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## *A contribution to sustainable management of integrated material/energy networks in process industries*

**Shabnam Morakabatchiankar**

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A contribution to Sustainable Management of Integrated  
Material/Energy networks in Process Industries



**A contribution to Sustainable Management of  
Integrated Material/Energy networks in Process  
Industries**

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A Thesis Presented for the degree of  
Doctor of Philosophy

Advised by

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To my father

– to whom I promised to dedicate this dissertation before he left this world

To my mother

for her endless love, support and encouragement.



*"Science knows no country because knowledge belongs to humanity and is the torch which illuminates the world."*

Louis Pasteur (1849-1895)





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## *Summary*

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Towards sustainability forces process industries to change their traditional patterns. Therefore, efficient retrofitting has been a significant challenge and raised several issues, motivating the process system engineering (PSE) to develop models. These models mainly aim to optimize profitability, cost reduction, energy consumption, demand satisfaction, the environmental impact associated with the production process, and social acceptance. Nevertheless, such optimization is significantly complicated if considering the presence of uncertainty and seeking compromised outcomes.

This thesis aims to extend a general model to facilitate retrofitting in industrial processes and expedite optimization of the issues. Such a contribution based on developing efficient mathematical models allows coordinating many decision variables synchronizing the production and distribution tasks in terms of economic and environmental criteria.

This thesis presents an overview of the retrofitting requirement towards sustainable material/energy networks, describing and analyzing the current methods, tools, and models used and identifying the most relevant open issues.

The second part focused on developing current models stressing energy integration in the processing system. This part first explores how the economic performance of the network can be enhanced and environmental impacts improved simultaneously by integrating an energy generation unit into the production system. Furthermore, the network sustainability performance was explored under demand uncertainties. Additional risk indicators (including financial and environmental risk metrics) have been included to add risk management capability to the model. This part also explores the strategies that efficiently select the number of scenarios.

Consequently, a novel generalized mathematical formulation that integrates equations regarding energy generation and material production decision variables is efficiently solved. The effect of uncertainty on the economic and environmental performance is analyzed by using risk analysis. Finally, the model was extended to solve multi-renewable energy generation integrated into the multi-product production process under demand uncertainty. The importance and effect of the

energy/material integration over the network configuration are analyzed through sensitivity analysis.

The third part of this thesis provides the conclusions and further work to be developed.

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## *Resumen*

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El camino hacia la sostenibilidad obliga a las industrias de procesos a cambiar los patrones de trabajo tradicionales. La modernización eficiente es un importante desafío que plantea múltiples problemas, lo que ha llevado a la ingeniería de sistemas de procesos (PSE) a desarrollar modelos que intentan no solo optimizar la rentabilidad, reducir de costes o satisfacer demanda de productos y servicios, sino también afrontar el impacto ambiental asociado al proceso productivo y la aceptación social de dicho proceso, en entornos volátiles, en los que la consideración de la incertidumbre asociada al escenario de trabajo es esencial.

Esta tesis tiene como objetivo ampliar y flexibilizar los modelos de gestión de cadena de suministro existentes para facilitar la retroadaptación de los procesos industriales y agilizar la optimización de los problemas de toma de decisiones en este entorno. Tal aporte está basado en el desarrollo de modelos matemáticos eficientes que permite coordinar diferentes variables de decisión, sincronizando las tareas de producción y distribución en términos de criterios económicos y ambientales.

Para ello, en primer lugar se presenta una visión general del requisito de adaptación hacia redes de materiales / energía sostenibles, describiendo y analizando los métodos, herramientas y modelos actuales utilizados e identificando los problemas abiertos más relevantes.

La segunda parte de esta Tesis se centra en el desarrollo de modelos que enfatizan la integración energética en el sistema de proceso. Esta parte explora primero cómo se pueden mejorar simultáneamente el desempeño económico de la red y los impactos ambientales mediante la integración de unidades de generación de energía en el sistema de producción. Además, se ha explorado el rendimiento de la sostenibilidad de la red bajo incertidumbre en la demanda. Se han incluido indicadores de riesgo adicionales (incluidas métricas de riesgo financiero y ambiental) para incorporar en el modelo la capacidad de gestión de riesgos. Esta parte también explora las estrategias que seleccionan de manera eficiente el número de escenarios a considerar.

En consecuencia, se resuelve de forma eficiente una formulación matemática novedosa que generaliza e integra ecuaciones relativas a decisiones de producción energética y de materiales. El efecto de la incertidumbre sobre el desempeño económico y ambiental se analiza mediante

análisis de riesgo. Finalmente, el modelo se amplía para abordar la utilización coordinada de diferentes formas de energía renovable, y su integración en el proceso de producción multi-producto bajo incertidumbre en la demanda. La importancia y el efecto de la integración de la toma de decisiones sobre la configuración de la red se discuten a través de diferentes análisis de sensibilidad.

La tercera parte de esta tesis resume las conclusiones de todos estos trabajos y plantea ampliaciones y nuevas líneas de mejora que surgen a partir de los modelos y procedimientos desarrollados en esta tesis.

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*Part I*

*Overview*



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## MOTIVATIONS, OBJECTIVES & INTRODUCTION

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This chapter presents an overview of challenges in process industries. Generally, the challenges are listed as increasing economic performance, reducing resource consumption, and minimizing environmental impact issues. These challenges have been arising since the industries were forced to keep their pace with sustainable development. This chapter has focused on the challenges associated with sustainability in energy/material supply chains. Furthermore, this chapter proposes the research scope and objectives of this thesis. Generally, these objectives focus on improving the sustainability of process industries, specifically energy management and renewable resources exploitation.

### **1.1. Introductory perspective and global issues**

Attention regarding the energy consumptions of existing process industries and environmental concerns such as more restrictive regulations on greenhouse gases (GHG) emissions has been growing for recent decades. This attention has made industrial sectors modify their energy and environmental performance using innovative retrofitting strategies, particularly integrating renewable energy sources (RES) in the production process. Hence efficient management of integrated systems is one of the most significant challenges of our time.

To that end, the design optimization based on new resources and technologies, alternative materials, and equipment seems to be essential. Also, environmental and economic assessments are crucial in the retrofitted production process since many policies are pursuing to reduce climate change risks by developing strategies and technologies to reduce emissions.

In this line, significant efforts have been made to improve the energy efficiency in the industrial sector, mainly focused on various energy savings strategies such as management, technologies, and policies during the last years (Abdelaziz, Saidur, & Mekhilef, 2011). However, it is still required innovative and efficient strategies such as integrated solutions combining different technologies and approaches are still required. Besides, despite the efforts to change the current trend, the International Energy Agency (Koirala, 2017) reports that industries are half as energy-efficient as they could be according to the thermodynamic laws. So, the opportunities to enhance the performance and reduce the environmental impacts are still very high. Consequently, intensive work in strategies is needed for worldwide enterprises to recover/maintain market leadership, disregarding the chaotic and competitive environment. For this purpose, studying the following issues have to be simultaneously addressed:

- An efficient model for highly complex networks through a well-balanced policy for material, energy, costs, and environmental concerns
- Efficient resource occupation (optimal process management)
- Intensive collaboration in integrative areas, promoting the development of integrated frameworks
- Reducing and preventing unfavorable environmental and improving costs (e.g., “Green engineering”).

Hence, Process System Engineering (PSE) is an adequate response to the above needs linking the concepts of modeling, simulation, optimization, and process control for the analysis, evaluation, and optimization for the design and operation of process systems. However, the significant advancement in approaches, methodologies, and computational procedures, has been done to address the above issues, the following particular challenges remain as open issues for PSE researchers regarding recent studies (Filho, Angeli, & Fraga, 2018; Grossmann, 2017):

- To develop integrated frameworks for the management of complex process systems.
- To improve the use and quality of the environmental indicators for the design of eco-friendly processes.
- To facilitate the procedure of design under uncertainty for process scale-up.
- To represent the treatment of uncertainty in process design and optimization through the development of novel modeling frameworks.
- Developing hybrid approaches (dynamic and discrete strategies integration).
- Multi-scale dynamic modeling.

The majority of mentioned issues have their limitations and specific application requirements to process problems; since the design and management of complex sustainable processes under uncertainty are a particular interest, it has to be applied for all the industrial activities worldwide. Thus, this thesis focuses on developing an integrated framework to facilitate the management of large-scale and complex process industries and represents treatment for issues associated with sustainability problems under uncertainty.

Moving toward sustainability and mainly being aware of the scarcity of resources, climate change, and environmental pollution requires revising current production and consumption patterns while enhancing the robustness of process industries. Currently, researchers are making an effort to develop approaches that promote sustainable solutions. Their solutions aim to a) facilitate the efficient management of natural resources (i.e., water, biomass, and fossil fuels) (Bernardi, Giarola, & Bezzo, 2012), b) reduce emissions, and c) develop alternative energy generation processes (i.e., reduce fossil-fuel dependency)(Martín & Grossmann, 2017).

In particular, these approaches assist in evaluating, identifying, and reducing the most damaging industrial activities; however, they have limitations and can apply to specific industries. Thus, the proposed models have not been general enough, including various technologies and resources.

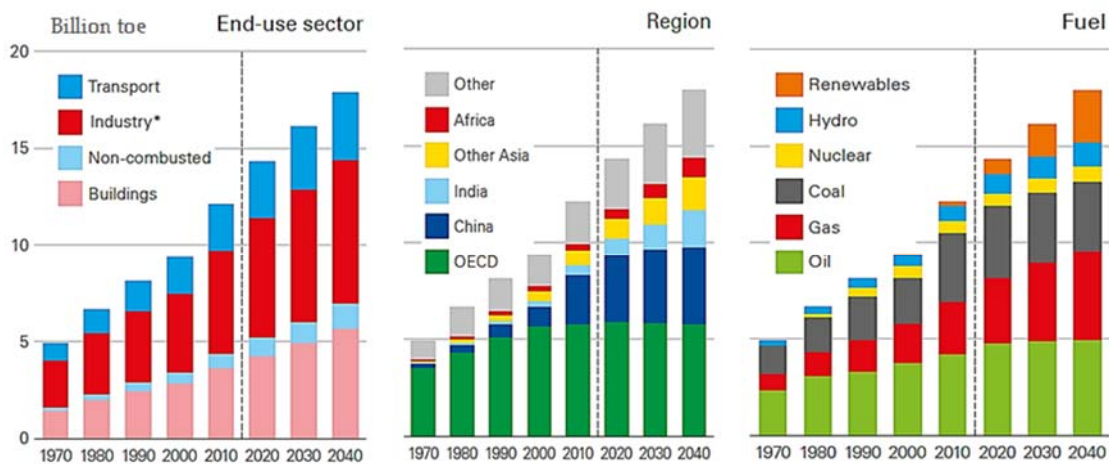
## 1.2. The Industrial energy demand situation

Global energy consumption is steadily increasing with economic growth as well as the population explosion. Due to International Energy Agency IEA reports conducted in 2019, worldwide consumption in 2018 has increased at nearly twice the average growth rate since 2010. The significant sources of energy are fossil-derived fuels, including petroleum, coal, and natural gases. Table. 1.1 displays the demand for all fuels has been increased.

Table. 1. 1. Global energy demand (Global Energy & CO2 Status Report 2019 – Analysis - IEA).

	Energy Demand (Mtoe)		Shares (%)	
	2018	Growth rate (%)	2000	2018
<b>Total Primary Energy Demand</b>	<b>14 301</b>	<b>2.3%</b>	<b>100%</b>	<b>100%</b>
Coal	3 778	0.7%	23%	26%
Oil	4 488	1.2%	37%	31%
Gas	3 253	4.6%	21%	23%
Nuclear	710	3.3%	7%	5%
Hydro	364	3.1%	2%	3%
Biomass and waste	1 418	2.5%	10%	10%
Other renewables	289	14.0%	1%	2%

Regarding the BP Statistical Review of World Energy conducted in 2019 (BP, 2019), crude oil and natural gas, the primary energy resources, maybe run out respectively in another 45 and 60 years, with the current global energy consumption rate.



\*Industry excludes non-combusted use of fuels

Fig. 1. 1. The energy consumption trend through three different lenses: sectors, regions and, fuels (BP p.l.c., 2019).

The energy transition from three different perspectives is illustrated in Fig 1.1, that each of these graphs illuminates different aspects of the transition: the sectors, the regions, and the consumption and production of different fuels. The industrial sector is the largest major energy consumer globally, representing more than 33% of total consumption. Total world energy utilized in the industrial sector reached 5 Billion tons of oil equivalent in 2010, and it forecasts that amount can be reached 7 Billion tons of oil equivalent in 2040.

All of the growth in energy demand centralizes fast-growing developing economies, led by India and China. In 1990, the Organization for Economic Co-operation and Development (OECD) accounted for almost two-thirds of energy demand, with the developing world just one-third. In the energy transition (ET) scenario, that position is almost exactly reversed by 2040, with the non-OECD accounting for over two-thirds of demand. China remains the most prominent energy market: in 2040, roughly twice the size of India. Energy consumption in Africa keeps small relative to its size: in 2040, Africa accounts for almost a quarter of the world's population but only 6% of energy demand.

Renewables and natural gas account for 85% of energy growth. The substitution of a lower-carbon energy system with renewable energy and natural gas is gaining importance relative to oil and coal. The fastest-growing energy source belongs to renewable energy (7.1% p.a.), contributing half of the growth in global energy, with its share in primary energy increasing from 4% today to around 15% by 2040.

Besides, the continued use of fossil-based fuels is not sustainable due to its limited availability and greenhouse gases emission and other air contaminants, including carbon dioxide ( $CO_2$ ), carbon monoxide ( $CO$ ), sulfur dioxide ( $SO_2$ ), nitrogen oxides ( $NO_x$ ), in addition to particulate matter and volatile organic compounds, upon combustion (Patade, Meher, Grover, Gupta, & Nasim, 2018).

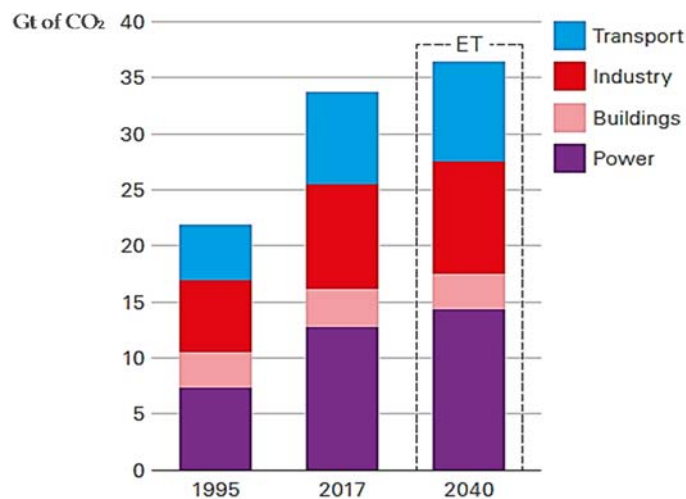


Fig. 1. 2.  $CO_2$  Emission by sector (BP p.l.c., 2019)

As Fig. 1.1 illustrates, the rapid growth in energy demand in the power and industry sectors means that they are the largest source of the increase in  $CO_2$  emissions over the same period (see Fig 1.2), with their share in the global energy system increasing to around 40% and 25% respectively by 2040. These are far higher than the transport sector, which accounts for around 10% of  $CO_2$  of energy use. Most importantly, carbon prices will increase to \$200 per tonne of  $CO_2$  in the OECD and \$100 in the non-OECD by 2040 (reported by BP p.l.c., 2019).

Therefore, the global energy system, particularly industrial sectors, faces a dual challenge: the need for ‘more energy and less carbon. Hence, for environmental and economic sustainability, renewable and carbon-neutral efficient biofuels are needed to displace or supplement the long run and complement the fossil-derived fuels soon.

Focusing on renewables studies reveals a global acceptance of the renewable resources to penetrate the global energy system more quickly than other alternatives (Fig. 1.3).

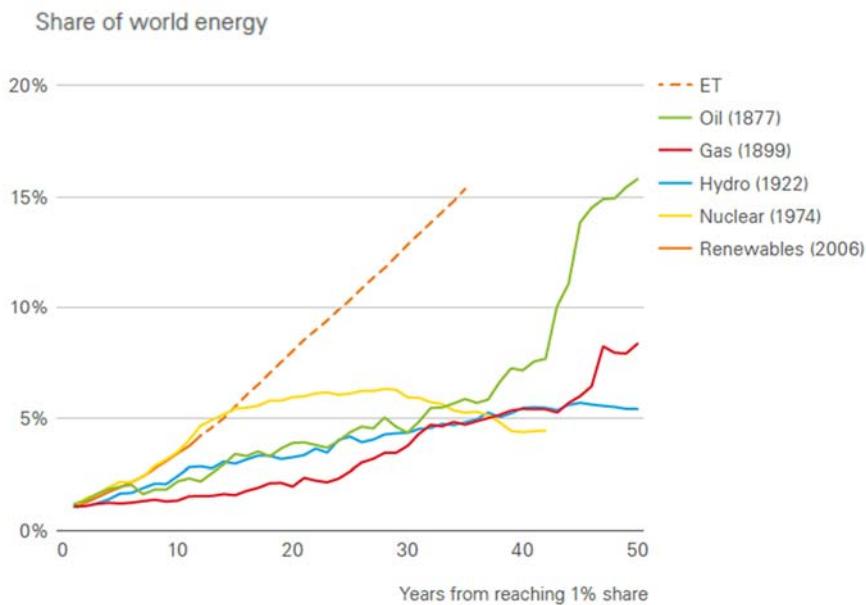


Fig. 1. 3. Speed of penetration of new fuels in the global energy system (BP p.l.c., 2019).

In short, renewable exploitation strategies have been implemented in the industrial context to optimize the design of energy networks (Martín & Grossmann, 2018). Nevertheless, the application of the exploitation of renewables strategies in industries is sometimes confined to address problems with the following assumptions:

- The regionalized problems in which the variability of renewable resource availability in medium/large scale problems,
- Multi-product problems.

Hence, the use of Supply Chain Management (SCM) concepts represents a powerful tool to manage the material/energy flows.



### 1.3. Supply chain management concepts

A Supply Chain (SC), as displayed in Fig. 1.4, is generally defined as an integrated process involving organizations to transform raw materials into final products and deliver them to the end-user. A Supply Chain typically consists of four echelons: supply (providing raw materials), production (converting these raw materials into final products), storage/distribution (storing and delivering demanded final products to retailers) and, market (selling these to end-users) (Lainez, Kopanos, España, & Puigjaner, 2009).

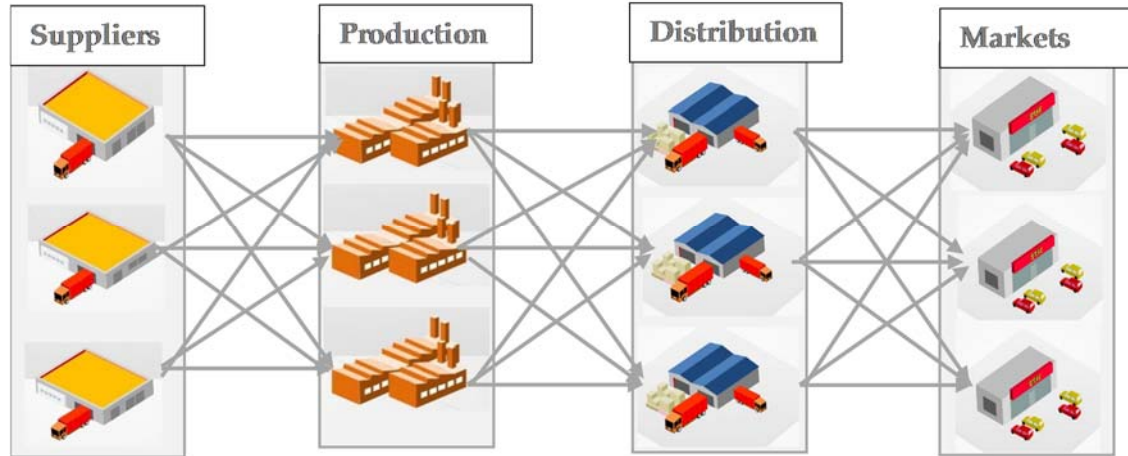


Fig. 1. 4. Generic multi-echelon Supply Chain Network.

The concept of Supply Chain Management (SCM) defines the governance of the exchangeable resources (i.e., material, information, and financial) flows within a conventional supply chain explained above. Supply Chain Management mainly aims to achieve an end-users satisfactory level and optimize economic performance by coordinating the SC activities.

#### 1.3.1. Sustainable supply chain management

Accelerated globalization and increased demands on being responsible for the environmental and social performance force organizations to evolve, and the concept of industrial symbiosis and circular economy plays an essential role in managing this evolution (Y. Zhang, Zheng, Chen, Su, & Liu, 2014).

Due to circular economy, Sustainable supply chain management involves integrating and financially viable practices into an overall supply chain lifecycle, from product design and development to material selection, including raw material extraction or agricultural, fabrication, packaging and transportation, storing, distribution and consumption, return to disposal. Environmentally conscious supply chain management and practices can assist organizations in reducing their total carbon footprint and optimize their end-to-end operations to achieve more efficiency. Sustainable aspects can apply to all supply chains that can be optimized. Sustainability in the SC encapsulates several different priorities:

- Environmental management

- Conservation of resources
- Reduction of carbon footprint
- Financial savings and viability
- Social responsibility.

In short, supply chain sustainability practices, to succeed, must deliver improved environmental performance within a financially viable operating construct.

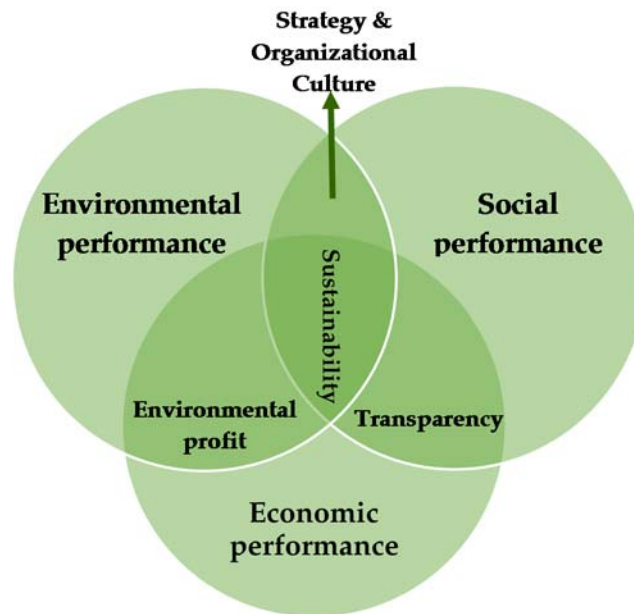


Fig. 1. 5. A Framework of Sustainable Supply Chain Management.

