineering Chemistry Research* 47: (2008) 3912–3919.

Alexander, B., G. Barton, J. Petrie, & J. Romagnoli. "Process synthesis and optimisation tools for environmental design: methodology and structure." *Computers and Chemical Engineering* 24: (2000) 1195–1200.

Amaro, A.C.S., & A.P.F.D. Barbosa-Póvoa. "Planning and scheduling of industrial supply chains with reverse flows: A real pharmaceutical case study." *Computers & Chemical Engineering* 32: (2008a) 2606–2625.

———. "Supply Chain Management with Optimal Scheduling." *Industrial & Engineering Chemistry Research* 47: (2008b) 116–132.

Applequist, G.E., J.F. Pekny, & G.V. Reklaitis. "Risk and uncertainty in managing chemical manufacturing supply chains." *Computers & Chemical Engineering* 24: (2000) 2211–2222.

Aytug, H., M.A. Lawley, K. Mckay, S. Mohan, & R. Uzsoy. "Executing production schedules in the face of uncertainties: A review and some future directions." *European Journal of Operational Research* 161: (2005) 86–110.

Azapagic, A. "Life cycle assessment and its application to process selection, design and optimisation." *Chemical Engineering Journal* 73: (1999) 1–21.

Azapagic, A., & R. Clift. "The application of life cycle assessment to process optimisation." *Computers & Chemical Engineering* 10: (1999a) 1509–1526.

———. "The application of life cycle assessment to process optimisation." *Computers and Chemical Engineering* 23: (1999b) 1509–1526.

Badell, M., J. Romero, & L. Puigjaner. "Planning, scheduling and budgeting value-added chains." *Computers & Chemical Engineering* 28: (2004) 45–61.

Bagajewicz, M.J. *Chemical Engineering: Trends and Developments*, West Sussex: John Wiley & Sons, 2005, Ch. Integration of Process Systems Engineering and Business Decision Making Tools: Financial Risk Management and Other Emerging Procedures.

Balasubramanian, J., & I.E. Grossmann. "Approximation to multistage stochastic optimization in multiperiod batch plant scheduling under demand uncertainty." *Industrial & Engineering Chemistry Research* 43: (2004) 3695–3713.

Balinski, M. "Integer programming: methods, uses, computation." *Management Science* 12: (1965) 254–313.

Banerjee, I., & M.G. Ierapetritou. "Parametric process synthesis for general nonlinear models." *Computers & Chemical Engineering* 27: (2003) 1499–1512.

Bansal, M., I.A. Karimi, & R. Srinivasan. "Selection of Third-Party Service Contracts for Chemical Logistics." *Industrial & Engineering Chemistry Research* 47: (2008) 8301–8316.

Barbaro, A.F., & M.J. Bagajewicz. "Managing financial risk in planning under uncertainty." *AIChE Journal* 50: (2004) 963–989.

Bauman, H., & A.-M. Tillman. *The Hitch Hiker's Guide to LCA*. Studentlitteratur AB, Lund Sweden, 2004.

Bazaraa, M.S., H.D. Sherali, & C.M. Shetty. *Nonlinear Programming, Theory and Algorithms*. New York: John Wiley & Sons, 1993, 2^{nd} Edition.

Beamon, B.M. "Supply Chain Design and Analysis: Models and Methods." *International Journal of Production Economics* 55: (1998) 281–294.

Berning, G., M. Brandenburg, K. Gürsoy, J.S. Kussi, V. Mehta, & F.-J. Tölle. "Integrating collaborative planning and supply chain optimization for the chemical process industry." *OR Spectrum* 24: (2002) 371–401.

Birge, Z., & S. Louveaux. *Principles on Stochastic Programming*. Springer Verlag, 1997.

Blanchard, B.S. *Logistics Engineering and Management*. New Jersey: Prentice Hall, 2004, 6th Edition.

Bok, J.W., I.E. Grossmann, & S. Park. "Supply chain optimization in continuous flexible process networks." *Industrial & Engineering Chemistry Research* 39: (2000) 1279–1290.

Bonfill, A., A. Espuña, & L. Puigjaner. "Addressing robustness in scheduling batch processes with uncertain operation times." *Industrial & Engineering Chemistry Research* 44: (2005) 1524–1534.

———. "Decision support framework for coordinated production and transport scheduling in SCM." *Computers & Chemical Engineering* 32: (2008) 1206–1224.

Bose, S., & J.F. Pekny. "A model predictive framework for planning and scheduling problems: a case study of consumer goods supply chain." *Computers & Chemical Engineering* 24: (2000) 329–335.

Bozarth, C.C., & W.L. Berry. "Measuring the congruence between market requirements and manufacturing: A methodology and illustration." *Decision Sciences* 28: (1997) 121–150.

Braun, M.W., D.E. Rivera, M.E. Flores, W.M. Carlyle, & K.G. Kempf. "A Model Predictive Control framework for robust management of multi-product, multi-echelon demand networks." *Annual Reviews in Control* 27: (2003) 229–245.

Brooke, A., D. Kendrik, A. Meeraus, R. Raman, & R.E. Rosenthal. *GAMS - A User's Guide*. GAMS Development Corporation, Washington, 1998.

Brown, G.G., G.W. Graves, & M.D. Honczarenko. "Design and Operation of a Multicommodity Production/Distribution System using Primal Goal Decomposition." *Management Science* 33: (1987) 1469–1480.

Buffet, W. "Annual report." Technical report, Berkshire Hathaway Inc., 1994.

Butner, K., D. Geuder, & J. Hittner. "Mastering carbon management: Balancing trade-offs to optimize supply chain efficiencies." *IBM Institute for Business Value* GBE03011-USEN-00.

Cakravastia, A., I.S. Toha, & N. Nakamura. "A two-stage model for the design of supply chain networks." *International Journal of Production Economics* 80: (2002) 231–248.

Camacho, E., & C. Bordons. *Model Predictive Control in the Process Industry*. Springer, 1995.

Castillo, E., A.J. Conejo, P. Pedregal, R. García, & N. Alguaci. *Building and Solving Mathematical Programming Models in Engineering and Science*. New York: John Wiley & Sons, 2001.

Castro, P., A.P.F.D. Barbosa-Póvoa, & H. Matos. "An improved RTN continuous-time formulation for the short-term scheduling of multipurpose batch plants." *Industrial and Engineering Chemistry Research* 40: (2001) 2059–2068.