Fig. 1.5 illustrates the three activities and the intersection between them that form sustainability. In the literature, most studies tackled the social and environmental dimensions of Sustainable Supply Chain Management (SSCM) towards the economic goal achievements of the firm and its supply chain (K. Xu & Cong, 2011).

### 1.3.2. Supply Chain Mathematical Modeling

Mathematical modeling, generally, intends to define a quantitative system as close to reality as possible through a set of equations. Supply chain modeling is mainly applied for control, coordination, identifying potential bottlenecks, and optimizing supply chain management. The SSCM contains a four-dimension structure consists of SCM, sustainability, modeling, and research directions. Hence, these four compromised dimensions define the modeling approaches. The model type keywords are pretty extensive and linked to many tools and techniques, and the employed solution approaches that Fig. 1.6 maps them.

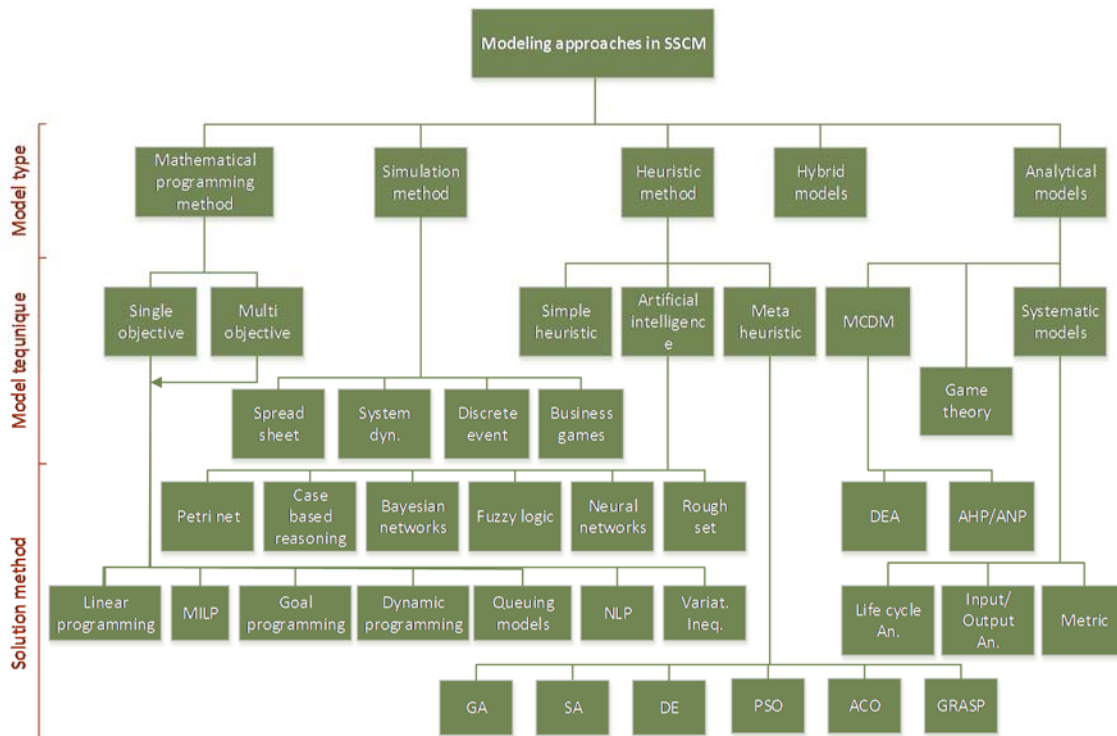


Fig. 1. 6. Analytic categories of the structural dimension “Modeling” (Brandenburg, et al., 2014).

Furthermore, as supply chains consist of sets of different task-oriented entities depending on the particular arrangement of the set’s elements, different organizational problems come up so that there are different decision-making policies to cope with them. Historically, two approaches have been proposed based on the decision-making domain: Centralized and Decentralized approaches (Saharidis, 2011).

The *centralized* approach considers a single entity that authorizes to take all the SC decisions. It significantly eases network coordination, although its application is inefficient and often leads to decisions that all the process members hardly accept.

Despite the centralized one, the *Decentralized* approach considers an active attitude of the entire supply chain members. Decision-makers take their own decisions as a function of their performances. This approach leads to a well-balanced solution-seeking of the highest benefit for all the entities. Nevertheless, the decisions of a supply chain member affect the overall system performance and other member’s decisions. Also, a lack of information between supply chain members’ performances, preferences, and behaviors influences the robustness/confidence of the final decisions.

Note that the Decision-making process runs while many alternative material suppliers and potential customers increase complexity and decrease efficient coordination. Thus, a classification based on the planning horizon can assist in easing the solution of SCM problems. It is explained this classification as below:

- Long-term planning (Strategic level): in this level, the planning horizon is yearly-based and in which the decisions include the number of facility locations and facilities capacities and the decisions that imply economic impacts.
- Medium-term planning (Tactical level): typically, in this level, it is assumed a monthly-based time horizon in which the optimization of production operations happens to satisfy the demand at a satisfactory level. Tactical decisions include the amounts of exchangeable resources (i.e., acquisition and distribution), optimal production targets, and inventory levels across time.
- Short-term planning (Operational planning): daily planning is usually, considered and decisions in this level are associated with the complex equipment operations (startup and shut down), the production quantities, and task sequencing to specific equipment.

#### **1.4. Research Scope and Objectives**

There has not yet been any quantitative methodology to retrofit large-scale integrated energy/material supply chains for process industries by reviewing the literature. Accordingly, developing an effective general model is necessary, specifically in highly competitive and uncertain situations. Hence this thesis aims to develop a model able to, generally, optimize the tactical/strategic decisions of large-scale process industries focusing on material/energy integrated supply chains. Regarding the overall goal, the following objectives are supposed to accomplish:

- Propose a mathematical model that represents integrated energy/material supply chains of process industries.
  - Develop a multi-objective model considering at least economic, environmental aspects.
  - Evaluate the effect of uncertainties over a centralized scheme.
- Develop and generalize tactical/strategic models for retrofitting multi-product multi-energy resource systems.
- Integrate renewables resources in process industries to offer the most effective method for reducing fossil energy consumption and greenhouse gas emissions.
- Address risk management in sustainability problems under uncertainty by extending the current multi-objective models.
- Analyze and compare integrated systems in comparison with current standalone models.

The capability of the proposed model must be well assessed under a holistic multi-objective approach (i.e., energy, environmental impact, and cost-effectiveness) to obtain conclusive results. Hence, the thesis applies the model to a case study, and its viability is analyzed. As concluded by the results, retrofitting energy/material systems with integrated renewable resources are most suitable for countries with a high share of carbon-rich sources.

Besides, the proposed model is general enough and applicable for different industries scales, including uncertainty of demand for products of process industries.

### 1.5. Thesis outline

The thesis structure devises to address the previously discussed sustainable supply chain management issues; multi-objective optimization and uncertainty approaches are the two critical elements across the different parts of the thesis.

In addition to the overview of the current sustainability problems, especially in supply chain management (Chapter 1), **part I** of this thesis consists of a detailed state of the art for Sustainable Supply Chain Management (SSCM), motivations, and general objectives of this thesis. The rest of part I consists of:

- ❖ a detailed state of the art for the Sustainable Supply Chain Management (SSCM), uncertainty, and mathematical programming applications (Chapter 2).
- ❖ The description of methodologies and tools and the advantages and disadvantages of the methods used to address sustainable SCM developed until now (Chapter 3).

Note that at the end of **part I**, significant challenges are identified. Basically, in this part, the different optimization techniques used throughout this thesis have been outlined. The main concepts briefly are explained to provide the reader with a general knowledge of the theories behind the solution techniques. Notably, it emphasizes techniques and algorithms for Multi-objective optimization and stochastic programming since their application to sustainability problems requires a solid knowledge of their principles (see Fig. 1.6).

**Part II** evaluates supply chain retrofitting for energy integration in the process industries to identify the overall better solution using multi-objective optimization. In particular, Chapter 4 explores the sustainability benefits of single renewable energy resource integration in material supply chains. The results are compared to non-integrated ones to observe the capability of the novel model through environmental impacts, and economic objectives improve simultaneously. In Chapter 5, the main challenge is uncertainty and its effect within a sustainable energy SC. In the same way, Chapter 6 proposes a design and planning optimization model of multi-renewable energy resources (as an internal energy supplier) integrating into process industries.

Finally, **Part III** summarizes the main contribution of this thesis and draws up concluding remarks for future work.

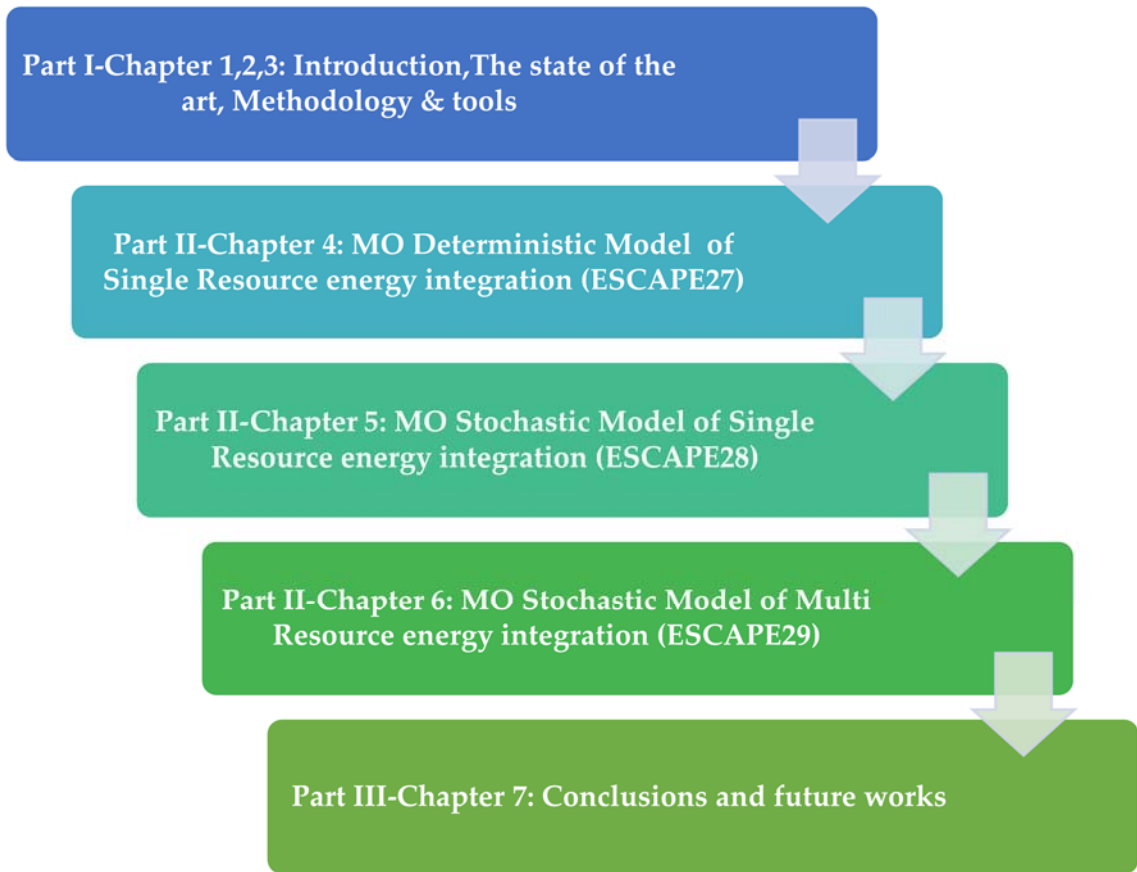


Fig. 1.7. Thesis outline.



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## THE STATE OF THE ART

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This chapter summarizes the main contributions to the optimization of Sustainable Supply Chain Management. Besides, it reviews studies addressing the challenges related to uncertainty management. Finally, this chapter identifies the most relevant open issues addressed in this thesis.

### 2.1. Sustainable Supply Chain Management

Recently, the application of Industrial Ecology (IE) and Industrial Symbiosis (IS) concepts in supply chain management creates a challenging area named sustainable supply chain management (Leigh & Li, 2015). Hence, several researchers provided frameworks for a common understanding of SSCM among supply chain managers to adopt it in practice and accept them during the last decades. In this line, (Carter & Rogers, 2008) performed a large-scale literature review and presented the rational relation between environmental, social, and economic performance within a supply chain management context by using conceptual theories. Later, the researchers conducted studies to modify, develop, and optimize conventional supply chains regarding sustainability. For instance, (Kleindorfer, Singhal, & Wassenhove, 2005) introduced a new pattern for extended supply chains and sustainable operation management. (K. Xu & Cong, 2011; Yen & Yen, 2012) proposed a framework to modify environmental logistics; these studies attempted to propose a sustainable modification at the managerial level. In this regard, the literature review classifies into 1) sustainable Material SCs, 2) Biomass SCs, and 3) Renewable resource SCs described the following.

#### 2.1.1. Sustainable Material Supply Chain Management

Several researchers have conducted studies to develop material supply chains at the operation and design level to be sustainably conscious. Recently, (A, Pati, & Padhi, 2019) have done a holistic literature review on Sustainable supply chain management in the chemical industry. Commonly, the primary approach towards sustainability in an SSC is carbon emission reduction, but some studies considered the other environmental metrics like (Mele, Guillen-Gosalbez, & Jimenez, 2009) that tried to optimized the biochemical oxygen demand.



One of the definitive studies in this field is the work proposed by (Guillen-Gosalbez & Grossmann, 2009); they developed a chemical supply chain to be more sustainable by controlling life cycle inventory associated with network operation. Later on, they developed the precedent work by using the damage assessment model. (Mele, Kostin, Guillén-Gosálbez, & Jiménez, 2011) applied their model to a fuel supply chain extended it by using GWP100 in addition to Eco-indicator 99 and optimized the SC in the presence of these two environmental indicators. Besides, (Azadeh, Shafiee, Yazdanparast, Heydari, & Fathabad, 2017) presented a bi-objective optimization model of crude oil supply chains minimizing environmental impacts damage assessment model while maximizing economic criteria simultaneously.

Generally, sustainable supply chains are modeled as multi-objective optimization problems to obtain trade-offs amongst economic, environmental, and social criteria. Nevertheless, most studies consider only the environmental and economic objective functions, neglecting the social criterion, and commonly are case-specific. The lack of a general SSC model has been a notable motivation for this thesis. Relatively, (Tautenhain, Barbosa-Povoa, & Nascimento, 2019) described a generic multi-objective formulation that includes the three pillars of sustainability and proposed a metaheuristic to obtain approximations of the Pareto frontier within a reasonable time.

### 2.1.2. Biomass Supply Chain Management

From the other perspective, the substitution of biofuels with fossil-based fuels is one way to move towards sustainable development. Biomass supply chains and biofuels/bioenergy production present paradigmatic case studies regarding the consideration of sustainability issues and the exploitation of industrial symbiosis (IS), industrial ecology (IE), circular economy (CE) opportunities in the process industries. Several studies have illustrated the advantages of these approaches as classified in the followings:

#### a) Biomass to bioenergy

- Cost-effectiveness approach of SC design and scheduling optimization (A. Dunnett, Adjiman, & Shah, 2007);
- Cost optimization of logistics (Y. Yu, Bartle, Li, & Wu, 2009);
- Costs optimization of logistics and network design (Parker, Fan, & Ogden, 2010);
- Multi-objective design optimization of SC (Pérez-Fortes, Laínez-Aguirre, Arranz-Piera, Velo, & Puigjaner, 2012);
- Cost and  $CO_2$  emission optimization of logistics (Kanzian, Kühmaier, Zazgornik, & Stampfer, 2013);
- Multi-objective design and planning optimization (Perez-Fortes, Laainez-Aguirre, Bojarski, & Puigjaner, 2014);
- Multi-objective design and planning optimization (Cambero, Sowlati, & Pavel, 2016);
- Multi-objective optimal planning (She, Chung, & Han, 2019);

- Cost evaluation of SC design (Ling et al., 2019);
- Multi-objective optimization of logistics network (C. Chen, Gan, Zhang, & Qiu, 2020);

**b) Biomass to biofuel**

- Production and logistics cost optimization (A. J. Dunnett, Adjiman, & Shah, 2008);
- Cost optimization of logistics (Zamboni, Shah, Bezzo, & others, 2009);
- Well-To-Tank (WTT) approach and multi-objective optimization (Zamboni, Shah, & Bezzo, 2009);
- Biorefinery logistics and design optimization (S. D. Ekşioğlu, Acharya, Leightley, & Arora, 2009);
- Cost optimization of design and logistic of SC (Ekşioğlu, Li, Zhang, Sokhansanj, & Petrolia, 2010);
- Cost optimization of SC design (Akgul, Zamboni, Bezzo, Shah, & Papageorgiou, 2010);
- Cost optimization of SC strategic planning (Huang, Chen, & Fan, 2010);
- Multi-objective design and planning optimization (You & Wang, 2011);
- Multi-objective planning optimization (Santibanez-Aguilar, Gonzalez-Campos, Ponce-Ortega, Serna-Gonzalez, & El-Halwagi, 2011);
- Optimal cost of SC design (Corsano, Vecchiotti, & Montagna, 2011);
- Optimal cost of SC design (Kim, Realff, Lee, Whittaker, & Furtner, 2011);
- Multi-objective design and planning optimization (Giarola, Zamboni, & Bezzo, 2011);
- Optimal Multi-objective design (You, Graziano, & Snyder, 2012);
- Optimal cost of planning and feedstock resource allocation (C. W. Chen & Fan, 2012);
- Multi-objective design optimization and risk management (Giarola, Bezzo, & Shah, 2013);
- Multi-objective design optimization (Liu, Qiu, & Chen, 2014a);
- Optimal multi-objective planning (Santibañez-Aguilar, Gonzalez-Campos, Ponce-Ortega, Serna-Gonzalez, & El-Halwagi, 2014);
- Economic evaluation considering carbon reduction in SC design and planning (Lainez-Aguirre, Pérez-Fortes, & Puigjaner, 2017);
- Optimal multi-objective design (Gao, Qu, & Yang, 2019);
- Optimal design cost-effectiveness (Sarker, Wu, & Paudel, 2019);

**c) Biomass/bioenergy integrated with renewable energy**

- Optimal cost of planning and logistics (Cucek, Martin, Grossmann, & Kravanja, 2014);
- Multi-objective design and planning optimization (Yue, You, & Snyder, 2014);
- Cost optimization of energy management of biomass-renewable SC (C. Wang et al., 2016);
- Cost-effectiveness of renewable resource supply chains (Giwa, Alabi, Yusuf, & Olukan, 2017);

- Cost optimization of biomass combined renewable energy resource supply chain (Zheng, Jenkins, Kornbluth, Kendall, & Træholt, 2018);

As mentioned above, biomass supply chain management consists of three main classes of **(a)**, **(b)**, and **(c)**. The studies of class **(a)** aim to optimize the economic and environmental performance of bioenergy SCs. Mathematical programming is applied to obtain optimal design or/and planning supply chains. These works responded to sustainability by demonstrating the viability of bio-based energy substitution with fossil-based energies. Besides, they optimize and control environmental impacts, mainly by  $CO_2$  emission reduction.

Class **(b)** were more widely studied. Mostly are bi-objective optimization to achieve minimizing costs and environmental impacts. Some of them considered social acceptance along with the economic performance of the SCs. The studies tried to obtain an optimal design or/and planning biomass for biofuel networks.

Class **(c)** consists of studies dedicated to optimizing the combination of biomass and renewable energy resources. Note that in this class, fewer studies exist.

### 2.1.3. Renewable resource Supply Chain Management

Renewable energy resources, or renewables, are naturally replacing fuel sources that can substitute with coal, oil, natural gas, and nuclear power and provide clean, safe, and reliable power with low or zero carbon emissions. Towards sustainability, several potential benefits make renewables an attractive option for the energy supply chains.

However, the significant renewable energy challenges are related to its fundamental characteristics. The most widespread renewable energy technologies – wind and solar – should tackle variability and uncertainty. In this line, researchers have mainly focused on optimizing these renewable energy resource characteristics, often summarized in the notion of intermittency, cause friction – technical, operational, financial - when integrating them in the energy system.

The most recent works have concentrated on **a)** optimization in microgrids (Borhanazad, Mekhilef, Gounder Ganapathy, Modiri-Delshad, & Mirtaheri, 2014; Fathima & Palanisamy, 2015; Hafez & Bhattacharya, 2012; Sanchez et al., 2014), **b)** optimal sizing (Ahadi, Kang, & Lee, 2016; Alabert, Somoza, De La Hoz, & Graells, 2016; Askarzadeh, 2017; Ogunjuyigbe, Ayodele, & Akinola, 2016; Tito, Lie, & Anderson, 2016), and **c)** multi-objective optimal design and planning (Baghaee, Mirsalim, Gharehpetian, & Talebi, 2016; Dufo-López, Cristóbal-Monreal, & Yusta, 2016; Kamjoo, Maheri, Dizqah, & Putrus, 2016; Maleki, Pourfayaz, & Rosen, 2016).

Generally, it is deduced through the literature review that the studies evolved by the time from single to multi-objective optimization, to be environmental and socially conscious, cover more concepts such as logistics, design, and planning at once, and finally to be more robust while considering uncertainty.

## 2.2. Multi-Objective Optimization

Historically, process industries focused on optimizing economic performance, and this concept includes unit installation, allocation, raw material, energy, and product flows and production rates. Since the sustainability concepts received strict attention, considering environmental and social aspects seems inevitable. Thus, it is necessary to adopt these objectives into the models that lead to multi-objective optimization models. There are two major numerical and analytical approaches.

Numerical methods application is for constructing an approximation of the Pareto front. These methods rely on the well-known scalarization approach proposed by Pascoletti and Serafini (Khorram, Khaledian, & Khaledyan, 2014). They generate a good distribution of the entire Pareto front for both convex and non-convex ones and commonly are preferred methods to apply to complex problems.

Analytical methods are capable of reaching an exact solution through detailed mathematical calculations. Hence, these methods usually require a large number of equations to approximate the solution realistically. PSE widely utilizes these methods, such as the  $\varepsilon$ -constraint method to address multi-objective problems (Cheng, Subrahmanian, & Westerberg, 2003; Guillén-Gosálbez & Grossmann, 2010; Guillen, Mele, Bagajewicz, Espuna, & Puigjaner, 2005; Mele et al., 2011; You, Tao, Graziano, & Snyder, 2012). In this method, the problem adjusts to a single objective, subject to the other objectives that act as the constraints. Using different epsilons leads to an optimal Pareto frontier. Nevertheless, the associated solution identification challenge remains unsolved. Therefore, several approaches exist to narrow down Pareto solutions, such as Pareto filters (Arora, 2012; Sudeng & Wattanapongsakorn, 2015) and, Data envelopment analysis (Seiford & Zhu, 2005). Besides, the evaluation of the feasible solution implies an additional computational effort to build the Pareto frontier. Therefore, various approaches bypass the mentioned procedure by promoting a single optimal solution directly right after solving the model. These approaches include **goal programming** (Charnes & Cooper, 1977; ROMERO, 1991), **multi-parametric programming** (Zeleny, 1974), **analytic hierarchy processes (AHP)** (Saaty, 2004), **weighted sum** (R. Timothy Marler & Arora, 2010), **metaheuristics** (Sudeng & Wattanapongsakorn, 2015), **lexicographic methods** (Arora, 2012), and **fractional programming** (Sakawa & Yano, 1985). These methods are applied extensively to a wide range of multi-objective problems, especially in sustainable supply chain management problems (Kanzian et al., 2013; Pérez-Fortes et al., 2012; Ruiz-Femenia, Guillen-Gosalbez, Jimenez, & Caballero, 2013; Tautenhain, Barbosa-Povoa, & Nascimento, 2019; You, Tao, et al., 2012; Zamboni, Shah, & Bezzo, 2009).

New trends force process managers to consider several conditions to obtain robust solutions that simultaneously satisfy multi objectives.

Solving a multi-objective problem is not the only challenge to be tackled; however, there are always issues to address. In addition, to obtain a value that accurately demonstrates the cause-effect of a particular objective, another open issue is the efficient integration of multi-objective

approaches with uncertainty management. Different efficiency indices and performance indicators such as financial and environmental metrics have gained widespread popularity.

**i) Financial indicators**

Financial management tries to reduce the rejection chance of robust solutions during the optimization process (Giarola et al., 2013; You, Wassick, & Grossmann, 2009). The application of financial metrics provides more precise and accurate information regarding the economic behavior of the system. Some of the most common financial risk metrics used in the literature are now briefly described:

- *Downside risk (DR)*: provides a statistical measure to calculate the loss value regarding changes in the economic conditions and uncertainty. Commonly, the loss associated with the financial return can be much less than the expected results. The DR mathematical formulation is relatively simple since it avoids using binary variables, and thus, it is very computationally efficient (Hahn & Kuhn, 2012). However, the main disadvantage of the downside risk is the lack of linear interconnection with the probability of occurrence.
- *Financial Risk (FR)*: is the probability of not meeting a specific economic target. Despite DR, considering financial risk in a mathematical model causes several binary variables (Guillen et al., 2005) and leads to a complex model. So an extensive computational effort is needed. The FR metric is an indicator that describes if the solution produces winnings, but it cannot quantify it. Thus, quantitative knowledge compromising the FR metrics' usefulness.
- *Value at Risk (VaR) and Conditional Value at Risk (CVaR)*: are measures of the investment loss and quantify it with the associated probability. In other words, these metrics evaluate the solution performance in the assumed region of the cumulative probability curve (Aseeri & Bagajewicz, 2004). CVaR, also known as the expected shortfall, measures the amount of tail risk by taking a weighted average of the extreme losses in the tail of the possible returns distribution over the VaR cutoff point (Ehrenstein, Wang, & Guillén-Gosálbez, 2019). Nevertheless, VaR is a statistic metric that quantifies financial risk over a specific time frame. This metric is commonly to determine the occurrence ratio of potential losses. However, VaR is a robust measurement and not a financial risk metric used in decision support.
- *Worst case (WC)*: is commonly used as an alternative regarding a conservative risk estimation is needed. The worst-case scenario is to control the probability of meeting unfavorable solutions. Hence, the decision-maker preliminarily defines a set of values in which the performance variations indicate neglected variations in the process performance (Ehrenstein et al., 2019; Ruiz-Femenia et al., 2013). Historically, WC was considered as a risk management metric since it associates the expected economic worst performance for a set of solutions (Guillen et al., 2005) for a low computational effort. The

major disadvantage of this metric is that it cannot be analyzed individually and depends on objective qualitative performance.

Despite the advantages of using robust decision support strategies by combining multiple metrics, developing a single one that efficiently correlates quantitative and qualitative measurements (probability and potential level of winnings/losses) simultaneously remains an open issue.

## ii) Environmental indicators

The Decision-making process under a sustainable environment requires scientifically-based information on sustainability. There are different environmental indicators to observe the fulfillment of sustainable targets. This section reviews the applied indicators (Dong & Hauschild, 2017).

- *Planetary Boundaries (PB)*: defines as a safe operating space by estimating impacts and aims to protect the function of the Earth system. Focusing on the stability of the Earth system processes, this indicator is concerned with impacts on the natural environment within boundaries. Several planetary boundaries have been recognized so far, such as climate change (i.e., atmospheric  $CO_2$  concentration, energy imbalance at top-of-atmosphere), acidification (i.e., carbonate ion concentration in oceans), ozone depletion (i.e., stratospheric  $O_3$  concentration), atmospheric aerosol loading (i.e., Aerosol Optical Depth (AOD)), eutrophication, change in biosphere integrity (i.e., extinction rate and biodiversity intactness index), freshwater use and, forest resources (i.e., area of forested land as % of original or potential forest cover). There are one or more developed indicators to demonstrate the distance to the boundary and indicate the transgression. As PB is a relatively new concept, there exist significant uncertainties of boundaries, so more research is needed (Bjørn, Diamond, Owsianiak, Verzat, & Hauschild, 2015). However, the PB indicator proposes a method to evaluate environmental impacts whereas, an absolute scale takes the whole earth as the system boundary (De Vries, Kros, Kroeze, & Seitzinger, 2013).
- *Sustainable Development Goals (SDGs)*: are the most recent indicators released by the UN. These indicators are parts of a plan of action to shift the world onto a sustainable path. The SDGs aim to guarantee common goals and comprehension among different stakeholders in worldwide sustainable development. These targets specifically focus on climate change, ocean acidity (measured as surface pH), and ozone depletion based on Millennium Development Goals (MDG) indicators, air/chemical pollution, waste treatment. Most of the targeted indicators have to reach a certain level within a limited time(Hák, Janoušková, & Moldan, 2016).

- *Life Cycle Assessment (LCA)*: measures all emissions and resource consumption and quantifies the associated environmental and health impacts. This robust and mature method is laid out in ISO standard (ISO 14040/14044) and widely applied in recent studies (Azapagic & Clift, 1999), particularly in sustainable supply chain management problems (Brandenburg et al., 2014). Commonly, LCA techniques are combined with a mathematical programming approach to create a systematic method. This method enables an assessment of the process and supply chain alternatives that may result in significant environmental and economic benefits simultaneously (Azadeh et al., 2017; Bojarski, Lainez, Espuna, & Puigjaner, 2009; Genovese, Acquaye, Figueroa, & Lenny Koh, 2015; Guillén-Gosalbez & Grossmann, 2010; Guillen-Gosalbez & Grossmann, 2009; Hugo & Pistikopoulos, 2005; Lainez-Aguirre et al., 2017; Liu, Qiu, & Chen, 2014b; Mele et al., 2011; Pérez-Fortes et al., 2012; Ruiz-Femenia et al., 2013; Santibañez-Aguilar et al., 2014; She et al., 2019; Tautenhain et al., 2019; You, Graziano, et al., 2012; You & Wang, 2011; Yue et al., 2014). The most widely-used LCA metrics include Global Warming potentials (GWP) (Buddadee, Wirojanagud, Watts, & Pitakaso, 2008), Eco-indicator 99 (Guillen-Gosalbez & Grossmann, 2009), IMPACT 2002 (Bojarski et al., 2009). GWP signifies greenhouse Gas (GHG) emissions causing the global warming effects, while Eco-indicator 99 and IMPACT 2002+ measure the environmental impacts in more extensive categories such as human health, ecosystem quality, and resources. Note that most searchers merely use LCA indicators as a post-optimization tool to evaluate environmental sustainability.

Despite the advantages of using robust decision support strategies by combining multiple metrics, developing a single one that efficiently correlates quantitative and qualitative measurements (probability and potential level of winnings/losses) simultaneously remains an open issue.

### 2.3. Uncertainty management

As mentioned in this chapter, different types of contingencies affect processes performance and the associated operating conditions. Uncertainty management techniques are the most commonly used to control these unexpected event effects. Hence, this section is describing uncertainty sources through a supply chain. Uncertainty management is becoming crucial for the PSE community since it ensures feasible/efficient processes regarding quality and applicability.

Uncertainties impact the performance of supply chains and affect the decision-making process. The main uncertainties in sustainable supply chains mainly include (I) raw material uncertainties, (II) production and operation uncertainty, (III) logistics uncertainty, (IV) demand and price uncertainty, (V) environmental impact uncertainty, and (VI) other uncertainties. These mentioned classifications explain in detail as the following:

- I. *Raw material supply uncertainties*: focus on supply quantity and quality uncertainties and arable land unavailability as an uncertainty source. Caesar, Riese, & Seitz (2007); Nagel

(2000) considered uncertain raw material **supply quantity**; while Nagel (2000) found it hard to maintain a stable supply that affects the environmental and economic viability of alternative fuel (Caesar et al., 2007) considered the shortage of feedstock caused by harvesting technology deficiencies. Uncertain **Supply quality** was studied by (Dautzenberg & Hanf, 2008) and recently (Medina-González, Espuña, & Puigjaner, 2018), and proposed an efficient model to handle the variation of raw material quality.

- II. *Production and operation uncertainty*: imply process or/and operation conditions (Cheng et al., 2003; Filho et al., 2018; Grossmann & Guillén-Gosálbez, 2010). They dealt with equipment deficiencies, production quality, and stability and, therefore, adopted a plant-wide control process.
- III. *Uncertainties in transportation and logistics*: mainly target delivery and intermodal. (Ekşioğlu et al., 2010) studied the impact of an uncertain intermodal facility on location and transportation decisions. (Choy et al., 2007) aimed to manage the information flow efficiency through the supply chain to reduce uncertainty. The literature indicates that various factors impinge on transport operations through a supply chain. Sanchez-Rodrigues, Potter, & Naim (2010) determined these key factors and consequently proposed a qualitative evaluation of different types of uncertainty impacting transport operations rather than estimating the risk that each of them involved.
- IV. *Demand and price uncertainties*: is historically the most common source of uncertainties in supply chains. Thus, it has a direct impact on potential sales revenue and raw material/required energy supply. Here several issues Market volatility (Markandya & Pemberton, 2010), market size (Jouvet, Le Cadre, & Orset, 2012), market conditions (Dal Mas, Giarola, Zamboni, & Bezzo, 2010; Zheng et al., 2018), uncertain demand quantity (Guillen et al., 2005) (You & Grossmann, 2008) (You et al., 2009) (Kostin, Guillén-Gosálbez, Mele, Bagajewicz, & Jiménez, 2012) (Hahn & Kuhn, 2012) (Ruiz-Femenia et al., 2013)(Govindan & Fattahi, 2017).
- V. *Environmental impacts uncertainties*: aim to evaluate uncertainties related to environmental damages, and commonly LCA uncertainty is taken to account. Guillen-Gosalbez & Grossmann (2009) indicated that the Eco-indicator 99 methodology is affected by three primary sources of uncertainty: the fundamental or model uncertainties, operational or data uncertainty, and uncertainty the completeness of the model. Later on, (Guillén-Gosálbez & Grossmann, 2010) focused on the environmental impact associated with operational uncertainty, and (Sabio et al., 2014) considered the uncertainty of the LCI data explicitly while this source of uncertainty does not affect the economic performance of the supply chain.
- VI. *Other uncertainty sources*: mainly can be environmental damages caused by carbon, methane, nitrogen emissions. (Hammond, Kallu, & McManus, 2008) considered carbon emission as a source of uncertainty leads to the inability to evaluate the actual carbon



emission to indicate a number in the market. In addition to carbon emission, (Mortimer & Elsayed, 2006) dealt with other particles such as methane and nitrogen emissions as it is complicated to fully determine the amount of methane and other nitrous gas effects on the environment, and it controlled the uncertain environmental damage caused by determining the amount of methane and other nitrous gas effects on the environment. Tax exemption can lead to uncertainty, and in this line, (Rozakis & Sourie, 2005) developed a model that estimated the cost and surplus by employing tax exemptions.

Initially, the uncertainty effects over a process were ignored and substituted by a safety factor. This factor adds a small percentage of the nominal/optimal operational value to the decision variables, including equipment capacity, inventory level, and production rate. In this way, it assures the operational feasibility and, to some extent, process robustness. However, the solutions obtained by this approach are typically costly and inefficient (Cheng et al., 2003; Jung, Blau, Pekny, Reklaitis, & Eversdyk, 2004; You & Grossmann, 2008); hence, it is required more efficient and sensitive approaches. Therefore, new approaches have been proposed recently and classified into two main groups: Reactive and preventive approaches described as the following.

### 2.3.1. Reactive approaches

These approaches aim to unveil the uncertainty by developing a deterministic model. The procedure is to be solved the model once to discover the uncertainty. Applying reactive approaches leads to constant plan adjustments that cannot be applicable to design problems. The principal used reactive approaches are Model Predictive Control, Multi-Parametric programming, Rolling Horizon approach, and Real-Time Optimization, which are the following described.

**Model Predictive Control (MPC)** is used to manage a dynamic system to predict the process performance by control variables. (Bose & Pekny, 2000; Braun, Rivera, Carlyle, & Kempf, 2002; Braun, Rivera, Flores, Carlyle, & Kempf, 2003; W. Wang, Rivera, & Kempf, 2007) controlled the customer satisfaction level by controlling the inventory level dynamic. Similarly, (Perea-López, Ydstie, & Grossmann, 2003) defined operational variables to manage the profit optimality of the system. (Niu, Zhao, Xu, Shao, & Qian, 2013) focused on process production management by controlling the demand price dynamic and inventory level. Velarde, Valverde, Maestre, Ocampo-Martinez, & Bordons (2017) applied MPC to energy supply chains to manage the delays and disturbances in distribution networks. However, the MPC approach cannot manage uncertainties associated with sustainability; thus, there is a need to integrate robust and accurate MO approaches with MPC strategies. (Kouvaritakis & Cannon, 2016) proposed details on the MPC application as a tool for sustainable development.

**Multi-Parametric optimization (MP)** is a strategy that operates as a function of different parameters and is commonly used to plot the optimized performances of objective functions and decision variables. The MP programming leads to a set of critical regions that implies the optimal

decision variables within uncertainty space (P. L. Yu & Zeleny, 1976). The advantage of this approach is that by using these regions, the required computational effort significantly reduces (Dua & Pistikopoulos, 2000; Pistikopoulos, 2009). Hence, several planning problems have extensively used the MP approach, specifically multi-stage MILP inventory design and planning (Guillen-Gosalbez & Grossmann, 2009; Rivotti & Pistikopoulos, 2014) and utility plants scheduling (Shokry & Espuña, 2017b). Besides, (Krieger & Pistikopoulos, 2014; Nascu, Lambert, Krieger, & Pistikopoulos, 2014) developed online parametric estimation by integrating the MPC and MP. Consequently, the integrated MPC-MP approach was applied to control and optimize batch processes dynamically (Shokry, Dombayci, & Espuña, 2016; Shokry & Espuña, 2017a). Regarding the capability of the MP to manage multiple sources of uncertainty, (Charitopoulos & Dua, 2016) applied it to sustainability problems. Furthermore, recent studies successfully approve the MP combination approaches within surrogate models to promote the sustainability of industrial problems (Lupera Calahorrano, Shokry, Campaña, & Espuña, 2016; Medina-González, Shokry, Silvente, Lupera, & Espuña, 2020).

**The Rolling Horizon approach (RH)** is well known as an iterative method that addresses deterministic problems involving a defined prediction horizon. Typically its application is when the problem aims to compare a short period with the entire horizon. Herein, the uncertain parameters are defined or easily forecasted. In each optimization phase, the forecast rolls forward until completing the whole horizon. The approach assumes that all parameters are known (based on the system feedback at each iteration) within the prediction horizon. The dynamic feature of the RH makes it worthwhile to apply it to planning and scheduling problems. Kostin, Guillén-Gosálbez, Mele, Bagajewicz, & Jiménez (2011) and (Silvente, Kopanos, Dua, & Papageorgiou, 2018; Silvente, Kopanos, Pistikopoulos, & Espuña, 2015) focused on the problems associated with the daily energy generation and storage. (Perea-López et al., 2003) successfully combined the RH and the MPC to manage the supply chain dynamics, and (Kopanos & Pistikopoulos, 2014) addressed reactive scheduling problems for heat and power units. However, it is required to justify its application to actual industrial processes in further studies.

**Real-Time Optimization (RTO)** focuses on managing continuous process operation and particularly its economic performance optimization. The RTO solution strategies are parameter estimation techniques that update vital parameters. They are commonly applied to nonlinear steady-state processes collaborating with the MPC to update the setpoints after optimizing the process management (H. Li & Swartz, 2019). Since applying the RTO to dynamics problems is complicated, the RTO has been developed to dynamic real-time optimization strategies to manage process dynamics precisely in which the bottleneck moves frequently. Alternatively, nonlinear MPC is used to address nonlinear dynamic optimization problems (H. Li & Swartz, 2019). Nevertheless, global optimization of a dynamic complex process can hardly achieve with the available computing resources.

### 2.3.2. Preventive approaches

This class of approaches is based on the known behavior of the uncertain parameters within the problem formulation and identified as a stochastic model. There are three classifications for these programming models, including **stochastic**, **robust**, and **fuzzy programming**.

**Stochastic programming** is an approach for modeling optimization problems that involve uncertainty, and it can estimate the variables as a function of the unpredictable variations through the set of scenarios with an associated probability distribution. As a scenario-based approach, stochastic programming aims to obtain the optimal decisions, disregarding the realization of the uncertainty parameters. The two-stage stochastic programming approach (Prékopa, 1995), and through MILP and MINLP formulations, is commonly used to solve PSE problems. Hence, this extensively addresses the planning of an industrial SC under supply and demand uncertainties (C. W. Chen & Fan, 2012; Grossmann & Guillén-Gosálbez, 2010), the risk management of SC design under demand uncertainty (Govindan & Fattahi, 2017; Kostin et al., 2012). Due to the existing potential to promote process sustainability, a wide range of studies were using scenario-based approaches to tackle sustainable SC problems under uncertainty such as SC design and planning under process life cycle uncertainty (Cheng et al., 2003), managing uncertainty in environmental damage and life cycle inventory (Guillén-Gosálbez & Grossmann, 2010), environmentally conscious supply chains under demand uncertainty (Ruiz-Femenia et al., 2013). Despite the extensive interest in applying the multi-objective stochastic approach, there is a need for further studies regarding decision-support strategies.

**Robust Optimization (RO)** is a new and active, and recently developed approach. Basic versions of the RO assume that constraint violation is not allowed to realize the data in the uncertainty set. RO is famous for its computational tractability for several classes of uncertainty sets and problem types (Gorissen, Yanikoğlu, & den Hertog, 2015). However, due to its proactive feature, it does not react to different uncertain events. So that it is inefficient for short-term problems (Grossmann, Apap, Calfa, García-Herreros, & Zhang, 2016; Rezaei, Khazali, Mazidi, & Ahmadi, 2020). Robust optimization attempts to find a solution that can remain feasible for the whole uncertainty space by optimizing the problem deterministically for the worst-case scenario (Ben-Tal Laurent El Ghaoui Arkadi Nemirovski, 2009). Historically, PSE problems have effectively used the RO techniques to deal with the SC operation (Verderame & Floudas, 2009), SC operational risk (Hahn & Kuhn, 2012), process scheduling (Z. Li & Ierapetritou, 2008; Mirzapour Al-E-Hashem, Malekly, & Aryanezhad, 2011), and inventory sizing (Ben-Tal, Goryashko, Guslitzer, & Nemirovski, 2004). The RO application requires a significantly high computational effort; hence this approach is integrated with decomposition strategies and forms a single framework to make it capable of solving complex process-scheduling problems (Q. Zhang, Grossmann, & Lima, 2016). The RO demonstrates the capability to address multi-objective problems to promote process sustainability (Bairamzadeh, Saidi-Mehrabad, & Pishvaei, 2018; Sabio et al., 2014). Nevertheless, the RO application in PSE has been relatively limited and usually

restricted to operational/tactical problems. Even if the RO strategies can address MO problems, further studies must ensure the systematic generation/identification of sustainable and robust solutions.

**Fuzzy Programming** is applied when there is no particular distribution for uncertain data, but it is possible to determine its boundaries and membership functions. Commonly, the uncertainties representation using a set of fuzzy constraints. The fuzzy approach has addressed many industrial problems under uncertainty, including chemical product design (Ng, Chemmangattuvalappil, & Ng, 2015), close-loop SC design (J. Xu, He, & Gen, 2009), logistics design (Pishvaei, Torabi, & Razmi, 2012), SC planning and scheduling (Su, 2017), material supply planning (Sun, Liu, & Lan, 2010). Fuzzy programming deals with multi-objective problems addressing different aspects of sustainability, including industrial hazardous waste management (Ghezavati & Morakabatchian, 2015), environmental conscious multi-objective SC network design (Tsao, Thanh, Lu, & Yu, 2018), and (Tsao & Thanh, 2020) proposed a strategy to address the design and management of integrated networks. However, two main challenges remain unsolved to address sustainability problems under uncertainty; first, a clear definition of membership functions that determine the objective behavior and the detailed impacts of uncertain conditions on the process performance. The second challenge is to develop approaches to make decision-makers able to consider their preferences into the fuzzy model.

The reactive and preventive uncertainty approaches are not capable of tackling the main limitations in:

- I) the study uncertainty effects for the hierarchical levels individually (Elluru, Gupta, Kaur, & Singh, 2019),
- II) a single uncertainty source consideration (Moret, Peduzzi, Gerber, & Maréchal, 2016),
- III) application capability for multi-objective problems (Moret, Codina Gironès, Bierlaire, & Maréchal, 2017),

that hinder their application to further and complex problems, as stated above. Besides, the increasing concern about sustainability and green engineering obliges industries and academia to develop integrated/holistic approaches to manage multiple and unexplored uncertainty sources simultaneously for multi-objective/multi-criteria problems. In particular, this thesis tries to contribute to such a line, as described in the following chapters.