CEFIC. "Facts and Figures: The European chemical industry in a worldwide perspective." Technical report, Conseil Européen des Fédérations de l'Industrie Chimique, 2009.

Cerdá, J., G.P. Henning, & I.E. Grossmann. "A mixed-integer linear programming model for short-term scheduling of single-stage multiproduct batch plants with parallel lines." *Industrial and Engineering Chemistry Research* 36: (1997) 1695–1707.

Chen, C.L., & W.C. Lee. "Multi-objective optimization of multi-echelon supply chain networks with uncertain demands and prices." *Computers & Chemical Engineering* 28: (2004) 1131–1144.

Chen, C.L., B.W. Wang, & W.C. Lee. "Multi-objective optimization for a multi-enterprise supply chain network." *Industrial & Engineering Chemistry Research* 42: (2003) 1879–1889.

Chen, H., & D. R. Shonnard. "Systematic Framework for Environmentally Conscious Chemical Process Design: Early and Detailed Design Stages." *Industrial & Engineering Chemistry Research* 43: (2004) 535–552.

Chen, X., & D. Simchi-Levi. "Coordinating inventory control and pricing strategies with random demand and fixed ordering cost: The finite horizon case." Technical report, Massachusetts Institute of Technology, 2002.

Cheng, L., E. Subrahmanian, & A.W. Westerberg. "Design and planning under uncertainty: Issues on problem formulations and solutions." *Computers & Chemical Engineering* 27: (2003) 781–801.

———. "Multiobjective decisions on capacity planning and inventory control." *Industrial & Engineering Chemistry Research* 43: (2004) 2192–2208.

Christopher, M. *Logistics and Supply Chain Management. Creating Value-Adding Networks.* Prentice Hall, 2005.

Colvin, M., & C.T. Maravelias. "A stochastic programming approach for clinical trial planning in new drug development." *Computers & Chemical Engineering* 32: (2008) 2626–2642.

Conejo, A.J., E. Castillo, R. Mínguez, & R. Bertrand. *Decomposition Techniques in Mathematical Programming.* Berlin: Springer-Verlag, 2006.

Conejo, A.J., F.J. Nogales, & F.J. Prieto. "A decomposition procedure based on approximate Newton directions Mathematical Programming." *Mathematical Programming, Series A* 93: (2002) 495–515.

Dantzig, G.B., & M.N. Thapa. *Linear Programming 1: Introduction.* Springer Series in Operations Research. New York: Springer-Verlag, 1997a.

———. *Linear Programming 2: Theory and Extensions.* Springer Series in Operations Research. New York: Springer-Verlag, 1997b.

Domenech, X., J.A. Ayllon, J. Peral, & J. Rieradevall. "How Green Is a Chemical Reaction?, Application of LCA to Green Chemistry." *Environmental Science and Technology* 36: (2002) 5517–5520.

Dondo, R., C.A. Méndez, & J. Cerdá. "Optimal management of logistic activities in multi-site environments." *Computers & Chemical Engineering* 32: (2008) 2547–2569.

Dua, P., K. Kouramas, V. Dua, & E.N. Pistikopoulos. "MPC on a chip–Recent advances on the application of multi-parametric model-based control." *Computers & Chemical Engineering* 32: (2008) 754–765.

Duffie, N.A., & R.S. Piper. "Non-hierarchical control of a flexible manufacturing cell." *Robotics and Computer-Integrated Manufacturing* 3: (1987) 175–179.

Duran, M., & I.E. Grossmann. "An outer-approximation algorithm for a class of mixed-integer nonlinear programs." *Mathematical Programming* 36: (1986) 307–339.

Ecoinvent-V1.3. "The Ecoinvent database V1.3." Technical report, Swiss Centre for Life Cycle Inventories, 2006.

Ehrgott, M., & X. Gandibleux, Eds. *Multiple Criteria Optimization: State of the Art Annotated Bibliographic surveys*, Dordrecht: Kluwer Academic Publisers, 2002. International Series in Operations Research & Management Science.

Eliashberg, J., & R. Steinberg. *Marketing-Production Joint Decision Making*, Amsterdam: Elsevier Science Publishers, 1997, Vol. 5 of *Handbooks in Operations Research* *and Management Science*, Ch. 18.

Eo, S.Y., T.S. Chang, D. Shin, & E.S. Yoon. "Cooperative solving in diagnostic agents for chemical processes." *Computers & Chemical Engineering* 24: (2000) 729–734.

Eppen, G.D., R.K. Martin, & L. Schrage. "A scenario approach to capacity planning." *Operations Research* 37: (1989) 517–527.

Erdirik-Dogan, M., & I.E. Grossmann. "Planning Models for Parallel Batch Reactors with Sequence-Dependent Changeovers." *AIChE Journal* 53: (2007) 2284–2300.

Fan, L.T., Y. Kim, C. Yun, B. Park, S. Park, B. Bertok, & F. Friedler. "Design of optimal and near-optimal enterprise-wide networks for multiple products in the process industry." *Industrial & Engineering Chemistry Research* 48: (2009) 2003–2008.

Fandel, G., & M. Stammen. "A general model for extended strategic supply chain management with emphasis on product life cycles including development and recycling." *International Journal of Production Economics* 89: (2004) 293–308.

Felthouse, T.R., J.C. Burnett, B. Horrell, M.J. Mummey, & Y. Kuo, Eds. *Kirk Othmer Encyclopedia of Chemical Technology*, New York: John Wiley & Sons, 2001, Ch. Maleic Anhydride, Maleic Acid And Fumaric Acid, 1–58.

Ferrer-Nadal, S., E. Capón-Garcia, C.A. Méndez, & L. Puigjaner. "Material Transfer Operations in Batch Scheduling. A Critical Modeling Issue." *Industrial & Engineering Chemistry Research* 47: (2008) 7721–7732.

Ferrio, J., & J. Wassick. "Chemical supply chain network optimization." *Computers & Chemical Engineering* 32: (2008) 2481–2504.

Ferris, M. "MATLAB and GAMS: Interfacing optimization and visualization software." Technical report, University of Wisconsin, 1999.

Fiacco, A.V. *Introduction to Sensitivity and Stability Analysis in Nonlinear Programming.* New York: Academic Press, 1983.

Fine, C.H, & A.C. Hax. "Manufacturing Strategy: A Methodology and an Illustration." *Interfaces* 15: (1985) 28–46.