## **2.4. Trends and Challenges**

An extensive literature review has been made over this chapter, focusing on practical and integrated solution methods and strategies proposed for supply chain management, particularly sustainable supply chain management. This survey emphasizes the motivation to drive further research efforts in four main topics (i.e., multi-objective decision-support, uncertainty management, and sustainability issues) and the combined/integrated effect of the above challenges. The strategies aim to simultaneously consider many objectives in a systematic

framework to identify the best global solution. A considerable proportion of the multiple objectives optimization models focus on just economic optimality. The economic criteria are the most desirable objective, and the economic formulations for the additional criteria successfully represent the system performance. Apart from economic criteria, several motivations, such as social and environmental issues, remain to be addressed. Since it is not very easy to propose an effective method for optimizing the environmental and social regulations/concerns in industrial processes thus, to facilitate problem-solving, future studies must address the following challenges:

#### ☞ **Multi-Objective issues**

It is vital to develop and improve the objectives and model formulations to increase the accuracy concerning real-life process industries' performance to tackle these issues. In this regard, further studies should consider the following hints:

- ☛ The economic objectives mainly focus on optimizing Net present Value (NPV) subjected to fixed capital cost and an adjusted interest rate. Using a set of financial risk metrics provides more details about system behavior.
- ☛ Historically, researchers have extensively used Life Cycle Assessment (LCA) among other methods as a systematic environmental analysis method. The practical application of LCA provides efficient knowledge about process conditions/constraints. Commonly, these methods relax the multi-objective problems by integrating linear programming with weighted-sum approaches. However, there are insufficient studies about the effects of resource quality and associated consumption (i.e., biomass, renewable energy resources). As a particular case, even if material/energy integration within LCA enables a comprehensive assessment of the environmental impact, its application for a large-scale material/energy supply chain remains an open issue.

In addition to all mentioned above, an adequate multi-objective function formulation affects the entire system. Accordingly, an efficient formulation for each SC echelon is needed to identify the activities with the highest impacts for each objective. In this regard, some studies assess the objectives systematically to form a hierarchy/importance based on the decision-maker perspective to effectively industrial changes.

In general, many PSE problems, including those that addressed sustainability, aim to improve the robustness and quality of the obtained solutions. Even with the highest quality of the obtained solutions, a huge decision maker issue remains unattended and poorly addressed. Hence, problem solvers require an accurate decision support strategy in a multi-objective framework.

#### ☞ **Uncertainties Management issues**

Commonly, uncertainty issues are the primary process industries challenges to tackle. Thus, it is necessary to develop a framework to model these uncertainties, and studies ultimately aim to obtain an easy way to interpret and implement solutions. Recently, the studies have achieved a

significant advancement in this regard, although some challenges remain to address as the following:

- ☛ Decision-makers have faced a high level of uncertainty in supply chain management due to the dynamic and complex nature of influential factors in supply chain management. Hence, modeling under uncertainty has become an active research field, and several studies have considered this concept, particularly the effect of demand and price uncertainty. Nevertheless, the studies have scarcely addressed the simultaneous analysis of uncertainty sources, and thus, the absence of a proper approach severely affects supply chain performance. Besides, such a study would represent a huge opportunity area and lead to a particular challenge. In this line:
  - The multi-parametric programming has been applied to the detailed information on the effect of the different uncertainty parameters over the system behavior while considering their interactions—however, its potential to define the uncertainty importance has remained unattended.
  - Data management is an important and complicated process and is needed to stabilize data variation. Besides, current stochastic models generate a large amount of output information; therefore, there is also a need for data-driven tools to integrate analytical tools with tailor-made databases. Hence, future studies should focus on implementing a strategy that accurately manages a large amount of process information, data variations, and the different data flows. Knowledge management systems (i.e., surrogate models and ontologies) can be successful alternatives.
- ☛ Besides dealing with various sources of uncertainty, another critical issue is the number of scenarios. Various approaches and methods are introduced in the literature to deal with scenario-based uncertainty models, including stochastic programming, robust optimization, and fuzzy programming. Multi-stage stochastic programming is the most used approach, and it should be able to manage uncertainty efficiently. So far, dealing with small scenarios has been studied extensively, but its application to medium-large scale industrial problems has remained an open issue.
- ☛ Ultimately, performance indexes are needed to represent uncertainties and quantify the robustness of the proposed solutions. The application of reactive and preventive approaches integrated into Multi-Objective problems will represent a promising research direction.

#### ☛ **Sustainability issues**

Regarding sustainability principles, exploiting renewable resources in process industries turns to be a particular interest. This challenging issue requires addressing simultaneously many uncertainties affecting the resources and resulting in multi-objective problems. In this regard,

several studies have been dedicating to improving strategies. Nevertheless, it is still necessary to propose applied strategies to deal with large-scale problems. Hence, the following challenges remain to consider in further studies.

☛ The integration of Industrial Symbiosis (IS) strategies within a holistic approach is a significant issue. This concept in an industrial context aims to efficiently exploit resources (i.e., material, energy, information) between companies/process plants. IS strategies address decentralized problems by considering at least two actors who manage the operations independently while seeking win-win solutions. This strategy creates a contentious evaluation of the relationship between the network and the player's coordination/collaboration. However, in real-life problems, information flows are limited, which hinders the IS strategies application.

☛ Besides the technical/conceptual challenges mentioned above, complex model formulation is another main issue to address. Here, there are two main challenges are needed to mention:

- A scenario-based dynamic framework is responsible for dealing with the market conditions variations. This strategy is capable of reacting to the constant changes in the market conditions within a single model. However, this framework uses to simplify the uncertainty approach compromising its representativeness. Therefore, the adequate combination of the dynamic scenario-based framework with uncertainty approaches remains an open issue.
- Here, several metrics can quantify the objectives and each entity's performance in the decentralized scheme. Hence, it is needed to explore and develop them to improve decision-making strategies.

#### ☞ **Integration issues**

Under sustainable development obligations, process industries are moving towards an optimization to integrate operational decisions into a general model. Despite several conflicting objectives and decision variables, this model should optimize the overall system performance. Thus, the main challenge is defining an efficient model that simultaneously represents the individual and global system performance and the synergy between different SC decision levels. This section proposes some particular challenges in the following:

☛ As noted before, in terms of decision quality, multi-objective techniques development is required. These techniques are supposed to function accurately and represent the decision-maker preferences systematically. Besides, these developed techniques can adequately identify the standard variables that allow connecting the different hierarchical levels.

☛ Current researchers dedicate their efforts to manage the prices, production rate, and distribution decisions to break the traditional organizational obstacles. A proper

framework is needed to examine the trade-offs between the impact of the operational decisions over the entire SC.

So far, the high computational burden is required to solve large-size multi-scale optimization problems so that the computational effort reduces a critical issue to achieve a monolithic optimization model. Hence, researchers must dedicate themselves to developing and improving decomposition strategies to manage information flows, especially within a decentralized structure. Currently, knowledge-based algorithms (e.g., Metamodeling) are in use to expedite a feasible space.

Ultimately, the critical factor in sustainable supply chain management is a systematic and general model to facilitate the decision-making coordination and integration processes. Such an objective can be a proposal of general PSE methods and tools for an advanced system management sustainable supply chain and integrated material/renewable energy resource supply chains. By studying the literature review and considering the above cases, it seems necessary to provide a general model that combined a sustainable material SC with a biofuel/bioenergy/renewable energy SC. Hence, this thesis dedicates to propose this general model. It demonstrates the advantages and discusses to enlighten a path to future studies.





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## METHODOLOGY AND TOOLS

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In the last decades, the process systems engineering community (PSE) has developed tools to facilitate the problem-solving process in the mentioned area using mathematical programming. Retrofitting the conventional supply chains and optimize tactical decisions have got extensive attention in industries. Decisions at these levels have a long-lasting effect on the firm, and hence they play a significant role in Supply Chain Management, particularly with sustainability considerations. The following, it is discussing some key aspects and tools that the studies commonly utilize.

### 3.1. Optimization

As the industrial world is getting more and more competitive, efficiency has become the main concern for many business activities. Such efficiency can generally define optimization problems and a well-studied area in academia (Yang, 2018).

According to the various definitions, an optimization problem is finding and proposing optimal solutions that optimize objective functions. Optimization is applicable for a diverse range of areas such as process industries and production facilities, material/energy supply chain management, such as improving profit, energy consumption, or/and decreasing pollutant generation. Optimization is a wise step procedure as mentioned below:

- The first step to implementing optimization is to identify all available data.
- The second step is to determine an objective function and decision variables.
- The third step is to translate the objective function and decision variables into a mathematical model.

Moreover, the optimization procedure can include a single objective or the consideration of multiple criteria in the decision-making process.

### 3.2. Mathematical model

Generally, models illustrate the perceptions about how the world functions. A mathematical model is a translation of the perceptions into the language of mathematics. A mathematical model aims to define a system using mathematical approaches and expressions. Besides, mathematics is an exact and concise language with well-defined rules to formulate ideas (Lawson & Glenn, 2008). The application of mathematical programming for decision-making problems implies the combination of mathematical representation and optimization algorithms. A mathematical model consists of several equation/inequation blocks such as:

- Mass/energy balances, in addition to momentum, integral/differential and dynamic/stationary state, and other related information;
- Conditional equations like thermodynamic and kinetic statements and chemical properties;
- Design spec like capacity constraints, costs, and revenue.

#### Convexity

If  $x$  and  $y$  and all points on the straight line connecting  $x$  and  $y$  belong to  $S$ , therefore,  $S$  is convex. Note that  $S$  is a set in a natural or complex vector space. Fig. 3.1 illustrates Convex and non-convex definitions.

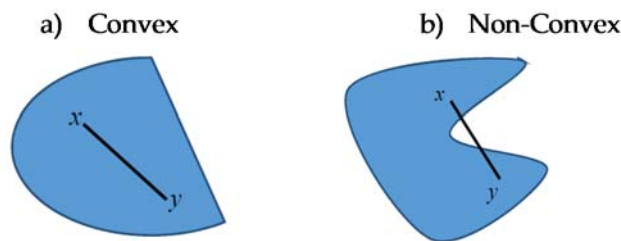


Fig. 3. 1. Definition of Convex (a) and Non-Convex(b) set (Kopanos & Puigjaner, 2019).

This definition can be expressed mathematically as below:

$$S \text{ is convex} \Leftrightarrow \forall (x, y) \in S \wedge \lambda \in \{0,1\}: \lambda x + (1 - \lambda)y \in S$$

The following section discusses some commonly used techniques for solving optimization problems. Depending on the characteristic of each problem, the solution techniques differ.

### 3.3. Optimization techniques

A combination of mathematical representation and optimization algorithms results in mathematical programming approaches focusing on optimization problems. The optimization model, in general, consists of an objective with/without several constraints that form constrained/non-constraint optimization, and also, there are two classes of continuous

optimization and discrete optimization. Regarding the structure, mathematical models are classified as linear and, Non-linear.

### 3.3.1. Linear programming (LP)

Linear programming is a particular case of the constrained optimization problem in which the objective function is linear and the set of equations and inequalities. Linear programming methods propose a technique to find the optimum solution among a finite number of possible points (Thie & Keough, 2011). Commonly, a linear model has a canonical form as:

$$\begin{aligned}
 &\text{Minimize} && F(x) = c^T x \\
 &\text{Subject to} && Ax = b \\
 &&& x \geq 0
 \end{aligned} \tag{3.1}$$

Where  $c \in \mathbb{R}^n, b \in \mathbb{R}^m$  and  $A \in \mathbb{R}^{m \times n}$ . The term  $x \geq 0$  represents nonnegative variables. The intersections of the hyperplanes associated with each constraint geometrically define the solution space of the LP problem, and the optimal solution is in each vertex of the feasible n-dimensional polytope (Fig. 3.2).

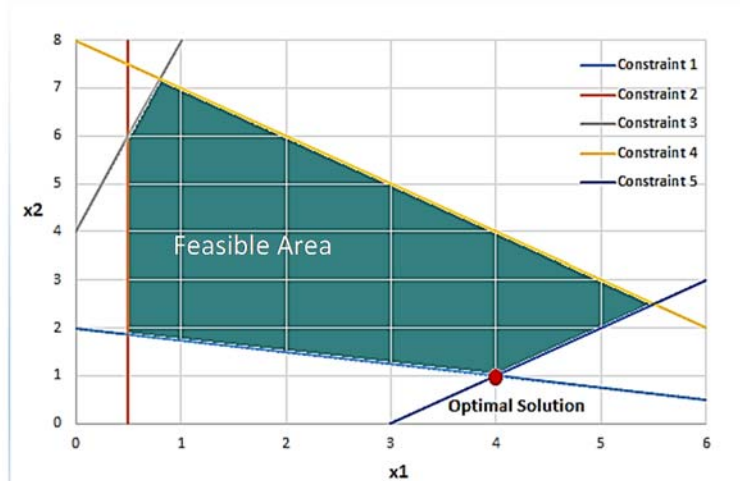


Fig. 3. 2. Geometric solution of a linear program.

There are two solution methods used traditionally to solve linear problems: The simplex method and Interior-point Methods.

#### a) Simplex Method

In mathematical optimization, the Simplex algorithm is a method for solving Linear programming (LP) problems first proposed and then developed by Dantzig (1963). The Simplex algorithm proceeds to move from one basic feasible solution (an initial vertex) to another until finding an optimal basic feasible solution (Fig. 3.3).

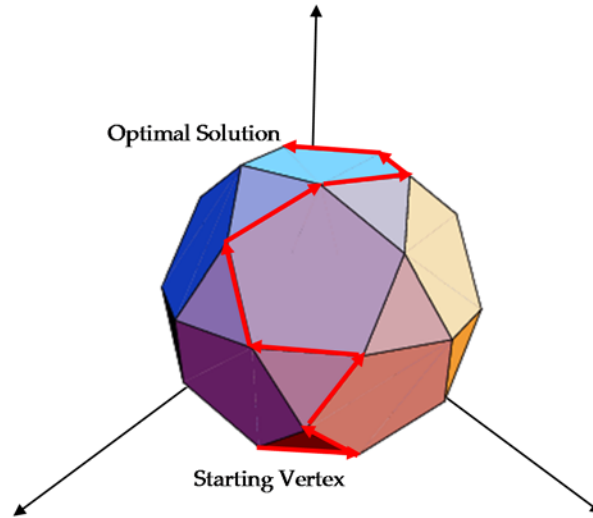


Fig. 3. 3. Illustration of Simplex Method (Kopanos & Puigjaner, 2019).

**a) Interior-point Methods**

Karmarkar, in 1984, proposed a new algorithm that had polynomial complexity and could solve real-world optimization problems more efficiently than the Simplex method. Karmarkar's work led to the development of many other non-Simplex methods commonly referred to as interior-point methods. Well-implemented types of these methods are very potent, specifically for the problems with many variables (Thie & Keough, 2011).

While the Simplex method considers the vertex of the feasible area, the interior-point methods infer an initial feasible interior-point and follow through the feasible region moving in one direction and stop with an approximate optimal solution when the difference between two iterations is sufficiently small in the original space (Fig. 3.4).

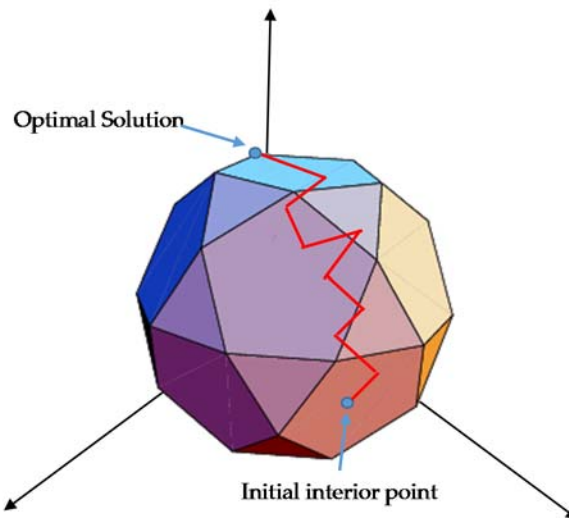


Fig. 3. 4. Illustration of Interior-point Method (Kopanos & Puigjaner, 2019).

### 3.3.2. Nonlinear Programming (NLP)

In mathematics and science, nonlinearity is a system in which the output change is not proportional to the input change. Nonlinear problems appear in engineering, biology, physics, mathematics, and many other sciences because most systems are inherently nonlinear.

Typically, in a nonlinear system, there are variables of a polynomial of degree higher than one or in the argument of a function that is not a polynomial of degree one. In nonlinear mathematical models, all variables are continuous and contain nonlinearities in either objective function and or the constraints.

In general, it is analytically hard to solve non-linear equations. Therefore, using iterative methods such as the First methods and the Newton-Raphson method, and the Bisection method (Kelley, 1995) allows to approach the solutions. There are algorithms and methods proposed to deal with the complexity of these problems belong to constrained and unconstrained optimization methods, such as Penalty Methods, Interior point, and Sequential quadratic programming (Buchanan, 2008).

#### Unconstrained optimization

The mathematical representation of unconstrained optimization is as below:

$$\begin{aligned} \text{Minimize } & F(x) \\ & x = (x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n \end{aligned} \tag{3.2}$$

The objective function  $F(x)$  is a nonlinear function, and the algorithms proposed to solve are divided into two main groups:

- **Line search methods**

This method is a basic iterative approach to find a local minimum  $x$  of the objective function  $F(x)$ . The approach first finds a descent direction along with the objective function  $f$  that will reduce and then calculates a step size that determines how far  $x$  should move along that direction. The gradient descent can compute the descent direction, Newton's method, and Quasi-Newton method.

- **Trust region methods**

In optimization, a Trust region is the subset of the objective function region approximated using a quadratic function. If a suitable model of the objective function exists within the trust region, then the region is expanded; conversely, the region gets contracted if the approximation is insufficient. Trust-region methods are also known as restricted-step methods.

Trust-region methods are dual to line-search methods: trust-region methods first, choose a step size (the size of the trust-region), and then a step direction, while line-search methods first choose a step direction and then a step size.

#### Constrained optimization

A general constrained optimization problem is mathematically defined as follows:

$$\begin{aligned}
 &\text{Minimize } F(x) \\
 &\text{Subject to } h(x) = 0 \\
 &\quad \quad \quad g(x) \leq 0
 \end{aligned} \tag{3.3}$$

Where  $h: \mathbb{R}^n \rightarrow \mathbb{R}^m$  and  $g: \mathbb{R}^n \rightarrow \mathbb{R}^p$ .

In constrained optimization, it aims to optimize the objective function in the presence of constraints. There are two classes of constraints: hard and soft constraints. Hard constraints fix conditions for decision variables, while soft constraints penalize the objective function if the determined condition remains unsatisfied. Commonly a penalty method can readjust many unconstrained optimization algorithms to the constrained case.

### 3.3.3. Mixed-integer Programming

Mixed-integer optimization problems arise in many real-world applications. Integer variables are often required to model logical relationships, fixed charges, piecewise linear functions, disjunctive constraints, and non-divisibility of resources.

A mixed-integer programming (MIP) problem is when some of the decision variables are constrained to be integer values at the optimal solution. Generally, in this optimization method, they are combined with continuous and discrete variables to respond to yes/no decisions. The use of integer variables dramatically expands the scope of practical optimization problems. Linear programming LP and nonlinear programming NLP models that contain integer variables are Mixed-Integer Linear Programming (MILP) and Mixed-Integer Non-Linear Programming (MINLP), respectively.

To solve MILP problems, two highlighted algorithms of [Branch and Bound \(B&B\)](#) and [Branch and Cut \(B&C\)](#) are standard algorithms for discrete and combinatorial optimization problems that consist of a systematic enumeration of candidate solutions through state-space search.

Nonlinear functions are required to accurately reflect physical properties, covariance, and economies of scale. Mixed-Integer Non-Linear Programming (MINLP) is applied to design problems, and its complexity is related to the non-convexity of the feasible region. Accordingly, various methods such as [Branch & Bound](#), [Branch & Cut](#), [Generalized Benders Decomposition](#), and [Outer-Approximation](#) are generally known for solving MINLP problems. The following subsection explains the algorithms applied to MILP and MINLP.

- **Branch and Bound (B&B)**

The Branch and bound approach was developed independently by (Land & Doig, 2010), focusing on mixed discrete programming problems. This algorithm aims to find a value  $F(x)$  that optimizes a real-valued function  $F(x)$ , among feasible search space of  $S$  or candidate solutions, while B&C involves running a branch and bound algorithm and using cutting planes to tighten the linear programming relaxations (Brusco & Stahl, 2005).

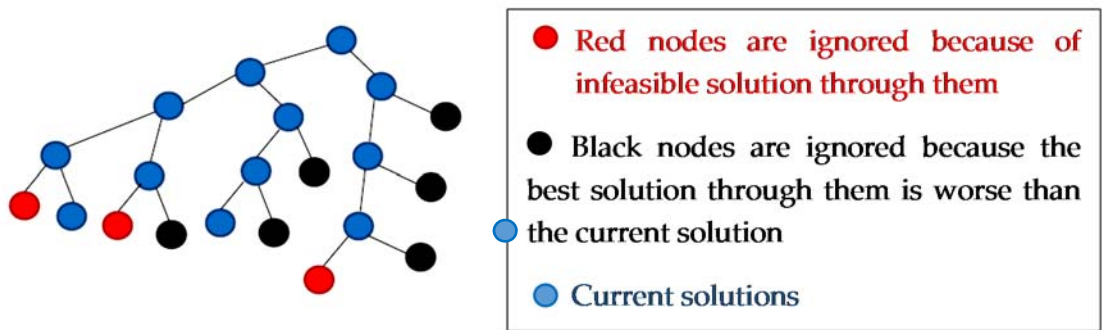


Fig. 3. 5. Graphical representation of the Branch and Bound algorithm.

There are two main phases in the B&B algorithm: a) the search phase; and b) the verification phase; in the first phase, the algorithm does not find an optimal solution, while in the second phase, the binding solution is optimal, although there are neglected subproblems that the algorithm cannot cut them back. Note that a binding solution cannot be proven optimal until no neglected subproblems remain.

According to these two mentioned phases of operation, the three algorithm components of search strategy, branching strategy, and cut back rules play distinct roles in B&B algorithms (Fig. 3.5). The search strategy and the cut back rules mainly impact the search and verification phases, whereas the branching strategy impacts both.

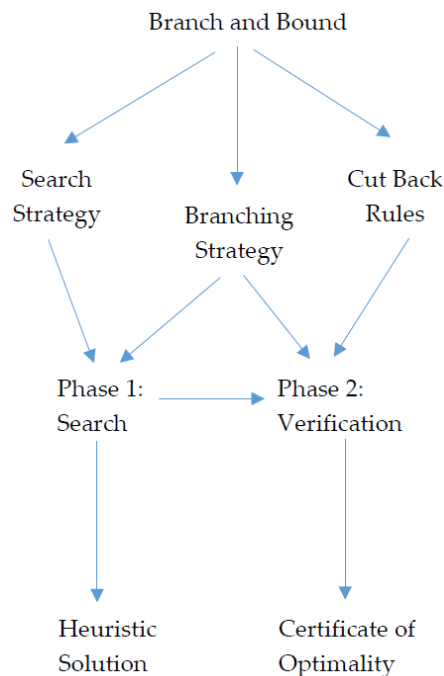


Fig. 3. 6. A diagram of the three main B&B components.

Furthermore, cut back rules usually aim at the verification phase, especially in an objective-based bounding, comparatively weak before an optimal solution is recognized. In this case, if the



binding solution has a poor objective value early in the search process, the lower bounds will not be able to cut back effectively, even if they are very tight. Nonetheless, there are also situations in which cutting back rules contribute to the searching phase, such as when cutting planes in a mixed-integer program (MIP) is to find feasible solutions.

- **Cutting-plane method**

Gomory (2010) introduced the cutting-plane method to solve MILP based on the notion that each subgradient of the objective function or the violated/operational constraints designates a half-space kept out from a set that contains an optimal solution. The Cutting-plane algorithm moves towards a global minimum of any pseudoconvex sub differentiable function. Such procedures generally exist to find integer solutions to mixed-integer linear programming problems. The cut reduces the solution space for a fractional solution graphically displayed in Fig. 3.7.

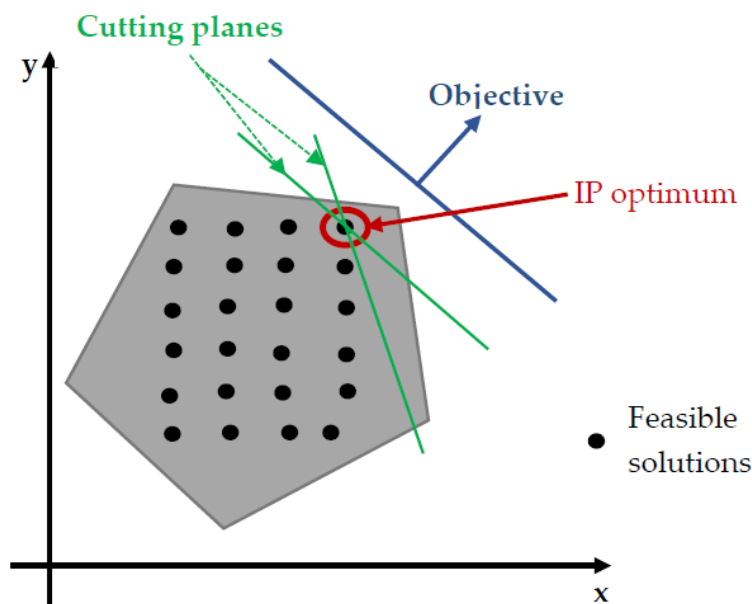


Fig. 3. 7. Classical cutting plane method.

This methodology can be more effective if combined with branch and bound methods and Gomory cuts in all MIP solvers.

- **Generalized Benders Decomposition (GBD) and Outer-Approximation (OA)**

Generalized Benders Decomposition (GBD) and Outer-Approximation (OA) are two methods mainly applied to Mixed-Integer Non-Linear Problems (MINLP). (Geoffrion, 1972) generalized Benders' approach to a broader range of programs. In Benders' approach, a linear program was a parametrized sub-problem, but Geoffrion employed nonlinear convex duality theory to derive the natural families of cuts corresponding to those in Benders' case. The proposed algorithm divides variables into two classes of complicated and non-complicated variables. Fixing the binary variables split the problem into a sequence of NLP sub-problems and MILP master problems. Specifically, the upper bound of the problem is generated by the NLP sub-problem, while the MILP master problems generate a combination of discrete variables to be used as lower

bounds for the NLP sub-problems. The optimal solution will be achievable by converging the upper and lower bounds.

Like GBD, the Outer-Approximation algorithm suggested by (Duran & Grossmann, 1986) divides the MINLP non-convex problem into NLP sub-problems and MILP master problem. Hence, solving the NLP sub-problems results in a feasible region, and approximating the nonlinear constraints of the feasible region generates the master problem.

### 3.4. Multi-Objective Optimization

The systematic and simultaneous optimization process of several objective functions is called multi-objective optimization (MOO) or vector optimization. Multi-objective Optimization is a multi-criteria decision-making tool applied to mathematical optimization problems. Hence, optimal decisions happen in the presence of trade-offs between two or more conflicting objectives. The general Multi-objective Optimization problem formulation is as below:

$$\begin{aligned}
 &\text{Minimize} && F(x) = [F_1(x), F_2(x), \dots, F_k(x)]^T \\
 &\text{Subject to} && g_j(x) \leq 0, && j = 1, 2, \dots, m \\
 &&& h_l(x) = 0, && l = 1, 2, \dots, e
 \end{aligned} \tag{3.4}$$

Where  $x \in E^n$  is a vector of decision variables,  $n$  is the number of independent variables  $x_i$  and  $F_i(x)$  are called objective functions. The feasible decision space  $X$  is:

$\{x \mid g_j(x) \leq 0, j = 1, 2, \dots, m; \text{ and } h_l(x) = 0, l = 1, 2, \dots, e\}$  while the feasible criterion space  $Z$  is the set  $\{F(x) \mid x \in X\}$ .

Despite the single-objective optimization (SOO), the solution of a multi-objective optimization problem (MOO) is more conceptual than a definition. It is necessary to define a set of points that fit a predetermined definition for an optimal solution. Non-dominated points of Pareto optimality (R. T. Marler & Arora, 2004) defined as Non-dominated points of Pareto optimality below:

A point  $x^* \in X$  is Pareto optimal if no other point  $x \in X$  exists such that  $F(x) \leq F(x^*)$ , and for at least one single function  $F_i(x) < F_i(x^*)$ . All Pareto optimal points spread on the boundary of the feasible criterion space  $Z$ .

**Definition 3.1.** *Non-dominated and Dominated points: a vector of objective functions,  $F(x^*) \in Z$ , is nondominated if there is no other vector  $F(x) \in Z$ , such that  $F(x) \leq F(x^*)$  with at least one  $F_i(x) < F_i(x^*)$ . Otherwise,  $F(x^*)$  is dominated.*

The curve that connects the set of feasible (all non-dominated) solutions is known as the Pareto frontier (see Fig. 3.8).

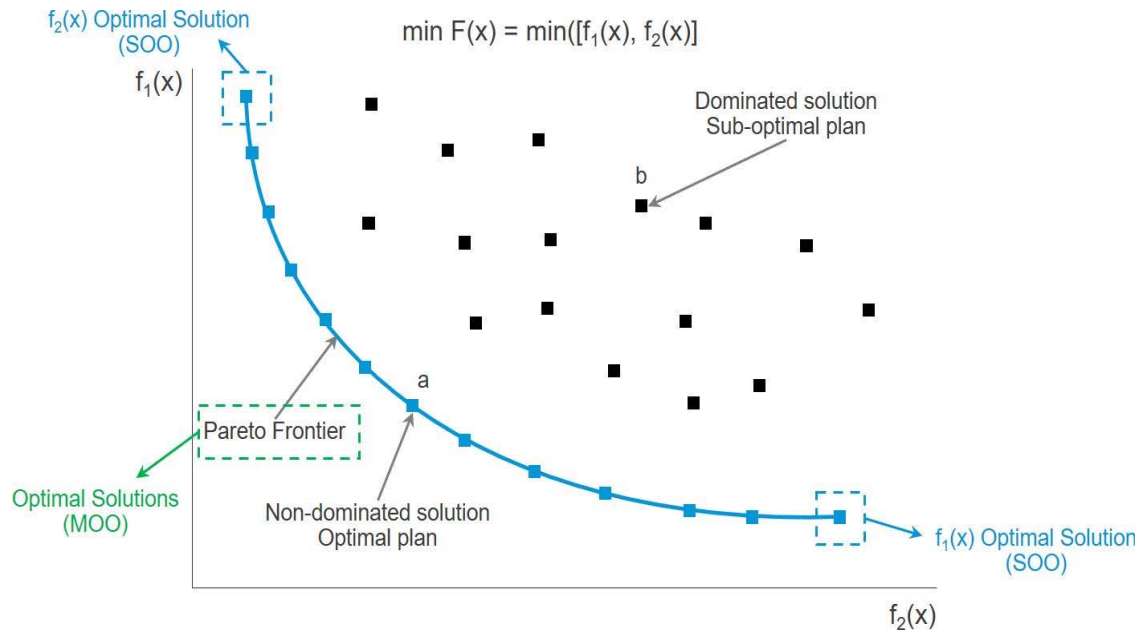


Fig. 3. 8. Pareto frontier for a multi-objective optimization problem (Dieter Vermeulen, 2020).

There are three categories of multi-objective mathematical programming methods: a priori, interactive, and a posteriori regarding decision-making and decision-maker preference. In a priori methods, the preference of the decision-maker (DM) must be specified in advance, like before the solution process, although the DM is not necessarily aware of possible attainments and the extent to which the expectation is realistic. The a priori methods include Value Function Method, Lexicographic Ordering, and Goal Programming (Charnes, Cooper, & Ferguson, 1955). Despite a priori methods, the interactive and the a posteriori methods transfer much more information to the decision-maker. Especially the a posteriori methods give the whole picture (i.e., the Pareto set), to the decision-maker, before the final decision reinforcing, thus, the DM confidence.

In the **interactive methods**, there is a constant interchange between the decision-maker and phases of calculation, and after a few iterations, the process converges to the most favored solution. This approach includes **Analytical Hierarchical Processes (AHP)** (Saaty, 2004), **Weighted sum** approach (R. Timothy Marler & Arora, 2010), **Step Method (STEM)** (Benayoun, de Montgolfier, Tergny, & Laritchev, 1971), **Fuzzy programming** and **Fractional approach** (Sakawa & Yano, 1985).

The **a posteriori** or generation methods are not very common as previously mentioned methods due to their computational effort and the lack of extensively available software. However, they have some notable advantages. The solution process consists of two independent phases: First, the generation of efficient solutions and the decision-makers' involvement when all the information is available. Hence, the DM is involved only in the second phase, having all the possible alternatives (the Pareto set or an adequate representation). Besides, all the discovered

potential solutions reinforce the decision maker's confidence in the final decision. The most commonly used generation methods are the **weighting method** (W. Zhang & Yang, 2001) and the  **$\epsilon$ -constraint method** described profoundly in the next section as it is the primary strategy of this thesis.

### 3.4.1. The $\epsilon$ -constraint method

Since a generation method can identify all finite numbers of Pareto optimal solutions, a wide range of algorithms, such as heuristics and exact methods are used, in this context. However, this must be taken into account that the weighted sum method, for instance, is the only capable method to find supported Pareto optimal solutions, i.e., those existing in the convex region of the objective-space and non-supported ones that can coincidentally exist like intermediate solutions. In the  $\epsilon$ -constraint method, one of the objective functions roles as the only objective of the problem, and the remaining ones are constraints. Therefore, it is possible to obtain different elements of the Pareto front by a systematic variation of constraint bounds. Assume that the following MOMP problem (Bérubé, Gendreau, & Potvin, 2009):

$$\begin{aligned} \text{Maximize} \quad & F_1(x), F_2(x), \dots, F_p(x) \\ \text{Subject to} \quad & x \in S, \end{aligned} \tag{3.5}$$

Where  $x$  is the decision variable vector,  $S$  is the feasible region, and objective functions are  $F_1(x), \dots, F_p(x)$ . In the  $\epsilon$ -constraint method, the model is as shown below:

$$\begin{aligned} \text{Maximize} \quad & F_1(x) \\ \text{Subject to} \quad & F_2(x) \geq e_2, \\ & F_3(x) \geq e_3, \\ & \vdots \\ & F_p(x) \geq e_p, \\ & x \in S. \end{aligned} \tag{3.6}$$

By parametrical alternation of the constrained objective functions ( $e_i$ ), efficient solutions are found. The following presents the global algorithm of the  $\epsilon$ -constraint method applied to bi-objective and related definitions:

**Definition 3.2.** *Utopia or Ideal point represents a situation that each objective achieves its optimal value individually. Although this point describes the ideal situation of a MOP, it cannot be a solution because the objectives conflict.*

**Definition 3.3.** *Nadir's point opposed to Utopia describes the worst performance of every single objective derived from the extreme points in a non-dominated solution set.*

**Definition 3.4.** *Extreme points are two points of the Pareto frontier.*

**Algorithm 3.1.**

Step 1. Set  $i = 1, j = 2$ .

Step 2. Compute the Utopia and Nadir points.

Step 3. Set Pareto Front  $PF = \{(z_i^U, z_j^N)\}$  and  $e_j = z_j^N - \Delta$  ( $\Delta = 1$ ).

Step 4. While  $e_j \geq z_j^U$ , do:

Step 4.1. Solve  $P_i(e_j)$  through branch and cut and add the optimal solution value  $(z_i^*, z_j^*)$  to  $PF$ .

Step 4.2. Set  $e_j = z_j^* - \Delta$ .

Step 5. Remove dominated points from  $PF$  if required.

Finally, the  $\varepsilon$ -constraint method produces a set of feasible solutions to propose to the decision-makers. Fig 3.9 depicts Pareto frontier, Utopia, and Nadir points.

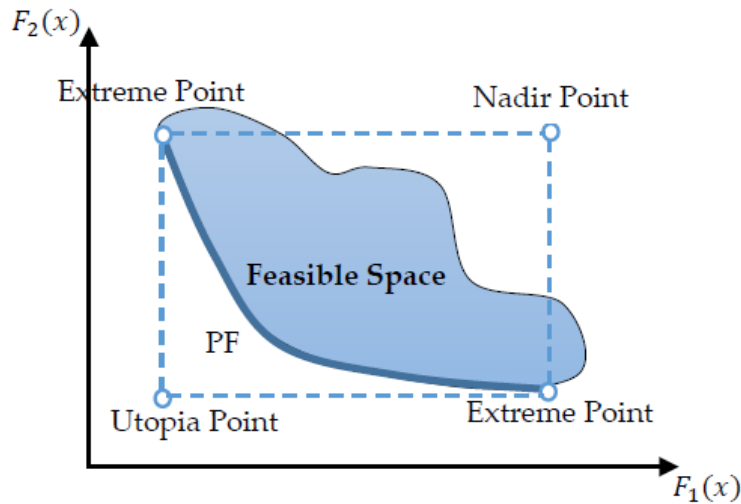


Fig. 3. 9. Illustration of Pareto frontier and essential points for multi-objective optimization problems. In this line, various Multi-Objective Decision Making (MODM) strategies have been introduced, as explaining in the following.

### 3.4.2. Multi-objective Decision Making

The multi-objective decision-making process implies the whole process of problem-solving, including fundamentally of five steps depicted in Fig. 3.10 (Chankong & Haimes, 1983).

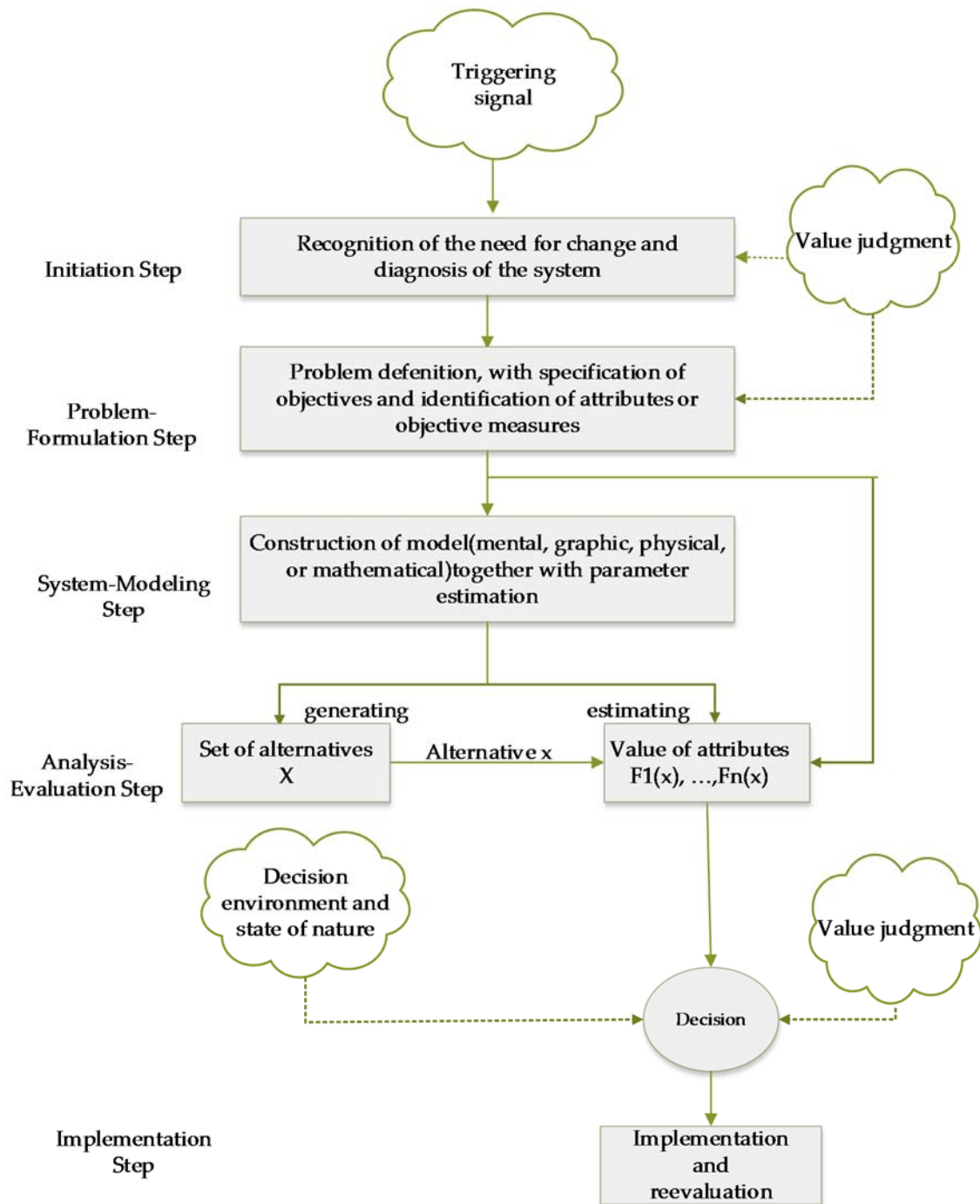


Fig. 3. 10. Multi-Objective Decision-Making Process.

Several methods exist for the evaluation of a multi-objective decision-making model. Depending on the phase and data type receiving from the decision-maker, these methods estimate the utility function. There are different ways to evaluate a MO model and are classified into two groups: DM information and independent evaluation methods, as described below.

### 3.4.3. Independent MODM Evaluation

- **$L_p$  metric methods**

These methods function independently from data obtained by DM and aim to minimize the distance of existing objective functions of a multi-objective model to an ideal solution.  $L_p$  Methods use metric deviations to measure the proximity of an existing solution to the ideal solution. Compromise functions will do this measurement of deviation as follows (Ringuest, 1997):

$$L_p = \left[ \sum_{j=1}^K (\gamma_j |F_j(x^{*j}) - F_j(x)|)^P \right]^{1/p} \quad (3.7)$$

here  $P$  is the parameter that determines which of  $L_p$  metric family is to be applied. The  $P$ 's effect emphasizes the relative contribution of individual deviations, i.e.,  $P = \infty$  (called the Tchebycheff metric) is the largest of deviations that completely dominate the distance measure. In addition to  $P = \infty$ , using the values  $P = 1$  and  $P = 2$  are very common. In maximization of the objective functions,  $x^{*j}$  represents the ideal solution of the objective  $F_j$ , and  $\gamma_j$  is a gradation weight associated with the  $j^{th}$  objective with all  $\gamma_j > 0$ . To minimize the deviations, the  $L_p$  Compromise minimized functions.

### 3.4.4. Evaluating MODM depending on DM information

#### A priori methods

These methods function by getting basic information from DM before solving the problem. This type of information may be from quantitative scales applicable for utility function and value function methods, rating scales, or a mixture of them applicable to the **Lexicographic method** and **Goal programming**.

- **Goal programming**

Perhaps Goal programming is the oldest and widely applied approach to multi-criteria decision-making. The initial formulations were proposed by (Charnes & Cooper, 1977) that ordered the unwanted deviations into several priority levels. The minimization of a deviation at a higher priority level is infinitely more important than any deviations at lower priority levels.

The initial goal programming formulations ordered the unwanted deviations into several priority levels, with the minimization of a deviation at a higher priority level is infinitely more important than any deviations at lower priority levels.

In the formulation, the first step is to establish attributes considered in the problem situation. Hence, for each attribute, it is necessary to determine the target value  $b_i$ . The next step is to introduce negative or positive deviation variables into the GP model. The positive deviation variable  $p_i$  and the negative deviation variable  $n_i$  represent the quantification of the achievement and non-achievement of the  $i^{th}$  goal. Generally, the  $i^{th}$  goal is:

$$F_i(x) + n_i - p_i = b_i \quad (3.8)$$

Where  $x$  is the vector of decision variables. If  $F_i(x) \geq b_i$ , then it is necessary to minimize  $n_i$ , if  $F_i(x) \leq b_i$  then  $p_i$  must be minimized and if the  $i$ th goal is to be satisfied concerning the achievement level, it is needed to minimize  $(n_i + p_i)$ .

The GP aims to minimize the deviations between the achievement of the goals and the related aspiration levels. Hence the minimization process can be done by various methods, and each one leads to a different GP variant that the main ones are such as the Weighted goal programming (WGP) variant, Lexicographic goal programming (LGP), and MINMAX GP.

The WGP consists of a compound objective consists of all goals. This objective minimizes the summation of deviations that exist between the goals and associated aspirational levels. Note that according to the DM preference for each goal, the deviations get weights.

The other GP variant, as mentioned above, is lexicographic goal programming (LGP). The concept of this method is the pre-emptive or non-Archimedean priorities. Here, different goals are divided into several levels of pre-emptive priorities so that the fulfillment of the goals in a specific priority  $Q_j$  is infinitely preferred to any other set of goals situated in a lower priority. In other words, in LGP, higher priority goals are satisfied first, i.e., the goals are satisfied regarding a lexicographic order.

The final step is to form the achievement function that substitutes the objective function concept in conventional mathematical programming models and compound function in WGP models. This achievement function consists of an ordered vector whose dimensions coincide with the number of priority levels established in the model. Each component in this vector represents the deviation variables. The minimization of these variables ensures that the goals ranked in this priority come closest to the established achievement levels.

$$\text{lex Minimize } a = [h_1(n, p), h_2(n, p), \dots, h_q(n, p)] \quad (3.9)$$

While it is not straightforwardly applicable for solving LGP problems, several adopted algorithms exist to solve LGP problems. These algorithms are the sequential linear method, the partitioning algorithm, which iteratively uses the Simplex, or the modified simplex method that uses a multi-phase simplex algorithm.