Fleischmann, M., P. Beullens, J.M. Bloemhof-Ruwaard, & L.N. van Wassenhove. "The impact of product recovery on logistics network design." *Production and Operations Management* 10: (2001) 156–173.

Forrester, J.W. *Industrial Dynamics.* Cambridge, MA: The Massachusetts Institute of Technology., 1961.

Fransoo, J.C., & M.J. Wouters. "Measuring the bullwhip effect in the supply chain." *Supply Chain Management: An International Journal* 5: (2000) 78–89.

Freeman, H., T. Harten, J. Springer, P. Randall, M. Curran, & K. Stone. "Industrial pollution prevention: A critical review." *Journal of the air and waste management association* 42: (1992) 617–656.

Gill, P.E., W. Murray, M.A. Saunders, J.A. Tomlin, & M.H. Wright. "George B. Dantzig and systems optimization." *Discrete Optimization* 5: (2008) 151–158.

Gjerdrum, J., N. Shah, & L.G. Papageorgiou. "Transfer prices for multienterprise supply chain optimization." *Industrial & Engineering Chemistry Research* 40: (2001) 1650–1660.

Glover, F., & G.A. Kochenberger. *Handbook of Metaheuristics*, Dordrecht: Kluwer academic publishers, 2003, Ch. Preface. Series in Operations Research and Management Science.

Goedkoop, M., & R. Spriensma. "The Eco-Indicator 99: A damage oriented methods for Life Cycle Impact Assessment, Methodology Report." Technical report, Pré Consultants B.V., Amersfoort, The Netherlands, 2001.

Goodwin, R., P. Keskinocak, S. Murthy, F. Wu, & R. Akkiraju. "Intelligent decision support for the e-supply chain." In *Artificial Intelligence for Electronic Commerce, AAAI Workshop 99.* 1999, 770.

Grant, J.L. *Foundations of Economic Value Added.* John Wiley and Sons, 2003.

Graves, S.C., & B.T. Tomlin. "Process Flexibility in Supply Chains." *Management Science* 49: (2003) 907–919.

Graves, S.C., & S.P. Willems. *Handbooks in Operations Research and Management Science Vol. 11, Supply Chain Management: Design, Coordination and Operation.* Elsevier Publishing Company, 2003.

Grossmann, I.E. "Challenges in the new millennium: product discovery and design, enterprise and supply chain optimization, global life cycle assessment." *Computers & Chemical Engineering* 29: (2004) 29–39.

———. "Enterprise-wide Optimization: A New Frontier in Process Systems Engineering." *AIChE Journal* 51: (2005) 1846–1857.

Guignard, M., & S. Kim. "Lagrangean decomposition: a model yielding stronger bounds." *Mathematical Programming* 39: (1987) 215–228.

Guillén-Gosálbez, G., M. Badell, A. Espuña, & L. Puigjaner. "Simultaneous optimization of process operations and financial decisions to enhane the integrated planning/scheduling of chemical supply chains." *Computers & Chemical Engineering* 30: (2006a) 421–436.

Guillén-Gosálbez, G., M.J. Bagajewicz, S. E. Sequeira, A. Espuña, & L. Puigjaner. "Management of Pricing Policies and Financial Risk as a Key Element for Short Term Scheduling Optimization." *Industrial & Engineering Chemistry Research* 44: (2005a) 557–575.

Guillén-Gosálbez, G., J.A. Caballero, & L. Jiménez. "Application of Life Cycle Assessment to the Structural Optimization of Process Flowsheets." *Industrial & Engineering Chemistry Research* 47: (2008) 777–789.

Guillén-Gosálbez, G., A. Espuña, & L. Puigjaner. "Addressing the scheduling of chemical supply chains under demand uncertainty." *AIChE Journal* 52(11): (2006b) 3864–3881.

Guillén-Gosálbez, G., & I.E. Grossmann. "Optimal Design and Planning of Sustainable Chemical Supply Chains Under Uncertainty." *AIChE Journal* 55: (2009) 99–121.

Guillén-Gosálbez, G., F.D. Mele, M.J. Bagajewicz, A. Espuña, & L. Puigjaner. "Multiobjective supply chain design under uncertainty." *Chemical Engineering Science* 60: (2005b) 1535–1553.

Guillén-Gosálbez, G., F.D. Mele, A. Espuña, & L. Puigjaner. "Addressing the design of chemical supply chains under demand uncertainty." *Industrial & Engineering Chemistry Research* 45(22): (2006c) 7566–7581.

Guillén-Gosálbez, G., C. Pina, A. Espuña, & L. Puigjaner. "Optimal Offer Proposal Policy in an Integrated Supply Chain Management Environment." *Industrial & Engineering Chemistry Research* 44: (2005c) 7405–7419.

Guinee, J.B., M. Gorree, R. Heijungs, G. Huppes, R. Kleijn, A. de Konig, L. van Oers, A.W. Sleeswijk, S. Suh, H.A. Udo de Haes, H. de Brujin, R. van Duin, M.A.J.

Huijbregts, E. Lindeijer, A.A.H. Roorda, B.L. van-der Ven, & B.P. Weidema. *Life cycle assessment. An operational guide to the ISO standards Part 3: Scientific Background.* Ministry of Housing, Spatial Planning and the Environment (VROM) and Centre of Environmental Science - Leiden University (CML), 2001.

Gupta, A., & C.D. Maranas. "A two-stage modelling and solution framework for multisite midterm planning under demand uncertainty." *Industrial & Engineering Chemistry Research* 39: (2000) 3799–3813.

———. "Managing demand uncertainty in supply chain planning." *Computers & Chemical Engineering* 27: (2003) 1219–1227.

Gupta, A., C.D. Maranas, & C.M. McDonald. "Mid-term supply chain planning under demand uncertainty: customer demand satisfaction and inventory management." *Computers & Chemical Engineering* 24: (2000) 2613–2621.

Haimes, Y.Y., L.S. Lasdon, & D.A. Wismer. "On a bicriterion formulation of the problems of integrated system identification and system optimization." *IEEE Transactions on Systems, Man and Cybernetics* 1: (1971) 296–297.

Hameed, S. "How Should We Define Supply Chain Management?" Technical report, SAP Labs, 2007.

Han, C., J.M. Douglas, & G. Stephanopoulos. "Agent-based approach to a design support system for the synthesis of continuous chemical processes." *Computers & Chemical Engineering* 19: (1995) S63–S69.

Handfield, R.F., & E.L. Nichols. *Introduction to supply chain management.* New Jersey: Prentice Hall, 1999.

Harsanyi, J.C. "Rational Behavior and Bargaining Equilibrium in Games and Social Situations." Technical report, Cambridge University, 1977.

Hart, S.L. "Beyond greening: Strategies for a sustainable world." *Harvard Business Review* 75: (1997) 66–76.

Hax, A.C., & H.C. Meal. *Hierarchical integration of production planning and scheduling*, Amsterdam: Elsevier, 1975, Vol. 1 of *Studies in the Management Sciences: Logistics.*

Heijungs, R., & S. Suh. *The Computational Structure of Life Cycle Assessment.* Kluwer Academic Publishers, Dordrecht The Netherlands, 2002.

Hené, T.S., V. Dua, & E.N. Pistikopoulos. "A Hybrid Parametric/Stochastic Programming Approach for Mixed-Integer Nonlinear Problems under Uncertainty." *Industrial & Engineering Chemistry Research* 41: (2002) 67–77.

Hendricks, K.B., & V.R. Singhal. "An empirical analysis of the effect of the effect of supply chain disruptions on long-run stock price performance and equity risk of the firm." *Production and Operations Management* 14: (2005) 35–52.

Hoeffer, E. "The worst is over." *New Steel* 15: (1999) 48–51.

Howard, B.B., & M. Upton. *Introduction to Business Finance.* New York: McGraw Hill, 1953.

Hugo, A., & E.N. Pistikopoulos. "Environmentally conscious long-range planning and design of supply chain networks." *Journal of Cleaner Production* 13: (2005) 1471–1491.

Humbert, S., M. Margni, & O. Jolliet. "IMPACT 2002+: User Guide Draft for version 2.1." Technical report, Industrial Ecology & Life Cycle Systems Group, GECOS, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland, 2005.

Hynes-III, M. “Addressing escalating drug development cost through improved resource management: a pharmaceutical product resear and development case study.” In *Proceedings Foundations of Computer-Aided Process Operations (FOCAPO 2008)*, edited by M. Ierapetritou, M. Bassett, & S. Pistikopoulos. CACHE-AIChE-Informs, CACHE Corp, 2008, 103–107.

Ierapetritou, M.G., & E.N. Pistikopoulos. “Batch plant design and operations under uncertainty.” *Industrial & Engineering Chemistry Research* 35: (1996) 772–787.

ILOG-Optimization. “ILOG CPLEX 10.0.” Technical report, ILOG Optimization, 2008.

IMS-Health. “IMS Retail Drug Monitor.” Technical report, IMS, 2006.

IRAM-ISO-14040. *Gestión ambiental - Análisis del ciclo de vida - Principios y marco.* 1997.

ISBM-Newsletter. Technical Report Spring, Institute for the Study of Business Markets, Pennsylvania State University, 1998.

Iyer, R.R., & I.E. Grossmann. “A bilevel decomposition algorithm for long-range planning of process networks.” *Industrial & Engineering Chemistry Research* 37: (1998) 474–481.

Jackson, J.R., & I.E. Grossmann. “Temporal Decomposition Scheme for Nonlinear Multisite Production Planning and Distribution Models.” *Industrial and Engineering Chemistry Research,* 42: (2003) 3045–3055.

Jensen, P.A., & J.F. Bard. *Operations Research Models and Methods.* John Wiley & Sons, 2003.

Jetlund, S., & I.A. Karimi. “Improving the logistics of multi-compartment chemical tankers.” *Computers & Chemical Engineering* 28: (2004) 1267–1283.

Jordan, W.C., & S.C. Graves. “Principles on the benefits of manufacturing process flexibility.” *Management Science* 41: (1995) 577–594.

Jung, J.Y., G.E. Blau, J.F. Pekny, G.V. Reklaitis, & D. Eversdyk. “A simulation based optimization approach to supply chain management under demand uncertainty.” *Computers & Chemical Engineering* 28: (2004) 2087–2106.

———. “Integrated safety stock management for multi-stage supply chains under production capacity constraints.” *Computers & Chemical Engineering* 32: (2008) 2570–2581.

Kall, P., & S.W. Wallace. *Stochastic programming.* Wiley, 1994.

Kallrath, J. “Combined strategic and operational planning: An MILP success story in chemical industry.” *OR Spectrum* 24: (2002) 315–341.

Klassen, R.D., & N.P. Greis. “Managing environmental improvement through product and process innovation: Implications of environmental life cycle assessment.” *Industrial and Environmental Crisis Quarterly* 7: (1993) 293–318.

Klassen, R.D., & P.F. Johnson. *Understanding Supply Chains: Concepts, Critiques & Futures*, Oxford: Oxford University Press, 2004, Ch. The Green Supply Chain, 229–251.

Klibi, W., A. Martel, & A. Guitouni. “The Design of Robust Value-Creating Supply Chain Networks: A Critical Review.” *European Journal of Operational Research* Doi:10.1016/j.ejor.2009.06.011.

Klöpffer, W., & G. Rippen. “Life cycle Analysis and ecological balance: Methodological approaches to assessment of environmental aspects of products." *Environmental international* 18: (1992) 55–61.

Kondili, E., C.C. Pantelides, & R.W. Sargent. "A general algorithm for short term scheduling of batch operations." *Computers & Chemical Engineering* 17: (1993) 211–227.

Kouvelis, P., & M. Rosenblatt. "A mathematical programming model for global supply chain management: Conceptual approach and managerial insights." In *Supply Chain Management: Models, Applications and Research Directions*, Springer, 2000, Vol. 62 of *Applied optimization*, Ch. 10.

Kuo, T.H., & C.T. Chang. "Application of a Mathematic Programming Model for Integrated Planning and Scheduling of Petroleum Supply Networks." *Industrial & Engineering Chemistry Research* 47: (2008) 1935–1954.

Lababidi, H.M., M.A. Ashmed, I.M. Alatiqi, & A.F. Al-Enzi. "Optimizing the supply chain of a petrochemical company under uncertain operating and economic conditions." *Industrial & Engineering Chemistry Research* 43: (2004) 63–73.

Lakkhanawat, H., & M.J. Bagajewicz. "Financial Risk Management with Product Pricing in the Planning of Refinery Operations." *Industrial & Engineering Chemistry Research* 47: (2008) 6622–6639.