MINMAX GP is the third variant to be presented. In this variant, despite a pre-emptive (LGP) or non-pre-emptive (WGP), which implies the minimization of the sum of deviational variables, the maximum of deviations is minimized. The MINMAX GP model is defined mathematically as below:

*Minimize*  $d$

$$\begin{aligned} \text{s. t. } & \alpha_i n_i + \beta_i p_i \leq d \\ & F_i(x) + n_i - p_i = b_i \\ & x \in F \\ & x \geq 0, n \geq 0, p \geq 0 \end{aligned} \quad (3.10)$$

Where  $d$  is the maximum deviation, as the model (Eq. 3.10) is an LP problem, the conventional Simplex can solve it (ROMERO, 1991).



- **Lexicographic method**(Arora, 2012)

In this method, ordering the objective functions impose preferences regarding their importance rather than by assigning weights. So that the following optimization problems are solved:

$$\begin{aligned}
 & \text{Minimize } F_i(x) \\
 & \text{s. t. } F_j(x) \leq F_j(x_j^*) \\
 & \quad j = 1 \text{ to } (i - 1) \\
 & \quad i > 1, \quad i = 1, \dots, k
 \end{aligned} \tag{3.11}$$

Where  $i$  is a function's position in the preferred sequence, and  $F_j(x_j^*)$  represents the minimum value for  $j^{\text{th}}$  objective function found in the  $j$ th optimization problem. However, determining the uniqueness within the feasible objective space can be difficult. The algorithm terminates once to obtain a unique optimum. Often, with continuous problems, this approach terminates after finding the optimum of the first objective  $F_1(x)$ , Moreover, in any case, the solution is always Pareto optimal. Note that it is best to use a global optimization engine with this approach. Besides, this method is classified as a vector multi-objective optimization method because it treats each objective independently. The advantages of this method are:

- a) the uniqueness of the approach in specifying preferences;
- b) no need to normalize the objective functions;
- c) to provide a Pareto optimal solution.

### Interactive methods

In these methods, the decision-maker would not be able to make a prior evaluation before solving the problem due to its complexity but will be able to evaluate during the solution of an example or in the presence of a local solution. In this way, the DM is allowed to intervene in the solution process and learn more about the current problem, and he intervenes and checks his preferences in a trade-off between levels of different goals constantly during the solving process. There are two categories of Interactive methods in terms of possible trade-offs of the available levels for different objectives.

- a) The methods in which the explicit information of the trade-offs exist.
- b) The methods in which the implicit information are estimating preferred trade-offs.

Fig. 3.11 shows these methods classification, and the following subsection briefly describes the basic ideas behind the most appropriate ones.

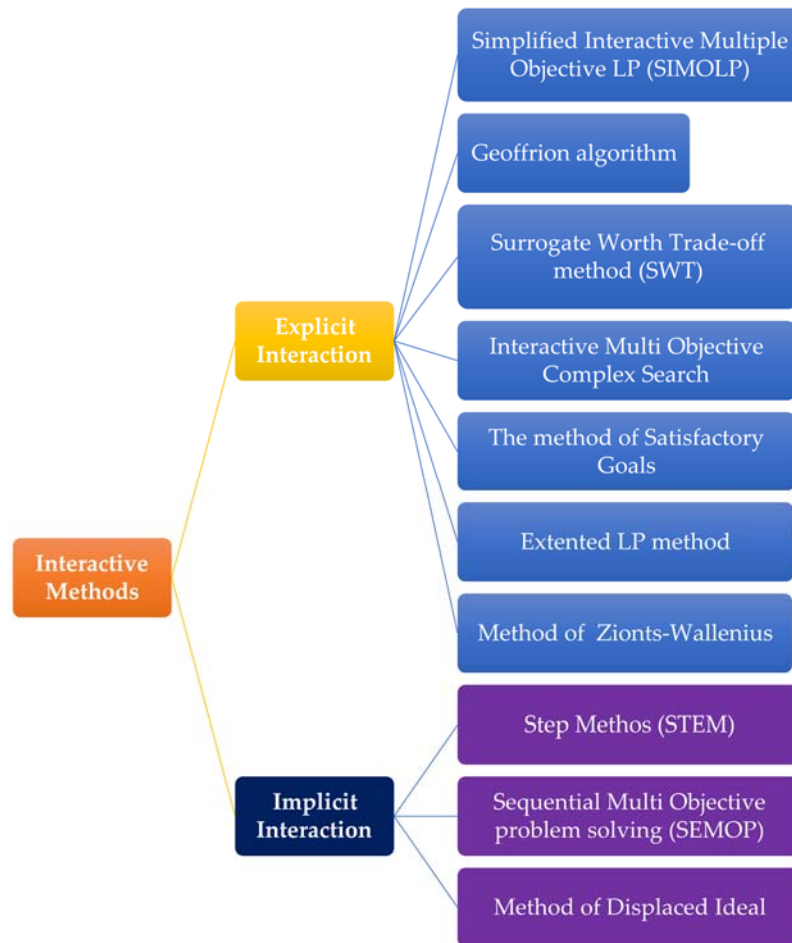


Fig. 3. 11. Interactive Methods in Multi-Objective decision Making Evaluation Methods.

### Explicit interaction

- **Simplified Interactive Multiple Objective LP (SIMOLP)**

In this algorithm, first, a multi-objective linear problem is solved like a series of single objective linear problems, and then the problem is evaluated and optimized by information received from the DM, using weights in each transformation and linear estimation of the value function.

- **Geoffrion algorithm**

This algorithm can solve a linear and nonlinear Vector Maximum Problem (VMP) if the DM can identify the utility function among all available ones. This algorithm is in the form of the Frank & Wolfe method (Frank & Wolfe, 1956), mainly intended for nonlinearities. This method changes a nonlinear problem to a linear one by outer linearization and employing  $\nabla F(x).d > 0$  (for maximizing a problem) to do sequential optimization.

- **Surrogate Worth Trade-off method (SWT)**

This method consists of two steps: the first step aims to obtain efficient solutions, and the trade-off functions are available in the objectives space; the second step includes a search for selecting a preferred solution among efficient solutions.

- **Interactive Multi-Objective Complex Search**

Box (1965) developed this searching method to solve single-objective nonlinear programs. Later on, Biles & Swain (1979) presented a complex search procedure for multi-objective optimization of simulated systems. In their method, a simulated model evaluates the objective functions at each vertex of the search procedure.

$$y_j = g_j(x_1, \dots, x_n | z_1, \dots, z_p) + \varepsilon_j, \quad j = 1, \dots, m \quad (3.12)$$

A simulation trial estimates the system response at a particular set of values  $x_i^k$  by controllable input variables  $x_i$ ,  $i = 1, \dots, n$  and yields responses  $\eta_j$ .

$$E(y_j) = \eta_j = g_j(x_1, \dots, x_n), \quad j = 1, \dots, m \quad (3.13)$$

This method has the advantage that the decision maker's underlying value function need not be explicitly specified.

- **The method of Satisfactory Goals**

This method is similar to Bounded objective methods, but the evaluation process by interaction with DM can result in a more improved final solution. The DM determines acceptable and practical satisfactory levels  $L_i$  for goals intentions and then identifies the objective that its goal has a minimum satisfactory level  $LS$  and optimizes this objective for main problem constraints and other objectives constraints.

$$\begin{aligned} & \text{Maximize } f_{LS}(x) \\ & \text{Subject to } g_j(x) \leq 0, \quad j = 1, 2, \dots, m \\ & \quad \quad \quad f_i(x) \geq L_i, \quad i = 1, 2, \dots, k; \quad i \neq LS \end{aligned} \quad (3.14)$$

- **Extended  $L_p$  method**

These kinds of methods are explained before in section 3.4.2.1. Applying the method may cause several efficient solutions. Therefore, a set of efficient solutions and their multiplicity might make the decision-making process complicated. Hence, reducing the current set to a smaller subset seems necessary. The Filtering method is a reductive method that the following describes concisely.

- **Filtering method**

Here it is tried to eliminate excess points and record a subset of heterogeneous points. Here, a compromise function of  $L_p$  calculates the heterogeneity of each pair of efficient points:

$$L_p = \left[ \sum_{i=1}^k (\gamma_i |F_i^t - F_i^h|)^p \right]^{1/p} < d \quad (3.15)$$

Where  $\gamma_i$  represents the degree of importance for  $i$ th objective,  $F_i^h$  is  $i$ th element of the efficient point of  $h$  has crossed the filter and  $F_i^t$  is  $i^{th}$  element of the efficient point  $t$  that is under study to

control heterogeneity. Besides,  $d$  is a distance parameter that adjusts the heterogeneity process and  $1 \leq P \leq \infty$ .

In addition to the Filtering method, there are other reductive methods like the Clustering method, value function assessment, and Ranking method.

- **Method of Zionts-Wallenius**

(Zionts & Wallenius, 1976) proposed a method based on the progressive preference information given in the interactive programming methods. In this method, the utility function is linear since the accurate weights in such functions are not explicitly known. Hence, the method chooses an arbitrary set of positive multipliers or weights  $\gamma_i \geq \varepsilon$  satisfying  $\sum_{i=1}^p \gamma_i = 1$  in the first step. Moreover, it generates a composite objective function or utility function using these multipliers.

$$\begin{aligned} & \text{Maximize} && \sum_{i=1}^k \gamma_i f_i(x) \\ & \text{Subject to} && g_j(x) \leq 0, \quad j = 1, 2, \dots, m \\ & && x \geq 0, \end{aligned} \quad (3.16)$$

The composite objective function is then optimized to produce an extremely efficient solution  $x^*$  to the problem. The utility function is not known explicitly; therefore, the set of all nonbasic variables consists of two subsets:

- (1) Those nonbasic variables lead to efficient adjacent extreme points when introduced into the basis.
- (2) Those nonbasic variables, when introduced into the basis, do not lead to efficient adjacent extreme points.

The first subset of variables is known as efficient variables, and the second subset is inefficient variables. In finding efficient variables set from the set of nonbasic variables, essentially,  $w_{ij}$  values must be estimated based on implicit information around the optimal solution at hand. These  $w_{ij}$  values represent the decrease in the objective function  $F_i$  due to some specified increase in  $x_j$ . For estimating  $w_{ij}$  values. After value estimation of  $w_{ij}$ , the following model is solved for each nonbasic variable  $x_l$  ( $l \in N$ ):

$$\begin{aligned} \text{Min:} & \sum_{i=1}^p w_{il} \gamma_i \\ \text{s. t.} & \sum_{i=1}^p w_{il} \gamma_i \geq 0, j \neq l, j \in NBV \\ & \sum_{i=1}^p \gamma_i = 1 \\ & \gamma_i \geq 0 \end{aligned} \quad (3.17)$$

Step 3 is to examine if the variable  $x_l$  is efficient or not. Hence, if the optimal value of Eq. (3.17) is negative, the variable  $x_l$  is efficient while it is nonnegative the  $x_l$  is not efficient.

Step 4. For each variable  $x_j$  of a subset of efficient variables, the DM responds if he accepts a decrease in the objective function  $F_1$  to  $F_p$  of  $w_{1j}$  to  $w_{pj}$  or not.

a) If all the responses are “no” for all efficient variables, terminate the procedure and,  $\gamma_i$  is defined as the most efficient weight for the utility function.

b) If the DM response is “yes,” for each yes, an inequality of the below form is constructed:

$$\sum_{i=1}^p w_{il}\gamma_i \leq -\varepsilon \quad (3.18)$$

c) for each ‘no’ response, construct an inequality of the form (3.19)

$$\sum_{i=1}^p w_{il}\gamma_i \geq \varepsilon \quad (3.19)$$

d) for each response of indifference, construct equality of the form as below:

$$\sum_{i=1}^p w_{il}\gamma_i = 0 \quad (3.20)$$

Here is a feasible solution to all previously constructed constraints of the form (3.15)-(3.20), and the following set of constraints:

$$\sum_{i=1}^p \gamma_i = 1, \gamma_i \geq \varepsilon \quad (3.21)$$

When the resulting set of  $\gamma_i$  is obtained, the objective function is optimized to produce a new, extremely efficient solution to the problem. This process assures the convergence of an overall optimal solution concerning the DM’s implicit utility function.

### Implicit interaction

- **Step Methods (STEM)**

STEM is an iterative exploration procedure to reach after a certain number of cycles. Each cycle  $m$  consists of a calculation phase and a decision-making phase (i.e., a conversation between the analyst and the decision-maker). During the decision-making phase, the DM examines the results of the calculation phase to give new information about his objectives.

This method is to solve a MOLP as is shown below:

$$\begin{aligned} \text{Max: } & \{C_1^t x, C_2^t x, \dots, C_k^t x\} \\ \text{s. t. : } & Ax \leq b \\ & x \geq 0 \end{aligned} \quad (3.22)$$

under this model, the STEM algorithm description is as following:

**Step 0. Construction of a Pay-off table.** Before starting the first cycle, it is necessary to construct a pay-off table of the optimum objectives calculated for the feasible region.

	$F_1$	$F_2$	...	$F_j$	...	$F_k$
$F_1$	$F_1^*$	$Z_{21}$		$Z_{j1}$		$Z_{k1}$
$F_2$	$Z_{12}$	$F_2^*$		$Z_{j2}$		$Z_{k2}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$		$\vdots$
$F_j$	$Z_{1j}$	$Z_{2j}$		$F_j^*$		$Z_{kj}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$		$\vdots$
$F_k$	$Z_{1k}$	$Z_{2k}$		$Z_{jk}$		$F_k^*$

The  $Z_{ij}$  represents the value of the objective  $i^{th}$  when the objective  $j^{th}$  reaches to its ideal value of  $F_j^*$ .

**Step 1. Calculation phase.** For each cycle  $m$ , linear programming (3.18) aims to minimize the  $\gamma$  where implies the nearest, in the MINIMAX sense, to the ideal solution  $F_j^*$ :

$$\begin{aligned}
& \text{Min } \gamma \\
& \text{s.t.: } \gamma \geq (F_j^* - F_j(x)) \cdot \beta_j \\
& \quad x \in S^m \\
& \quad \gamma \geq 0
\end{aligned} \tag{3.23}$$

The coefficient  $\beta_j$  represents the relative importance of the distances to the optimized objectives, note that they are only locally effective and but not predominant as the weights in the Utility method.

**Step 2. Decision phase.** The compromise solution  $x_m$  is introduced to the decision-maker, who compares the objective  $F_m$  with an ideal value of  $F_j^*$ . If  $F_j^m$  is satisfactory and, the decision-maker must accept the value of relaxation of  $F_j^*$  to allow an improvement of the unsatisfactory ones in the next cycle.

**Step 3. Repetition.** Repeating previous steps until the value of all  $F_j^m$  will be satisfactory.

- **Sequential Multi-Objective problem solving (SEMOPS)**

SEMOPS, a sequential multi-objective problem-solving technique, allows the decision-maker to compromise one objective versus another in an interactive manner. SEMOPS cyclically uses a surrogate objective function based on goals and the decision maker's aspirations about achieving these goals. SEMOPS is a three-step algorithm involving setup, iteration, and termination.

- The DM defines aspiration levels  $AL = \{AL_1, \dots, AL_i\}$ .
- Lower and upper bounds of objective  $i^{th}$  is  $\{F_{il}, F_{iu}\}$ .

**Step 1. Setup.** To unscaling objectives, each  $F_i(x)$  is converted to  $H_i(x)$  (in the range of zero and aspiration level  $AL_i$  also are converted to  $A_i$ ).

$$H_i(x) = \frac{F_i(x) - F_{il}}{F_{iu} - F_{il}} + \varepsilon \quad \varepsilon \neq 0 \tag{3.24}$$

$$A_i = \frac{AL_i - F_{il}}{F_{iu} - F_{il}} + \varepsilon$$

**Step 2. Iteration.** This step is the interactive segment of the algorithm involving a cycle between an optimization phase and an evolution phase until achieving satisfaction. At the beginning of the  $i^{th}$  cycle, a principal problem is formed with goal formulation  $F_i(x)$ , and the remained objectives form sub-problems. They should reach their associated aspiration levels as the set goals. The achieved solutions are introduced to the DM to evaluate. New aspiration levels set goals.

**Step 3. Termination.** The optimum solution is introduced to DM to evaluate and decide about the next cycle. The steps above are repeating until achieving a satisfactory solution.

- **Method of Displaced Ideal**

This method was proposed by Zeleny (1974) for a MOLP, and  $L_p$  Metric is used in this method. However, the ideal solution is in the frontier point  $F(x^*)$ , it is not applicable for the objective-space. The efficient solutions set lies in the sides between A, and B but reducing these solutions to subset C leads to having efficient solutions with the least distance from the ideal point.

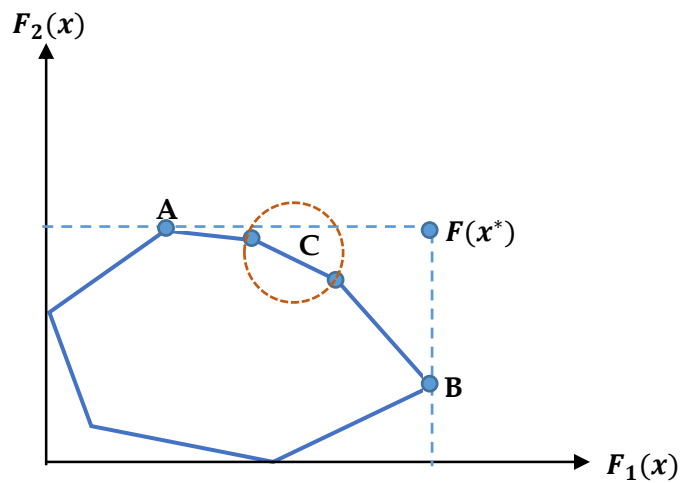


Fig. 3. 12. Method of Displaced Ideal for two objective functions.

Note that the method of the displaced ideal is an adequate method for problems with complex, heterogeneous, and conflicting objectives, and it is not necessarily needed to receive information from the DM.

### A posteriori methods

In these methods, when in the termination phase, a subset of an efficient solution is proposed to DM to select and evaluate the most satisfactory one. Also, there is no need for the utility function. Here, these methods include **Parametric methods**, the **limited  $b_L$  methods**, **Multi-objective linear programming**, and **Multi-criteria simplex method**.

- **Parametric methods**

This method is known for generating various efficient solutions to propose to the DM. It is assumed an additive linear utility function, and the different weight values are applied to generate efficient solutions. Its mathematical model is as below:

$$\begin{aligned} \text{Max} \quad & \sum_{j=1}^k \omega_j F_j(x) \\ \text{s. t.} \quad & x \in S \\ & \omega_j \geq 0, \sum \omega_j = 1 \end{aligned} \quad (3.25)$$

Note that weights  $\omega$  do not represent the relative importance of objectives, but they change parametrically to find efficient points. This method is illustrated in a two-dimensional objective space as follows:

$$\begin{aligned} L &= \omega_1 F_1 + \omega_2 F_2 \\ \text{Slope} &= -\frac{\omega_1}{\omega_2} \end{aligned}$$

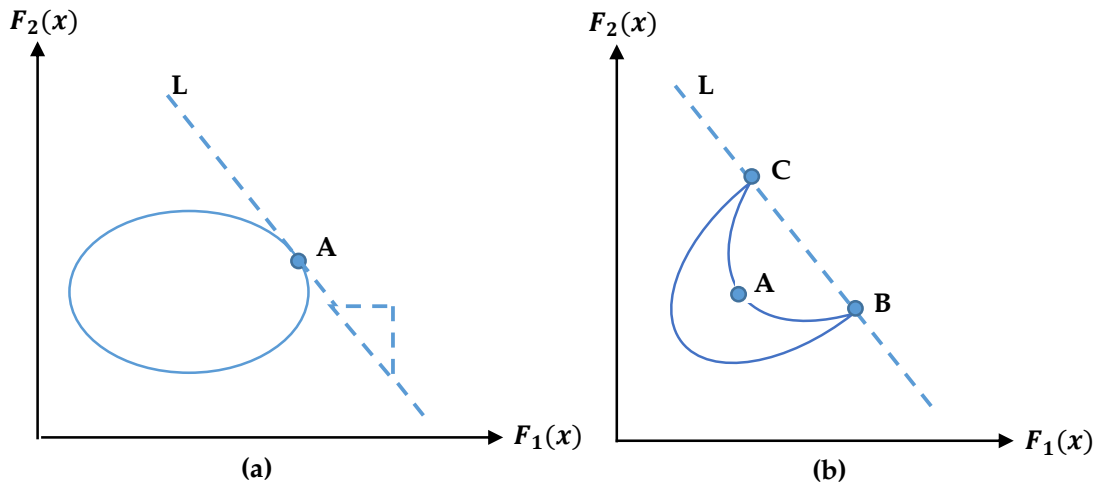


Fig. 3.13. Convex (a) and Non-Convex (b) objective functions.

Fig. 3.13 (a) shows function  $L$  is the tangent line surface  $S$  that defines point  $A$  as an efficient point in the solution space  $S$ . If solution space is non-convex, as Fig. 3.13 (b) shows, it may be impossible to find some efficient points such as  $A$ . Note that the mentioned method does not apply to non-linear problems even with convex solution space.

- **Multi-objective linear programming methods**

These methods are applicable for multi-objective linear programming, and therefore the available frontier points of a convex space can be found. A formulated MOLP is as below:

$$\begin{aligned} \text{Max:} \quad & C_{k \times n} x \\ \text{s. t.:} \quad & A_{m \times n} x = b \\ & x \geq 0 \end{aligned} \quad (3.26)$$

Most of the related algorithms include three steps as following:

**Step 1.** Finding a feasible frontier point.



**Step 2.** Detecting the first efficient frontier point.

**Step 3.** Detecting all efficient frontier points.

- **Multi-criteria Simplex method**

The multi-criteria simplex method is a natural generalization of the simplex method. This method was proposed by (P. L. Yu & Zeleny, 1975), and it is assumed:

$N$	Efficient solutions set
$X$	Available solutions set
$D = X - N$	Non-efficient solution set
$N_{ex}$	Efficient frontier points

They studied the connectedness of  $N_{ex}$  and derive an algorithm to locate the entire set  $N_{ex}$ . In this method, the set of efficient frontier points for a MOLP is a connected set, and any other efficient point is a convex linear composition of an efficient frontier points subset.

- **Optimization under uncertainty**

In deterministic models, the model's output is entirely determined by the parameter values and the initial conditions (i.e., all the required data is to know in advance). Stochastic models contain inherent randomness. The same set of parameter values and primary conditions result in an ensemble of different outputs.