Lamming, R. "Japanese Supply Chain Relationships in Recession." *Long Range Planning* 33: (2000) 757–778.

Lasschuit, W., & N. Thijssen. "Supporting supply chain planning and scheduling decisions in the oil and chemical industry." *Computers & Chemical Engineering* 28: (2004) 863–870.

Lee, H., I. Lee, & G.V. Reklaitis. "Capacity expansion problem of multisite batch plants withproduction and distribution." *Computers & Chemical Engineering* 24: (2000) 1597–1602.

Lee, S., & I.E Grossmann. "New algorithms for nonlinear disjunctive programming." *Computers & Chemical Engineering* 24: (2000) 2125–2141.

Levis, A., & L.G. Papageorgiou. "A hierarchical solution approach for multi-site capacity planning under uncertainty in the pharmaceutical industry." *Computers & Chemical Engineering* 28: (2004) 707–725.

Li, Z., & M.G. Ierapetritou. "Process Scheduling Under Uncertainty Using Multiparametric Programming." *AIChE Journal* 53: (2007) 3183–3203.

Lilien, G., & A. Rangaswamy. "The Marketing Engineering Imperative: Introduction to the Special Issue." *Interfaces* 31: (2001) S1–S7.

Lin, G.Y.J., & J.J. Solberg. "Integrated shop-floor control using autonomous agents." *IIE Transactions* 24: (1992) 57–71.

Lin, X., & C.A. Floudas. "Continuous-time optimization approach for medium-range production scheduling of a multiproduct batch plant." *Industrial and Engineering Chemistry Research* 41: (2002) 3884–3906.

———. "Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review." *Computers and Chemical Engineering* 28: (2004) 2109–2129.

Little, J.D. "BRANDAID: A Marketing-Mix Model, Part 1: Structure." *Operations Research* 23: (1975) 628–655.

Liu, M.L., & N.V. Sahinidis. "Optimization in Process Planning under Uncertainty." *Industrial & Engineering Chemistry Research* 35: (1996) 4154–4165.

Maguire, P.Z., A. Struthers, D.M. Scott, & W.R. Paterson. "The use of agents both to represent and to implement process engineering models." *Computers & Chemical Engineering* 22: (1998) S571–S578.

Majozi, T., & F. Friedler. "Maximization of Throughput in a Multipurpose Batch Plant under a Fixed Time Horizon: S-graph Approach." *Industrial and Engineering Chemistry Research* 45: (2006) 6713–6720.

Majozi, T., & X. Zhu. "A novel continuous-time MILP formulation for multipurpose batch plants. Part 1. Short-term scheduling." *Industrial and Engineering Chemistry Research* 40: (2001) 5935–5949.

Maravelias, C.T., & I.E. Grossmann. "Simultaneous Planning for New Product Development and Batch Manufacturing Facilities." *Industrial & Engineering Chemistry Research* 40: (2001) 6147–6164.

Matthews, H. S., C. Hendrickson, & C. Weber. "The Importance of Carbon Footprint Estimation Boundaries." *Environmental Science & Technology* 42: (2008) 5839–5842.

McDonald, C.M., & I.A. Karimi. "Planning and scheduling of parallel semicontinuous processes. 1. Production planning." *Industrial & Engineering Chemistry Research* 36: (1997) 2691–2700.

McGreavy, C., X.Z. Wang, M.L. Lu, M. Zhang, & S.H. Yang. "Objects, agents and work flow modelling for concurrent engineering process design." *Computers & Chemical Engineering* 20: (1996) S1167–s1172.

McKinnon, A. "Supply Chain Excellence in the European Chemical Industry." Technical report, CEFIC and The European Petrochemical Association, 2004.

Meixell, M.J., & V.B. Gargeya. "Global supply chain design: A literature review and critique." *Transportation Research Part E* 41: (2005) 531–550.

Mele, F.D., A. Espuña, & L. Puigjaner. "Environmental impact considerations into supply chain management based on life cycle assessment." In *Proceedings of Innovation by Life Cycle Management (LCM) International Conference*, edited by F. Castells, & J. Rieradeball. 2005a, 428–433.

———. "Environmental impact considerations into supply chain management based on life-cycle assessment." In *Innovation by Life Cycle Management LCM 2005 International Conference*. 2005b.

———. "A Simulation-Based Optimization Framework for Parameter Optimization of Supply-Chain Networks." *Industrial & Engineering Chemistry Research* 45: (2006a) 3133–3148.

———. "Supply Chain Management through Dynamic Model Parameters Optimization." *Industrial & Engineering Chemistry Research* 45: (2006b) 1708–1721.

Mele, F.D., G. Guillén-Gosálbez, A. Espuña, & L. Puigjaner. "An agent-based approach for supply chain retrofitting under uncertainty." *Computers & Chemical Engineering* 31: (2007) 722–735.

Mele, F.D., M.R. Hernández, & J.A. Bandoni. "Optimal Strategic planning of the bioethanol industry supply chain with environmental considerations." In *Proceedings Foundations of Computer-Aided Process Operations (FOCAPO 2008)*, edited by M. Ierapetritou, M. Bassett, & S. Pistikopoulos. CACHE-AIChE-Informs, CACHE Corp, 2008, 517–520.

Melo, M.T., S. Nickel, & F. Saldanha. "Facility location and supply chain management – A review." *European Journal of Operational Research* 196: (2009) 401–412.

Messac, A., A. Ismail-Yahaya, & C.A. Mattson. "The Normalized Normal Constraint Method for Generating the Pareto Frontier." *Structural and Multidisciplinary Optimization* 25: (2003) 86–98.

Mestan, E., M. Türkay, & Y. Arkun. "Optimization of Operations in Supply Chain Systems Using Hybrid Systems Approach and Model Predictive Control." *Industrial & Engineering Chemistry Research* 45: (2006) 6493–6503.

Miettinen, K.M. *Nonlinear multiobjective optimization.* Kluwer Academic Publishers: Boston, 1999.

Min, H., & G. Zhou. "Supply chain modeling: past, present and future." *Computers & Industrial Engineering* 43: (2002) 231–249.

Mitra, K., R.D. Gudi, S.C. Patwardhan, & G. Sardar. "Midterm Supply Chain Planning under Uncertainty: A Multiobjective Chance Constrained Programming Framework." *Industrial & Engineering Chemistry Research* 47: (2008) 5501–5511.

Méndez, C.A., & J. Cerdá. "An MILP framework for short-term scheduling of single-stage batch plants with limited discrete resources." In *Computer-Aided Chemical Engineering*, Elsevier Science Ltd., 2002, Vol. 12.

Méndez, C.A., J. Cerdá, I.E. Grossmann, I. Harjunkoski, & M. Fahl. "State-of-the-art review of optimization methods for short-term scheduling of batch processes." *Computers & Chemical Engineering* 30: (2006) 913–946.

Mokashi, S.D., & A.C. Kokossis. "Application of dispertion algorithms to supply chain optimisation." *Computers & Chemical Engineering* 27: (2003) 927–949.

Montgomery, D.C., L.A. Johnson, & J.S. Gardiner. *Forecasting and Time Series Analysis.* McGraw-Hill Companies, 1990.

Morris, W.T. "On the Art of Modeling." *Management Science* 13: (1967) B707–B717.

Mulvey, J.M., R.J Vanderbei, & S.A Zenios. "Robust optimization of large-scale systems." *Operations Research* 43: (1995) 264–281.

Mun, J. *Real options analysis: tools and techniques for valuing strategic investments and decisions.* Wiley finance series. New York: John Wiley & Sons, 2005, 2nd Edition.

Naraharisetti, P.K., I.A. Karimi, & R. Srinivasan. "Supply chain redesign through optimal asset management and capital budgeting." *Computers & Chemical Engineering* 32: (2008) 3153–3169.

Nash, J. "The bargaining problem." *Econometrica* 18: (1950) 155–162.

Neiro, S.M.S., & J.M. Pinto. "A general modeling framework for the operational planning of petroleum supply chains." *Computers & Chemical Engineering* 28: (2004) 871–896.

Nemhauser, G.L., & L.A. Wolsey. *Integer and Combinatorial Optimization.* New York: John Wiley & Sons, 1999.

Nocedal, J., & S.J. Wright. *Numerical Optimization.* Springer Series in Operations Research. New York: Springer-Verlag, 1999.

Oh, H., & I.A. Karimi. "Regulatory factors and capacity-expansion planning in global chemical supply chains." *Industrial & Engineering Chemistry Research* 43: (2004) 3364–3380.

———. "Global Multiproduct Production-Distribution Planning with Duty Drawbacks." *AIChE Journal* 52: (2006) 595–610.

Orlicky, J. *MRP, The New Way of Life in Production and Inventory Management.*

New York: McGraw Hill, 1975.

Pantelides, C.C. "Unified frameworks for optimal process planning and scheduling." In *Proceedings on the Conference on Foundations of Computer-Aided Operations*, edited by D. Rippin, & J. Hale. 1994.

Papageorgiou, L.G. "Supply chain optimization for the process industries: advances and opportunities." *Computers & Chemical Engineering* .

Papageorgiou, L.G., G.E. Rotstein, & N. Shah. "Strategic supply chain optimization for the pharmaceutical industries." *Industrial Chemistry Engineering Research* 40: (2001) 275–286.

Papalexandri, K.P., & T.I. Dimkou. "A Parametric Mixed-Integer Optimization Algorithm for Multiobjective Engineering Problems Involving Discrete Decisions." *Industrial & Engineering Chemistry Research* 37: (1998) 1866–1882.

Pedregal, P. *Introduction to Optimization.* Texts in Applied Mathematics. New York: Springer-Verlag, 2004.

Pekny, J.F., & G.V. Reklaitis. "Towards the Convergence of Theory and Practice: A Technology Guide for Scheduling/Planning Methodology." In *Third International Conference on Foundations of Computer-Aided Process Operations*, edited by J.F. Pekny, & G.E. Blau. 1998, 91–111.

Pennington, D.W., M. Margni, C. Amman, & O. Jolliet. "Multimedia Fate and Human Intake Modeling: Spatial versus Non-Spatial Insights for Chemical Emissions in Western Europe." *Environmental Science and Technology* 39: (2005) 1119–1128.

Perea-López, E., I.E. Grossmann, B.E. Ydstie, & T. Tahmassebi. "Dynamic modeling and decentralized control of supply chains." *Industrial & Engineering Chemistry Research* 40: (2001) 3369–3383.

Perea-López, E., B.E. Ydstie, & I.E. Grossmann. "A model predictive control strategy for supply chain optimisation." *Computers & Chemical Engineering* 27: (2003) 1201–1218.

PhRMA. "Pharmaceutical Industry Profile 2007." Technical report, Pharmaceutical Research and Manufacturers of America, Washington, D.C., 2007.

Pinto, J.M., & I.E. Grossmann. "A continuous time mixed integer linear programming model for short-term scheduling of multistage batch plants." *Industrial and Engineering Chemistry Research* 34: (1995) 3037–3051.

Pinto, J.M., M. Joly, & L.F. Moro. "Planning and scheduling models for refinery operations." *Computers & Chemical Engineering* 24: (2000) 2259–2276.

Pistikopoulos, E.N. "Perspectives in Multiparametric Programming and Explicit Model Predictive Control." *AIChE Journal* 55: (2009) 1918–1925.

Pistikopoulos, E.N., V. Dua, N.A. Bozinis, A. Bemporad, & M. Morari. "On-line optimization via off-line parametric optimization tools." *Computers & Chemical Engineering* 26: (2002) 175–185.

Pratt, S.P. *Cost of Capital : Estimation and Applications.* New York: John Wiley and Sons, 2002.

PRe-Consultants-bv. "SimaPro 7.1.6." Technical report, PRe-Consultants-bv, 2008.

Puigjaner, L., & A. Espuña. "Integration in Supply Chain Management." In *Computer Aided Product and Process Engineering*, WILEY-VCH, 2006, 695–730.

Puigjaner, L., & G. Guillén-Gosálbez. "Towards an integrated framework for supply chain management in the batch chemical process industry." *Computers & Chemical*

Engineering, 32: (2007) 650–670.

Raj, T.S., & S. Lakshminarayanan. "Multiobjective Optimization in Multiechelon Decentralized Supply Chains." *Industrial & Engineering Chemistry Research* 47: (2008a) 6661–6671.

———. "Performance Assessment/Enhancement Methodology for Supply Chains." *Industrial & Engineering Chemistry Research* 47: (2008b) 748–759.