In a large number of problems, it is necessary to decide in the presence of uncertainty. In production planning and engineering design, uncertainty manages issues such as fuel prices, the availability of electricity, and the demand for chemicals. The critical challenges in optimization under uncertainty are huge uncertainty space that frequently leads to very large-scale optimization models and decision making in the presence of integer decision variables.

### 3.4.5. Stochastic programming

Stochastic programming is a structure for modeling optimization problems that involve uncertainty. Whereas all the previously presented strategies and methodologies depend on the data required to be known in advance, real-world problems almost invariably include some unknown parameters. Stochastic programming models take advantage of probability distributions governing the data are known or can be estimated. This section describes the stochastic and particularly the two-stage stochastic program.

Stochastic programs are mathematical models where some of the data and parameters incorporated into objectives or constraints are uncertain. As described before, usually, a probability distribution on the parameters characterizes uncertainty. However, the uncertainty is rigorously defined; it can practically range from a few scenarios to specific and precise joint probability distributions.

The most frequent model used to tackle problems under uncertainty is the two-stage stochastic programming and generally consists of two distinct sets of decision variables: first-stage

structural decision variables that are fixed and free of any uncertainty, and second-stage control decision variables that are affected by the uncertainty in input data (Prékopa, 1995).

Let  $x$  and  $y$  define the first and second stage decision vectors, respectively, and let  $\xi$  be the random observed vector. Consequently, there are two optimization problems to be solved. The second stage problem is defined by assuming  $x$  and  $\xi$  to be fixed, and is the following:

$$\begin{aligned} \text{Min: } & q^T y \\ \text{s. t.: } & Tx + Wy = \xi \\ & y \geq 0 \end{aligned} \tag{3.27}$$

Here, the first stage decision vector  $x$  satisfies some deterministic constraints:

$$\begin{aligned} Ax &= b \\ x &\geq 0 \end{aligned} \tag{3.28}$$

Let  $K$  be the set of all those  $x$  vectors for which problem (3.27) has a feasible solution for every possible value of the random vector  $\xi$ .  $q(x, \xi)$  is designated the optimum value of the problem (3.21) and  $Q(x) = E[q(x, \xi)]$  where the function  $Q(x)$  is called the recourse function. Therefore, the first stage of problem formulation is as follows:

$$\begin{aligned} \text{Min: } & \{c^T x + Q(x)\} \\ \text{s. t.: } & Ax = b \\ & x \geq 0 \\ & x \in K \end{aligned} \tag{3.29}$$

To approximate a feasible global solution by using the two-stage model (Eq. (3.27) & Eq. (3.29)), a set of scenarios represents the problem variability using a scenario tree representation (Fig. 3.14).

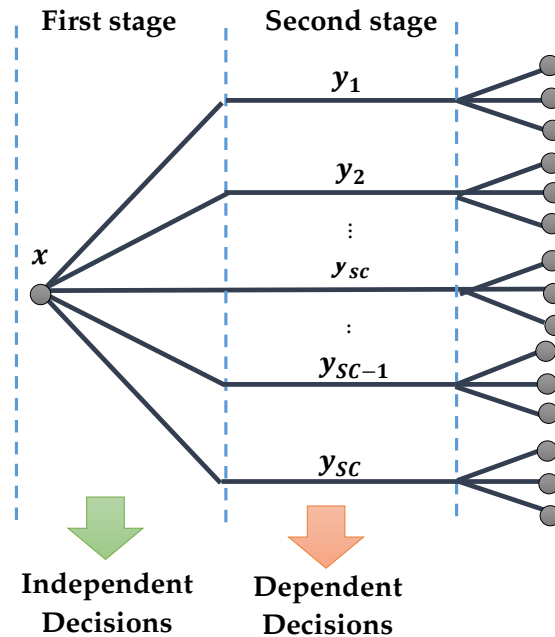


Fig. 3. 14. Uncertainties in two-stage stochastic programming.

**The scenario-based approach**

Generally, uncertain parameters  $\xi$  are represented by using a discrete number of possible scenarios; thus, a deterministic equivalent program can be formulated for a stochastic program as displayed in Eq. (3.24):

$$\begin{aligned} \min_{x, y_{sc}} F_{ob} &= \sum_{sc}^{SC} prob_{sc} F(x, y_{sc}, \xi_{sc}) \\ s. t. : & Ax = b \\ & x \geq 0, y_{sc} \geq 0, \xi_{sc} \geq 0 \\ & sc \in SC \end{aligned} \tag{3.30}$$

Here,  $\xi_{sc}$  is the vector of values taken by the uncertain parameters in the scenarios  $sc$  and  $prob_{sc}$  is the probability of occurrence of scenario  $sc$  belonging to the set  $SC$ .

Here, the better the representation of the scenarios used results in the better the robust solution approximates. Hence, the most common strategy is the Monte-Carlo sampling. This method aims to generate a random set of uncertain parameters considering a mean value and a standard deviation. In this thesis, Monte-Carlo sampling has been used as a unique sampling technique; however, other sampling techniques are used, such as polynomial-based methods, Sobol sampling, and methods based on low-discrepancy samples (also known as quasi-Monte Carlo methods).

Besides the representativeness of the set of scenarios, its size significantly affects the computational effort (i.e., optimization time). In this line, scenario reduction methods are proposed. These methods promote selecting a trim and representative set of scenarios, as displayed in Fig. 3.15.

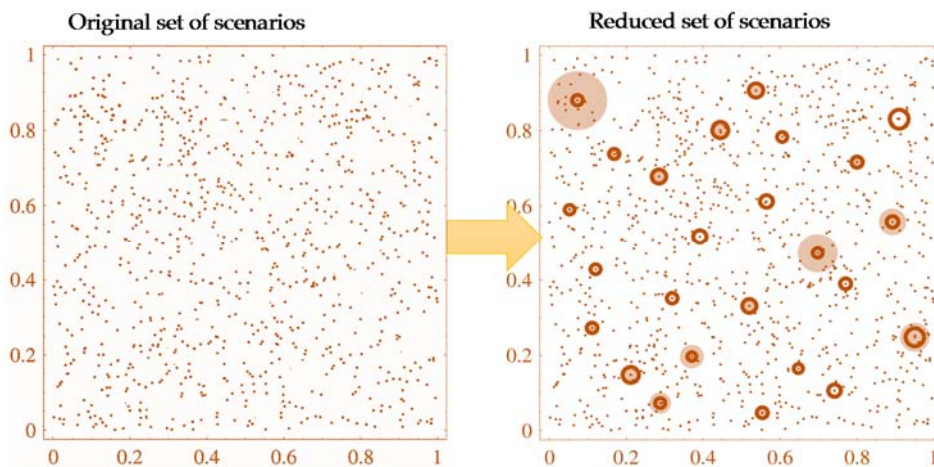


Fig. 3. 15. Graphical representation of the clustering technique for scenario reduction method (Römisch, 2009).

The most effective method for scenario reduction is the transportation distance-based scenario reduction initially proposed by Heitsch and Römisch (2003) and later extended by (Z. Li &

Floudas, 2014). This method systematically minimizes the distance (i.e., Kantorovich distance) among scenarios, finding the optimal subset representing the original set of scenarios.

### **3.5. Optimization software**

By putting into practice optimization methods and implementing optimal solutions, many optimization problems can be solved. However, real-life problems are more complicated than the theoretically stated pure base mathematical models. In some books or publications, there are several optimization software for solving different problem scales. For this purpose, there are some commercial tools including GAMS (General Algebraic Modeling System, (Bussieck & Meeraus, 2004)), AMPL (A Mathematical Programming Language, (Fourer, Gay, & Kernighan, 2003)), AIMMS (Advanced Interactive Multidimensional Modeling system, (Roelofs & Bisschop, 2020)), LINGO, LINDO, MATLAB, and the recently introduced PYOMO.

The conventional optimization software has common characteristics such as general mathematical language, different solvers to use. In this thesis, GAMS has been selected since it is a widely used modeling tool and optimization software in different fields, like the PSE, and promotes future comparisons.

#### **3.5.1. GAMS-General Algebraic Modeling System**

The General Algebraic Modeling System (GAMS) is a mathematical modeling tool for optimization. GAMS is designed for solving complex and large-scale models, specifically for modeling linear, nonlinear, and mixed-integer optimization problems.

Besides, GAMS has some advantages that encourage to select that listed as below:

- Strong virtual parallelism across set elements when solving an optimization problem makes programming very convenient to the user.
- A compelling bunch of options to the user regarding condition definitions-at set level, at the statement level, and solver level.
- "Dynamic" set definitions within parent set makes a variety of optimization solution space very convenient within nested loops or otherwise. It also makes multiple scenario programming very easy.

While the platform is designed for deterministic problems, it is also applicable to stochastic problems with a bit of effort and careful programming. The only thing that is challenging on GAMS is the realization of complex evolutionary optimization algorithms. Moreover, it is worth mentioning that the optimization algorithms 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).

### **3.5.2. Solvers**

Many solvers are available to solve MILP problems such as BARON, BDMLP, GUROBI, LINDO, MOSEK, and CPLEX. Similarly, some other solvers are used to address convex and non-convex problems, including DICOPT (convex/non-convex), GloMIQO (convex/non-convex quadratic), BARON (convex/nonconvex), and SCIP (convex/non-convex), among others. In this thesis, the main solver to be used is CPLEX.

### **3.6. Final remarks**

In this chapter, different optimization techniques have been delineated. The central notion behind each technique has been explained concisely to provide a general perspective of the theory associated with the solution techniques. Regarding implementing mathematical formulation in the optimization software, having a good understanding of the optimization principles is necessary to interpret results and debug skills. Notably, this thesis has focused on the combination and development of multi-objective optimization and uncertainty approaches. Besides, solution recognition strategies have been proposed extensively.



*Part II*

*Efficient Supply Chain Retrofitting towards  
Sustainability*





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**SIMPLIFIED TARGETING MODELS FOR SC RETROFITTING**

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Our traditional production system needs retrofitting to be more sustainable or adapted to sustainability criteria.

An environmentally, economically, and socially sustainable production system is supposed to deal with conflicting objectives. Hence, this chapter aims to formulate and solve multi-objective problems by exploiting mathematical programming techniques to simultaneously optimize the system's performance through supply chains and production processes. This thesis utilizes a real-world case study to validate the viability of the novel model.

Despite the comprehensive capability of multi-objective approaches to simultaneously evaluate several objectives, the studies so far have proposed models to optimize small-scale and non-complex problems. Notably, these approaches are practical to address complex sustainability problems. Hence, these approaches could be applied to improve supply chain management by considering both the quantified impact and its effects on more process conditions.

This chapter aims to propose a general systematic multi-objective strategic and tactical optimization model towards more sustainable and robust decision-making for large-scale supply chain superstructures. The proposed model exploits mathematical programming techniques to simultaneously optimize the performance of large-scale SCs, particularly integrated material bioenergy supply chains, in the presence of conflicting objectives (economic and environmental).

#### **4.1. Application of Multi-Objective approaches in sustainable supply chain retrofitting**

Optimization strategies should be improved within the framework of industrial symbiosis systems to meet sustainability goals. Thus, sustainable design and planning models for the process industries have strongly stimulated industries and academia during the last three decades. The industries and academia have set their goals to achieve a system with maximum sustainability adoption. Hence, their studies mainly have focused on retrofitting strategies, therefore, addressing fundamental improvements in energy, environmental, and cost performance. These strategies can involve industries in different levels, such as a unit, process segment, and overall system levels. Process industries, as the particular case, must address the following challenges:

- (i) The management strategies of material/energy integration in process industries;
- (ii) The integration of economic and environmental aspects within the framework of supply chain management;
- (iii) The development of efficient retrofitting techniques to production processes;

A holistic systems-based approach can tackle these challenges. Such an approach aims to propose an integrated formulation to optimize the global impact considering feasibility constraints. In this regard, the studies have applied mathematical programming to formulate the sustainability-conscious industrial systems (Arora, 2012; Grossmann & Guillén-Gosálbez, 2010). For example, in environmentally conscious optimization models, environmental impact metrics combine with mathematical programming. For instance, (Sabio et al., 2014) proposed an integrated LCA model through multi-objective mathematical programming to demonstrate that the combination of mathematical programming and LCA provides a powerful tool to optimize the environmental and economic performance of industrial processes.

Using environmental metrics to assess the environmental impact allows industries to control the contaminations and damages, mainly  $CO_2$  emissions caused by industrial activities. However, it is not a unique approach towards sustainability. As mentioned in Chapter 1, bioenergy substitution with fossil-based energies mitigates greenhouse gas emissions. A wide range of studies in the sustainability area has addressed bioenergy supply chain optimization using mathematical programming technics (mentioned in detail in Chapter 2). However, very few works have addressed bioenergy SCs optimization considering the byproducts as added-value products in the optimization process. For instance, Cambero et al. (2016) developed a bi-objective MIP model to optimize bioenergy SC network design. The novelty of their work is that modeling energy and material flows accurately estimates the quantities of exchanged material and energy and emissions across the supply chain simultaneously. However, the model neglected the added value of byproducts.

While very few approaches have addressed sustainable supply chain retrofitting, a general model is needed to simultaneously optimize the retrofitted supply chain's economic benefits and environmental impacts.

This chapter dedicates to introduce a novel model for the optimal retrofit and planning of large-scale material/energy networks based on multi-objective mathematical formulations that make use of linear programming. Here two conflicting objectives are net present value (NPV) and environmental damage that is the function of  $CO_2$  emissions. The first objective is commonly optimized in process industries reflecting the economic dimension of sustainability. The other one quantifies the environmental impacts. Hence, this chapter's significant contribution is a mathematical approach adoption capturing the cause-effect relationship between material/energy consumption/demand and the associated environmental impacts.

## 4.2. Problem statement

This chapter addresses the retrofitting of a production network system. Fig. 4.1 depicts the problem statement concisely. Each region involved in the production process has associated energy demand that should be satisfied. This energy can be provided by external resources traditionally. Here, retrofitting opens the opportunity to provide the required energy internally. The process industries include different production technologies coupled with internal multi-type energy generation technology. The energy generator unit receives and converts production plants' residues to energy in different types. The internally generated energy satisfies any energy demand, and the excess is transferrable to the grid. Note that, in any case, if the internal energy is not sufficient, the external resources can supply the shortage. The storage facilities are intermediaries to distribute the products to the markets.

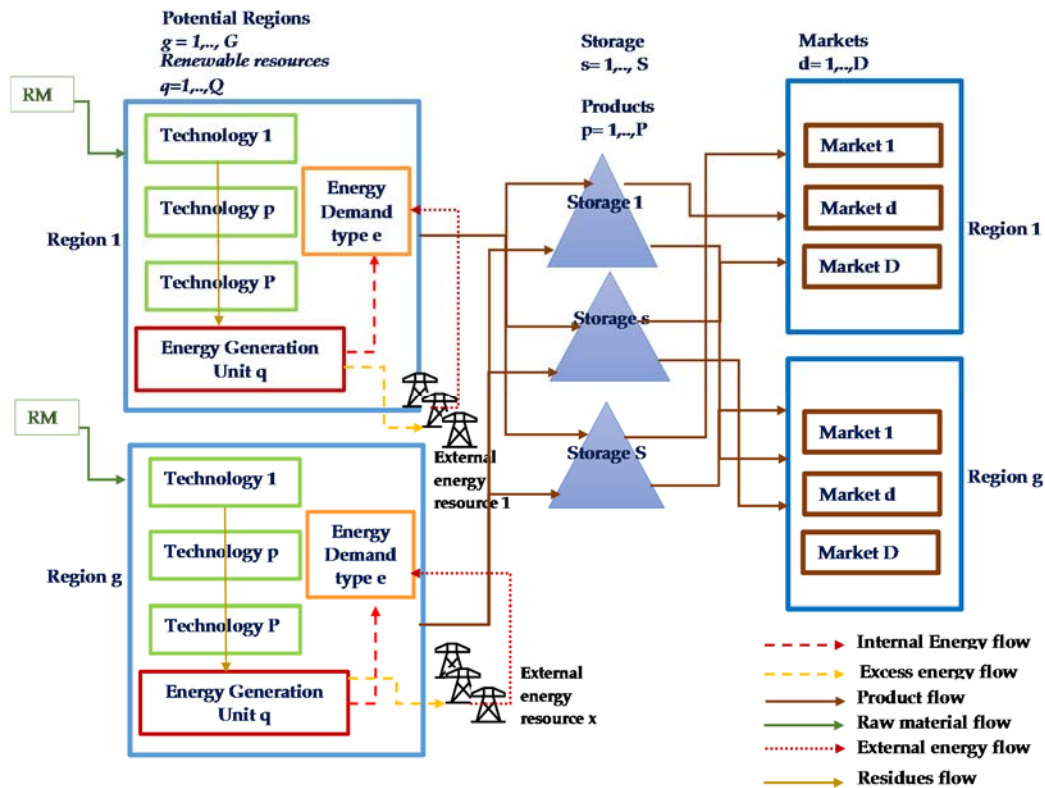


Fig. 4. 1. Multi-type energy integrated to material SC Network.

Note that material resources that play as the suppliers of the production process and internal energy generation units. The process industries include different production technologies coupled with internal energy generation technology, acting as raw material consumers and potential sites for storage technologies. The explicit production rate and material flow modeling among the plants and regions estimate the emissions across the supply chain.

The goal is to identify the optimum design of the network configuration and plan the operational processes in terms of economic performance and environmental impacts.

### 4.3. Mathematical Model

The mathematical equations formulate the network shown in Fig. 4.1. The formulations mainly describe mass and energy balances and capacity constraints of each section of the network. The mathematical model of this contribution is mixed-integer linear programming (MILP) and used to optimize the stated problem in this chapter. This MILP is an extension of the model introduced by (Mele et al., 2011). This contribution has extended the Melé model by integrating the energy generation section.

#### 4.3.1. Material production and associated constraints equations

##### Mass balances equations

Eq. (4.1) defines the mass balance for each potential site. In the equation, for each material type  $i$ , the is a mass balance, and it is the summation of initial inventory  $ST_{i,s,g,t-1}$  maintained in region  $g$  from the previous period added to the purchased raw material  $PU_{i,g,t}$ , the total produced material  $PT_{i,g,t}$  and input material flow rate  $Q_{i,l,g',g,t}$  that is equal to the current inventory  $ST_{i,s,g,t}$  added to delivered product  $DT_{i,g,t}$ , the output material flow  $Q_{i,l,g,g',t}$  and generated waste  $W_{i,g,t}$ .

$$\begin{aligned} \sum_{s \in IS(i,s)} ST_{i,s,g,t-1} + PT_{i,g,t} + PU_{i,g,t} + \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{i,l,g',g,t} = & \quad \forall i, g, t \quad (4.1) \\ \sum_{s \in IS(i,s)} ST_{i,s,g,t} + DT_{i,g,t} + \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{i,l,g,g',t} + W_{i,g,t} & \end{aligned}$$

Note that  $IS(i, s)$  is a subset that links material  $i$  to its adequate storage technology  $s$  and  $IL(i, l)$  is an ordered pair of material  $i$  and its suitable transportation mode  $l$ .

$$PT_{i,g,t} = - \sum_p sign \rho_{p,i} \times PE_{i,p,g,t} \quad \forall i, g, t \quad (4.2)$$

Equation (4.2) defines the total material production rate from the production rates of each technology  $p$  installed in each site  $g$ .

$$PE_{i,p,g,t} = |\rho_{p,i}| \sum_{i' \in IM(i',p)} PE_{i',p,g,t} \quad \forall i, p, g, t \quad (4.3)$$

In equation (4.3),  $IM(i, p)$  links the main product  $i$  to its production technology  $p$ . Note that the material balance coefficient  $\rho_{p,i}$  is associated with technology  $p$  that produces product/byproduct  $i$ .

##### Mass flow constraints

The purchase of the raw material in region  $g$  during period  $t$  is limited by its existing production capacity, as defined in Eq. (4.4).

$$PU_{i,g,t} \leq CapCrop_{g,t} \quad i = \text{Raw material}, \quad \forall g, t \quad (4.4)$$

In the following, the total product inventory  $ST_{i,s,g,t}$  is limited by the storage capacity during period  $t$ :

$$\sum_{i \in IS(i,s)} ST_{i,s,g,t} \leq SCap_{s,g,t} \quad \forall s, g, t \quad (4.5)$$

During the operation, the average inventory  $AII_{i,g,t}$  depends on the amount of material delivered to the associated market.

$$AIL_{i,g,t} = \sigma DTS_{i,g,t} \quad \forall i, g, t \quad (4.6)$$

Here,  $\sigma$  is the storage period defined as the average time a product can be stored by a storage technology. The total storage capacity in each site must be at least twice the average inventory level of product  $i$ , to manage the supply and demand fluctuations (Eq. (4.7)).

$$2AIL_{i,g,t} \leq \sum_{s \in IS(i,s)} SCap_{s,g,t} \quad \forall i, g, t \quad (4.7)$$

Notice that delivered product quantity  $DTS_{i,g,t}$  is supposed to be equal to or less the market demand amount  $SD_{i,g,t}$ .

$$DTS_{i,g,t} \leq SD_{i,g,t} \quad \forall i, g, t \quad (4.8)$$

A binary variable represents the transportation links between the two sites. It equals 1 if a transportation link is established between the two sites and 0 otherwise.

$$X_{l,g,g',t} + X_{l,g',g,t} = 1 \quad \forall l, g, g', t (g \neq g') \quad (4.9)$$

Note that a region can either import or export material  $i$ , but not both at the same time.

Besides, the total of material flows is between the lower and upper capacity of the flow rate.

$$\underline{Q}_l X_{l,g,g',t} \leq \sum_{i \in IL(i,l)} Q_{i,l,g,g',t} \leq \overline{Q}_l X_{l,g,g',t} \quad \forall l, g, g' (g \neq g'), t \quad (4.10)$$

In this equation, subset  $IL(i, l)$  represents the allowable combinations of material  $i$  and suitable transportation mode  $l$ .

### **Production and storage capacity constraints**

The production rate of each technology  $p$  in site  $g$  must be less than the capacity in use and more than the minimum capacity of the available technology. Note that  $\tau$  is the minimum desired percentage of the available technology.

$$\tau |\rho_{p,i}| PCap_{p,g,t} \leq PE_{i,p,g,t} \leq |\rho_{p,i}| PCap_{p,g,t} \quad \forall g, t, IM(i, p) \quad (4.11)$$

The capacity of technology  $p$  in each period equal to the summation of the available capacity of the previous period, plus the capacity expansion in the current period ( $PCapE_{p,g,t}$ ).

$$PCap_{p,g,t} = PCap_{p,g,t-1} + PCapE_{p,g,t} \quad \forall p, g, t \quad (4.12)$$

Besides, the capacity expansion is limited by upper and lower bounds capacities, as defined by Eq. (4.13).  $NP_{p,g,t}$  is an integer variable that indicates the number of plants installed in site  $g$  and period  $t$ .

$$\underline{PCap}_p NP_{p,g,t} \leq PCapE_{p,g,t} \leq \overline{PCap}_p NP_{p,g,t} \quad \forall p, g, t \quad (4.13)$$

Note that the capacity expansion must begin and finish within a period. Generally, in design problems, the period length can be one to several years. Therefore, the maximum allowable capacity expansion should be executed within one period.