Raman, R., & I.E. Grossmann. "Modeling and computational techniques for logic based integer programming." *Computers & Chemical Engineering* 18: (1994) 563–578.

Robins-Roth. "From Alchemy to IPO: The Business of Biotechnology." Technical report, Perseus publishing, 2001.

Rockafellar, R.T., & R. Wets. "Scenarios and policy aggregation in optimization under uncertainty." *Mathematics of Operations Research* 16: (1991) 119–147.

Romero, J., M. Badell, M.J. Bagajewicz, & L. Puigjaner. "Integrating Budgeting Models into Scheduling and Planning Models for the Chemical Batch Industry." *Industrial & Engineering Chemistry Research* 42: (2003) 6125–6134.

Romero, J., L. Puigjaner, T. Holczinger, & F. Friedler. "Scheduling Intermediate Storage Multipurpose Batch Plants Using the S-Graph." *AIChE Journal* 50: (2004) 403–417.

Ryu, J., V. Dua, & E.N. Pistikopoulos. "A bilevel programming framework for enterprise-wide process networks under uncertainty." *Computers & Chemical Engineering* 28: (2004) 1121–1129.

———. "Proactive Scheduling under Uncertainty: A Parametric Optimization Approach." *Industrial & Engineering Chemistry Research* 46: (2007) 8044–8049.

Ryu, J., & E.N. Pistikopoulos. "Design and Operation of an Enterprise-wide Process Network Using Operation Policies. 1. Design." *Industrial & Engineering Chemistry Research* 44: (2005) 2174–2182.

———. "Multiperiod Planning of Enterprise-wide Supply Chains Using an Operation Policy." *Industrial & Engineering Chemistry Research* 46: (2007a) 8058–8065.

———. "A novel approach to scheduling of zero-wait batch processes under processing time variations." *Computers & Chemical Engineering* 31: (2007b) 101–106.

Sabri, E.H., & B.M. Beamon. "A multi-objective approach to simultaneous strategic and operational planning in supply chain design." *Omega* 28: (2000) 581–591.

Sahinidis, N.V. "Optimization under uncertainty: state-of-the-art and opportunities." *Computers & Chemical Engineering* 28: (2004) 971–983.

Sanmartí, E., L. Puigjaner, T. Holczinger, & F. Friedler. "Combinatorial Framework for Effective Scheduling of Multipurpose Batch Plants." *AIChE Journal* 48: (2002) 2557–2570.

Santoso, T., S. Ahmed, M. Goetschalckx, & A. Shapiro. "A stochastic programming approach for supply chain network design under uncertainty." *European Journal of Operational Research* 167: (2005) 96–115.

Sauter, J.A., H.V.D. Parunak, & J. Goic. "ANTS in the supply chain." In *Workshop on agents for electronic commerce at agents 99*. 1999, 770.

Savelsbergh, M.W.P., & M. Sol. "The general pickup and delivery problem." *Transportation Science* 29: (1995) 17–29.

Schmidt, C.W., & I.E. Grossmann. "Optimization models for the scheduling of testing tasks in new product development." *Industrial & Engineering Chemistry Research* 35: (1996) 3498–3510.

Schmidt, G., & W.E. Wilhelm. "Strategic, tactical and operational decisions in multinational logistics networks: a review and discussion of modelling issues." *International Journal of Production Research* 38: (2000) 1501–1523.

Schultmann, F., B. Engels, & O. Rentz. "Closed-loop supply chains for spent batteries." *Interfaces* 33: (2003) 57–71.

Seferlis, P., & N. Giannelos. "A two-layered optimisation-based control strategy for multi-echelon supply chain networks." *Computers & Chemical Engineering* 28: (2004) 799–809.

Seppälä, J., L. Basson, & G.A. Norris. "Decision Analysis Frameworks for Life-Cycle Impact Assessment." *Journal of Industrial Ecology* 5: (2002) 45 – 68.

Shah, N. "Single and multisite planning and scheduling: current status and future challenges." In *FOCAPO 1998*, edited by J. Pekny, & G.E. Blau. 1998.

———. "Process industry supply chains: Advances and challenges." *Computers & Chemical Engineering* 29: (2005) 1225–1235.

Shapiro, J.F. "Challenges of strategic supply chain planning and modeling." *Computers & Chemical Engineering* 28: (2004) 855–861.

———. *Modeling the Supply Chain*. Duxbury, 2006.

Sharpe, W.F. *Portfolio Theory and Capital Markets*. McGraw-Hill Trade, 1999.

Shulz, P., M. Diaz, & J.A. Bandoni. "Supply chain optimization of large scale continuous processes." *Computers & Chemical Engineering* 29: (2005) 1305–1316.

Sousa, R., N. Shah, & L.G. Papageorgiou. "Supply chain design and multilevel planning - an industrial case." *Computers & Chemical Engineering* 32: (2008) 2643–2663.

Soylu, A., C. Oruç, M. Türkay, K. Fujita, & T. Asakura. "Synergy analysis of collaborative supply chain management in energy systems using multi-period MILP." *European Journal of Operational Research* 174: (2006) 387–403.

Srivastava, S.K. "Green supply chain management: A state of the art literature review." *International Journal of Management Reviews* 9: (2007) 53–80.

Stadtler, H. *Supply Chain Management and Advanced Planning*, Heidelberg: Springer, 2002, Ch. Supply Chain Management – An Overview.

Stefanis, S.K., A.G. Livingston, & E.N. Pistikopoulos. "Minimizing the Environmental Impact Of Process Plants: A Process Systems Methodology." *Computers and Chemical Engineering* 19: (1995) S39–S44.

Stern, N. "Stern Review on the Economics of Climate Change." *HM Treasury, London, UK* http://www.sternreview.org.uk/.

Subramanian, D., J.F. Pekny, & G.V. Reklaitis. "A Simulation-Optimization Framework for Research andDevelopment PipelineManagement." *AIChE Journal* 47: (2001) 2226–2242.

Subramanian, D., J.F. Pekny, G.V. Reklaitis, & G.E. Blau. "Simulation-Optimization Framework for Stochastic Optimization of R&D Pipeline Management." *AIChE Journal* 49: (2003) 96–112.

Sundaramoorthy, A., & I.A. Karimi. "Planning in pharmaceutical supply chain with outsourcing and new products introduction." *Industrial & Engineering Chemistry Research* 43: (2004) 8293–8306.

———. "A simpler better slot-based continuous-time formulation for short-term scheduling in multipurpose batch plants." *Chemical Engineering Science* 60: (2005) 2679–2702.

Sung, C., & C.T. Maravelias. "An Attainable Region Approach for Production Planning of Multiproduct Processes." *AIChE Journal* 53: (2007) 1298–1315.

Swaminathan, J.M., S.F. Smith, & N.M. Zadeh. "Modelling supply chain dynamics: a multi-agent approach." *Decision Sciences* 29: (1998) 607–632.

Talluri, S., & R.C. Baker. "A multi-phase mathematical programming approach for effective supply chain design." *European Journal of Operational Research* 141: (2002) 544–558.

Tang, C. S. "Perspectives in supply chain risk management." *International Journal of Production Economics* 103: (2006) 451–488.

The Mathworks, Inc. *Matlab: The Language of Technical Computing : Matlab Notebook User's Guide*. Natick: The Mathworks Inc., 1998.

The Mathworks, Inc. *MATLAB 7.0 (R14), Simulink 6.0, Stateflow 6.0. User's Manual*. The Math Works Inc., 2004.

Türkay, M., C. Oruç, K. Fujita, & T. Asakura. "Multi-company collaborative supply chain management with economical and environmental considerations." *Computers & Chemical Engineering* 28: (2004) 985–992.

Tsiakis, P., N. Shah, & C.C. Pantelides. "Design of multi-echelon supply chain networks under demand uncertainty." *Industrial & Engineering Chemistry Research* 40: (2001) 3585–3604.

USEPA, Ed. *AP 42, Fifth Edition, Volume I*, US Environmental Protection Agency, 1980, Ch. 6: Organic Chemical Process Industry, 6.14–1,6.14–5. Http://www.epa.gov/ttn/chief/ap42/ch06/final/c06s14.pdf.

Vargas-Villamil, F.D., & D.E. Rivera. "Multilayer optimization and scheduling using model predictive control: application to reentrant semiconductor manufacturing lines." *Computers & Chemical Engineering* 24: (2000) 2009 – 2021.

Varma, V.A., G.V. Reklaitis, G.E. Blau, & J.F. Pekny. "Enterprise-wide modeling & optimization - An overview of emerging research challenges and opportunities." *Computers & Chemical Engineering* 31: (2007) 692–711.

Verderame, P.M., & C.A. Floudas. "Integrated Operational Planning and Medium-Term Scheduling for Large-Scale Industrial Batch Plants." *Industrial & Engineering Chemistry Research* 47: (2008) 4845–4860.

———. "Integrated Operational Planning and Medium-Term Scheduling for Large-Scale Industrial Batch Plants." *Computers & Chemical Engineering* 33: (2009) 1036–1050.

Vidal, C.J., & M. Goetschalckx. "Strategic production-distribution models: A critical review with emphasis on global supply chain models." *European Journal of Operational Research* 98: (1997) 1–18.

———. "A global supply chain model with transfer pricing and transportation cost allocation." *European Journal of Operational Research* 129: (2001) 134–158.

Vonderembse, M.A., M. Uppal, S.H. Huang, & J.P Dismukes. "Designing supply chains: Towards theory development." *International Journal of Production Economics* 100: (2006) 223–238.

Wan, X., J.F. Pekny, & G.V. Reklaitis. "Simulation-based optimization with surrogate models. Application to supply chain management." *Computers & Chemical Engineering* 29: (2005) 1317–1328.

Wang, W., D.E. Rivera, & K.G. Kempf. "Model predictive control strategies for supply chain management in semiconductor manufacturing." *International Journal of Production Economics* 107: (2007) 56–77.

Weissenrieder, F. "Value Based Management: Economic Value Added or Cash Value Added?" Technical report, Department of Economics, Gothenburg University, Sweden, 1998.

Whitin, T.M. "Inventory control and price theory." *Management Science* 2: (1955) 61–80.

Wilkinson, S.J., A. Cortier, N. Shah, & C.C. Pantelides. "Integrated production and distribution scheduling on a Europe-wide basis." *Computers & Chemical Engineering,* S20: (1996) S1275–S1280.

Wooldridge, M., & N. Jennings. "Intelligent agents: theory and practice." *Knowledge Engineering Review* 10: (1995) 115.

WTO. "International Trade Statistics 2008." Technical report, World Trade Organization, 2008.

Xie, Y., D. Petrovic, & K. Burnham. "A heuristic procedure for the two-level control of serial supply chains under fuzzy customer demand." *International Journal of Production Economics* 37–50.

Yang, A., & Y. Yuan. "An object/agent based system modeling framework for integrated process plant operations." In *AIChE Annual Meeting*. 1999, 211f.

Ydstie, B.E. "Distributed decision making in complex organizations: the adaptive enterprise." *Computers & Chemical Engineering* 29: (2004) 11–27.

Yi, G., & G.V. Reklaitis. "Optimal design of batch-storage network with recycle streams." *AIChE Journal* 49: (2003) 3084–3094.

———. "Optimal design of batch-storage network with financial transactions and cash flows." *AIChE Journal* 50: (2004) 2849–2865.

———. "Optimal Design of Batch-Storage Network Considering Exchange Rates and Taxes." *AIChE Journal* 53: (2007) 1211–1231.

You, F., & I.E. Grossmann. "Design of responsive supply chains under demand uncertainty." *Computers & Chemical Engineering* 32: (2008) 3090–3111.

Young, D. M., & H. Cabezas. "Designing sustainable processes with simulation: the waste reduction (WAR) algorithm." *Computers and Chemical Engineering* 23: (1999) 1477–1491.

Young, T. "The beginners' guide to the UK's carbon trading schemes." *Business Green* http://www.businessgreen.com/business–green/analysis/2224,230/.

Zapata, J.C., V.A. Varma, & G.V. Reklaitis. "Impact of tactical and operational policies in the selection of a new product portfolio." *Computers & Chemical Engineering* 32: (2008) 307–319.

Zhou, G., H. Min, & M. Gen. "The balanced allocation of customers to multiple distribution centers in the supply chain network: a genetic algorithm approach." *Computers & Industrial Engineering* 43: (2002) 251–261.

Zhou, Z., S. Cheng, & B. Hua. "Supply chain optimization of continuous processes industries with sustainability considerations." *Computers & Chemical Engineering* 24: (2000) 1151–1158.

Author Index

Subject Index