Storage capacity in any period is the summation of the existing capacity of the previous period and the expanded capacity in the current period.

$$SCap_{s,g,t} = SCap_{s,g,t-1} + SCapE_{s,g,t} \quad \forall s, g, t \quad (4.14)$$

The storage capacity expansion is confined between the maximum and minimum available storage capacity of each technology, as stated in Eq. (4.15).  $NS_{s,g,t}$  is an integer variable that indicates the number of plants installed in site  $g$  and period  $t$ .

$$\underline{SCap}_s NS_{s,g,t} \leq SCapE_{s,g,t} \leq \overline{SCap}_s NS_{s,g,t} \quad \forall s, g, t \quad (4.15)$$

### 4.3.2. Energy generation and associated constraints equations

#### Energy balances and flows equations

Due to single-resource energy generation, the total energy demand ( $TotalDemand_{g,t}$ ) is equal to the energy demand needed per unit of raw material ( $Demand_{g,t}$ ) multiplied by the amount of raw material amount ( $PU_{i,g,t}$ ) in region  $g$ , each period  $t$ .

$$TotalDemand_{g,t} = PU_{i,g,t} \times Demand_{g,t}$$

Eq.(4.16) defines the energy balance in each region and period:

$$\sum_e [EnI]_{e,g,t} \times EfI]_e + \sum_{e \in EX(e,x)} \sum_x [EnX]_{e,x,g,t} \times EfX]_{e,x} = TotalDemand_{g,t} \quad \forall g, t \quad (4.16)$$

Here, the total energy demand  $TotalDemand_{g,t}$  of the process plant located in region  $g$ , is equal to the total of internal energy flows  $EnI]_{e,g,t}$  (flows between an energy generator and the process plant), plus the total external energy flow  $EnX]_{e,x,g,t}$  that the process plant receives from the external resources  $EnX]_{e,x,g,t}$ . The conversion efficiencies between energy resources and the process plant are represented by  $EfI]_e$  and  $EfX]_{e,x}$ . In Eq. (4.16), subset  $EX(e, x)$  links the energy type  $e$  to its external supplier  $x$ .

The energy type  $e$  generated in the internal resource will satisfy the process plant demand or market to the external energy demanders (Eq. (4.17)) and indicate the energy balance between internal and external resources.

$$EnI]_{e,g,t} \times EfI]_e + EnIX]_{e,x,g,t} \times EfIX]_{e,x} = EnIG]_{e,g,t} \quad \forall g, t, EX(e, x) \quad (4.17)$$

Here,  $EfIX]_{e,x}$  represents the conversion efficiency of the excess energy  $EnIX]_{e,x,g,t}$  that can be sent to the external energy generation resources while,  $EnI]_{e,g,t}$  is the energy flow consumed in the production plant while  $EnIG]_{e,g,t}$  is the total generated energy of type  $e$  in region  $g$  and period  $t$ , respectively.

#### Installation and generation capacity constraints

The following equations define the installation capacity:

$$PwI]_g \leq PwIMax \quad \forall g \quad (4.18)$$

$$PwI]_g \times SurfPwl \leq SurfTMax \quad \forall g \quad (4.19)$$

Equations (4.20) to (4.23) correspond to the Big-M method, introducing the binary variable  $Gn_{g,t}$  (the generation decision variable) to avoid nonlinearity.

$$PwIG]_{g,t} \leq PwIMax \times Gn_{g,t} \quad \forall g, t \quad (4.20)$$

$$PwIG]_{g,t} \geq -PwIMax \times Gn_{g,t} \quad \forall g, t \quad (4.21)$$

$$PwIG_{g,t} \leq PwIGMax_{g,t} + PwIMax \times (Gn_{g,t} - 1) \quad \forall g, t \quad (4.22)$$

$$PwIG_{g,t} \geq PwIGMin_{g,t} - PwIMax \times (Gn_{g,t} - 1) \quad \forall g, t \quad (4.23)$$

It needs to choose a value of M sufficiently large to make the problem feasible and small enough to limit it. In this case, M corresponds to the maximum power capacity installation  $PwIMax$ . Here, parameters  $PwIGMax_{g,t}$  and  $PwIGMin_{g,t}$  are calculated based on specific energy resource models (see Eq. (4.24) to (4.26)).

$$PwIGMax_{g,t} = PwIG_{g,t} \quad \forall g, t \quad (4.24)$$

$$PwIGMin_{g,t} = PwIG_{g,t} \times MinPgCO \quad \forall g, t \quad (4.25)$$

$$PwIG_{g,t} = EnIG_{g,t}/SL \quad \forall g, t \quad (4.26)$$

### **External resource equations**

The following equations define the energy the flows between internal and external elements.

$$EnXP_{e,x,g,t} = enXJ_{e,x,g,t} \times EfXJ_{e,x} \quad \forall g, t, EX(e, x) \quad (4.27)$$

$$EnXS_{e,x,g,t} = enIX_{e,x,g,t} \times EfIX_{e,x} \quad \forall g, t, EX(e, x) \quad (4.28)$$

$$PwXP_{e,x,g,t} = EnXP_{e,x,g,t}/SL \quad \forall g, t, EX(e, x) \quad (4.29)$$

$$PwXS_{e,x,g,t} = EnXS_{e,x,g,t}/SL \quad \forall g, t, EX(e, x) \quad (4.30)$$

Here,  $EnXP_{e,x,g,t}$  and  $EnXS_{e,x,g,t}$  are the amount of energy purchased and sold in each external resource. The corresponding powers are  $PwXP_{e,x,g,t}$  and  $PwXS_{e,x,g,t}$  in each time interval  $SL$ .

### **4.3.3. Objective functions**

The model includes two objective functions, being the net present value (NPV) as the economic objective function versus the environmental impact quantified regarding the Life Cycle Assessment (LCA) principles based on the compilation and evaluation of the inputs, outputs, and the potential of environmental impacts of a product (goods and service) system throughout its life cycle. The following section presents a detailed description of the calculation of the objective function.

#### **4.3.3.1. Economic objective**

The economic objective is the net present value (NPV) from the discounted cash flows  $CF_t$  of each period  $t$  divided into the planning horizon (Eq. (4.31)).

$$NPV = \sum_t \frac{CF_t}{(1+ir)^{t-1}} \quad (4.31)$$

Here,  $ir$  is the interest rate and the net earning  $NE_t$  (the profit after taxes) plus the fraction of the total depreciable capital  $TOTAL_t$  determine the cash flow  $CF_t$  as the following:

$$CF_t = NE_t - TOTAL_t \quad t = 1, \dots, T - 1 \quad (4.32)$$

$$TOTAL_t = \frac{FCI}{T} + \frac{CIns}{T} + \frac{GHGIns}{T} \quad \forall t \quad (4.33)$$

The fixed capital investments (i.e.,  $FCI$ ,  $CIns$  and  $GHGIns$ ) can partially be recovered at the end of the planning horizon. This partial amount is the salvage value  $sv$  of the network that may vary

from one type of industry to another. Eq. (4.34) defines the cash flow at the end of the planning horizon.

$$CF_t = NE_t - TOTAL_t + sv(FCI + CIns + GHGIns) \quad t = T \quad (4.34)$$

The following section defines the net earnings and total fixed cost investments. Thus, the total fixed cost investments of the production plant and energy generation unit are first explained as the following.

### **Total fixed cost investment**

#### **i. The fixed costs of the production plant**

The total fixed cost investment of the production plant, denoted by  $FCI$ , is determined by the production capacity and storage expansions plus the cost of transportation units utilized during the entire planned horizon.

$$FCI = \sum_p \sum_g \sum_t [\alpha_{p,g,t}^{Pr} \times NP_{p,g,t} + \beta_{p,g,t}^{Pr} \times PCapE_{p,g,t}] + \sum_s \sum_g \sum_t [\alpha_{s,g,t}^{St} \times NS_{s,g,t} + \beta_{s,g,t}^{St} \times SCapE_{s,g,t} \times PCapE_{p,g,t}] + \sum_l \sum_t TMC_{l,t} \times NT_{l,t} \quad (4.35)$$

Here, parameters  $\alpha_{p,g,t}^{Pr}$  and  $\beta_{p,g,t}^{Pr}$  are the fixed and variable investment coefficients for the production technologies and  $\alpha_{s,g,t}^{St}$  and  $\beta_{s,g,t}^{St}$  are the fixed and variable investment coefficients for the storage technologies. Additionally, the investment cost associated with the transportation mode  $l$  is denoted by  $TMC_{l,t}$ .

#### **ii. The fixed costs of the renewable energy installation**

$CIns$  and  $GHGIns$  are the fixed costs variables corresponding to the installation of the renewable energy resource, and consequent  $CO_2$  emissions. Eq. (4.36) and Eq. (4.37) define in the following:

$$CIns = PrPwI \sum_g PwI_g \quad (4.36)$$

$$GHGIns = GHGPr [\sum_g GHGPwI \times PwI_g + \sum_{e \in EX(e,x)} \sum_x \sum_g \sum_t [(PwXP_{e,x,g,t} + PwXS_{e,x,g,t}) \times GHGPw_x]] \quad (4.37)$$

Here,  $CO_2$  emissions caused by installation energy generation units are translated to monetary value and added to the installation costs. Hence, in Eq. (4.37),  $GHGPwI$  and  $GHGPr$  are the emission quantity and price per unit of power installed, respectively.

#### **iii. Total fixed costs constraint**

There is a limitation in the total capital investment, and defined by Eq. (4.38):

$$FCI + CIns + GHGIns \leq \overline{FIC} \quad (4.38)$$

### **Net earnings**

The difference between the revenues and operating costs defines the net earnings  $NE_t$ .

$$NE_t = (1 - \varphi)(Rev_t - FOC_t - TOC_t - COP_t - GHGCOP_t) + \varphi DEP_t \quad \forall t \quad (4.39)$$



Here, the operation costs consist of the production cost  $FOC_t$ , transportation cost  $TOC_t$ , energy generation cost  $COP_t$  and operational emission costs  $GHGCOP_t$  associated with a renewable resource.  $\varphi$  denotes the tax rate and  $DEP_t$  defines the depreciation term.

**a) Total revenue and depreciation**

$$Rev_t = \sum_{i \in SEP(i)} \sum_g DTS_{i,g,t} \times PR_{i,g,t} \quad \forall t \quad (4.40)$$

The revenues are the result of selling the final products with the corresponding prices to the on-demand regions.  $DTS_{i,g,t}$  is the final product amount delivered to region  $g$  with the selling price  $PR_{i,g,t}$ .

In Eq. (4.40),  $SEP(i)$  represents the set of the final products. The depreciation term is calculated with the straight-line method, similarly as (Mele et al., 2011) did in their work (Eq. (4.41)).

$$DEP_t = (1 - sv) \times TOTAL_t \quad \forall t \quad (4.41)$$

**b) The production operating costs**

The production operating costs  $FOC_t$  depend on the production rates and average inventory levels. The unit production and storage costs are denoted by  $UPC_{i,p,g,t}$  and  $USC_{i,s,g,t}$ , respectively.

$$FOC_t = \sum_i \sum_{p \in IM(i,p)} \sum_g UPC_{i,p,g,t} \times PE_{i,p,g,t} + \sum_i \sum_{s \in IS(i,s)} USC_{i,s,g,t} \times ALL_{i,g,t} + DC_t \quad \forall t \quad (4.42)$$

This term includes the disposal cost  $DC_t$  that is a function of the generated waste amount and landfill tax  $LT_{i,g,t}$  defined as the followings:

$$DC_t = \sum_i \sum_g W_{i,g,t} \times LT_{i,g,t} \quad \forall t \quad (4.43)$$

**c) The transportation costs**

The transportation cost, denoted by  $TOC_t$  includes the fuel cost  $FC_t$ , labor cost  $LC_t$ , maintenance cost  $MC_t$  and general costs ( $GC_t$ ) expressed in Eq. (4.44).

$$TOC_t = FC_t + LC_t + MC_t + GC_t \quad \forall t \quad (4.44)$$

The fuel cost depends on fuel consumption and its corresponding unit price  $FP_{l,t}$ . Eq. (4.45) defines the fuel consumption as below:

$$Fuel\ Usage_{i,l,g,g',t} = \frac{2EL_{g,g'}}{FE_l} \times \frac{Q_{i,l,g,g',t}}{TCap_l} \quad \forall i, l, g, g', t \quad (4.45)$$

Here,  $2EL_{g,g'}$  determines the total distance traveled in a trip, and  $FE_l$  indicates the fuel consumption of each transportation mode  $l$ . The material flow rate  $Q_{i,l,g,g',t}$  obtains the number of trips consequently made in each period, dividing into the capacity of the transportation mode  $l$  ( $TCap_l$ ). Thereupon, the total fuel cost in each period is as the following:

$$FC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l Fuel\ Usage_{i,l,g,g',t} \times FP_{l,t} \quad \forall t \quad (4.46)$$

Note that Eq. (4.46) considers that the transportation units operate only between two predefined regions.

The labor transportation cost  $LC_t$  is a function of the driver wage  $DW_{l,t}$  and total delivery time ( $Total\ Delivery\ time_{i,l,g,g',t}$ ) that is defined as below:

$$Total\ Delivery\ time_{i,l,g,g',t} = \frac{Q_{i,l,g,g',t}}{TCap_l} \left( \frac{2EL_{g,g'}}{SP_l} + LUT_l \right) \quad \forall i, l, g, g', t \quad (4.47)$$

Here,  $SP_l$  and  $LUT_l$  represent the average speed and loading/unloading time of transportation mode  $l$ , respectively. Therefore, the labor cost  $LC_t$  is defined as the following:

$$LC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l Total\ Delivery\ Time_{i,l,g,g',t} \times DW_{l,t} \quad \forall t \quad (4.48)$$

The general maintenance cost of the transportation systems depends on the total distance driven and the unit cost of the traveled distance  $ME_l$ .

$$MC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l \frac{Q_{i,l,g,g',t}}{TCap_l} \times 2EL_{g,g'} \times ME_l \quad \forall t \quad (4.49)$$

Finally, in this part, the general costs include transportation insurance, license, registration, and finances. Therefore, the general expenses  $GE_{l,t}$  and the average number of transportation units  $NT_{l,t}$  define general costs  $GC_t$  as below:

$$GC_t = \sum_l \sum_{t' \leq t} GE_{l,t'} \times NT_{l,t'} \quad \forall t \quad (4.50)$$

Note that the transportation costs basely depend on the average number of transportation modes required. Hence, it is calculated from the total delivery time (obtained by Eq. (4.47)), divided by the transportation availability  $avl_l$ , stated in Eq. (4.51):

$$\sum_{t' \leq t} NT_{l,t'} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \frac{Total\ Delivery\ time_{i,l,g,g',t}}{avl_l} \quad \forall l \quad (4.51)$$

#### a) The operation costs of renewable energy resource

The operation costs of energy generation units consist of energy generation costs and purchased energy imported from external resources.

$$COP_t = \sum_e \sum_g PrEnI_e \times EnIG_{e,g,t} + \sum_{e \in EX(e,x)} \sum_x \sum_g [PrEnP_{e,x} \times EnXP_{e,x,g,t} - PrEnS_{e,x} \times EnXS_{e,x,t}] \quad \forall t \quad (4.52)$$

Here,  $GHGCOP_t$  is the cost of  $CO_2$  emissions caused by operating the energy generation unit added to the operational costs.

$$GHGCOP_t = GHGPr \left[ \sum_e \sum_g GHGenI_e \times EnIG_{e,g,t} + \sum_{e \in EX(e,x)} \sum_x GHGenX_{e,x} \times EnXP_{e,x,g,t} \right] \quad \forall t \quad (4.53)$$

Note that Eq. (4.54) defines the allowable emissions amount for the entire horizon.

$$GHGPwl \sum_g Pwl_g + \sum_e \sum_g GHGenI_e \times EnIG_{e,g,t} \leq GHGMax \quad \forall t \quad (4.54)$$

#### 4.3.3.2. Environmental objective

In addition to the economic objective of maximizing the net present value (NPV), the MILP model is integrated with LCA. As per ISO 14040:2006, Life Cycle Assessment (LCA) includes 4 phases; the goal and scope definition, inventory analysis, impact assessment, and interpretation. These phases have been done by (Mele et al., 2011), and this thesis applies their results. Hence, based on their work, the environmental objective is to minimize the total annual  $CO_2$ -equivalent GHG emissions resulting from the supply chain operation, i.e., the feedstock production and provision,

the manufacturing and storage processes, and the transportation between regions. Mathematically, the emissions inventory due to the network is a function of some continuous variables. The production rate  $PE_{i,p,g,t}$  particularly calculates the entries of the life cycle inventory and the transportation flow  $Q_{i,l,g,g',t}$  as stated in Eq. (4.55) to (4.57):

$$GWPCul = \omega_i^{PU} \sum_i \sum_g \sum_t PU_{i,g,t} \quad (4.55)$$

$$GWPPr = \sum_i \sum_p \sum_g \sum_t \omega_p^{Pr} \times PE_{i,p,g,t} \quad (4.56)$$

$$GWPQ = \sum_i \sum_l \sum_g \sum_{g'} \sum_t \omega_l^{Tr} \times EL_{g,g'} \times Q_{i,l,g,g',t} \quad (4.57)$$

$\omega_i^{PU}$ ,  $\omega_p^{Pr}$ , and  $\omega_l^{Tr}$  represent the heat absorbed by any greenhouse gas (as a multiple of the heat that the same mass of carbon dioxide would absorb) in the atmosphere by the feedstock production, the products operations, and material transportation process, respectively. The environmental impact, as an objective function, is defined by the variable  $DAM$  as an environmental metric to be minimized.

$$DAM = GWPCul + GWPPr + GWPQ \quad (4.58)$$

#### 4.3.3.3. Multi-objective equations

The mathematical model presented herein capitalizes on the mixed-integer linear programming (MILP) formulation and seeks to optimize simultaneously the NPV and DAM objectives described in the bi-dimensional objective function as represented in model  $M$ . The overall bi-MILP formulation can briefly be expressed as follow:

$$(M) \quad \min_{x,X,N} \{-NPV(x,X,N); DAM(x,X,N)\}$$

s.t. constraints (4.1)-(4.58)

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

Here,  $x$  represents the continuous variables such as capacities, production rates, inventory levels, and materials flows,  $X$  denotes the binary variables (i.e., the transportation links), and  $N$  refers to the integer variables like the number of plants, storage facilities, and transportation units of each selected mode.

A set of Pareto consists of solution alternatives representing the optimal trade-off between the objectives considered in the problem. In this thesis, the  $\varepsilon$ -constraint method (Ehrgott, 2005) determines the Pareto set of solutions, which involves solving a set of instances the single-objective problem M1 for different values of the auxiliary parameter  $\varepsilon$  :

$$(M1) \quad \min_{x,X,N} \{-NPV(x,X,N)\}$$

s.t. constraints (4.1)-(4.58)

$$DAM(x,X,N) \leq \varepsilon$$

$$\underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon}$$

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

where the lower and upper limits are obtained from the optimization of each scalar objective separately:

$$(M1a) \quad (\bar{x}, \bar{X}, \bar{N}) = \arg \min_{x, X, N} \{DAM(x, X, N)\}$$

s.t. constraints (4.1)-(4.58)

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

which defines the lower bound of the epsilon parameter, i.e.  $\underline{\varepsilon} = DAM(\bar{x}, \bar{X}, \bar{N})$  and

$$(M1b) \quad (\hat{x}, \hat{X}, \hat{N}) = \arg \min_{x, X, N} \{-NPV(x, X, N)\}$$

s.t. constraints (4.1)-(4.58)

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

defines the upper bound of the epsilon parameter, i.e.  $\bar{\varepsilon} = DAM(\hat{x}, \hat{X}, \hat{N})$ . Note that the proposed model in this chapter is an extension of Mele et al., (2011) contribution equations regarding production by adding the energy section. It leads to amplify solutions borders and create more opportunities to make more flexible decisions.

#### 4.4. Case Study: Retrofitting of integrated Sugar-bioethanol SCs

The proposed formulation is validated through its application to a retrofitting problem of SSCM based on the sugarcane industry. Comparing to different types of crops such as maize/corn, the advantage of sugarcane is that it can be readily integrated with cogeneration at a large scale (see Fig. 4.2.).

The problem addressed explores the optimal retrofitting and configuration of the sugar/ethanol production plants integrated with the cogeneration power plants. It is assumed a five-year time horizon (with yearly discretization). The current problem follows the same geographical and production data assumptions as in a former study with a similar case study (Mele et al., 2011).

The sugarcane industry has been selected as a case study due to the high energy cost while it has a high potential for exploiting renewable agricultural residues. Despite other crops such as corn/maize, sugarcane can readily integrate with cogeneration at a large scale. According to the ISO report (International Sugar Organization), sugar mills are generally involved in excess power generation that can market to the grid and contribute to the country's energy mix. While the energy demand is increasing worldwide, specifically in developing countries, exploring the sugar industry's energy generation potential can be considered an alternative energy supplier.

The following attributes identify conventional utility in sugar mills/ethanol distillery plants: Low pressure (20 to 30 bars)-low temperature (300 to 400°C) boilers. Back-pressure turbines (BPT) to provide steam to the mechanical equipment that in average produce 30-34 t steam/h (1kWh is

equal to 0.284 t steam/h) (Bocci, Di Carlo, & Marcelo, 2009), while the energy consumption in the sugar plant is an internal heat demand of 480–550 kg steam/t cane and approximately 16 to 22 kWh electricity (Birru, Erlich, & Martin, 2019).

The sugarcane industry of Argentina (as a developing country) is selected. According to the Foreign Agricultural Service report ("Argentina: Sugar Annual | USDA Foreign Agricultural Service," 2020), the sugar production for the marketing year (MY) 2020/21 is forecasted at 1.8 million tons (raw value), a moderate increase from last year on stable acreage while it is forecasted to produce 21.7 million tons of net sugar cane, equal to 24 million tons of gross sugar cane (including bagasse).

Here is a country-size case study, and the geographic scope of the problem has been defined based on the country's administrative divisions. Therefore, it has been considered 24 provinces with an associated sugar and ethanol demand. Data and additional parameter values employed in the analysis are provided in Appendix section B.1.

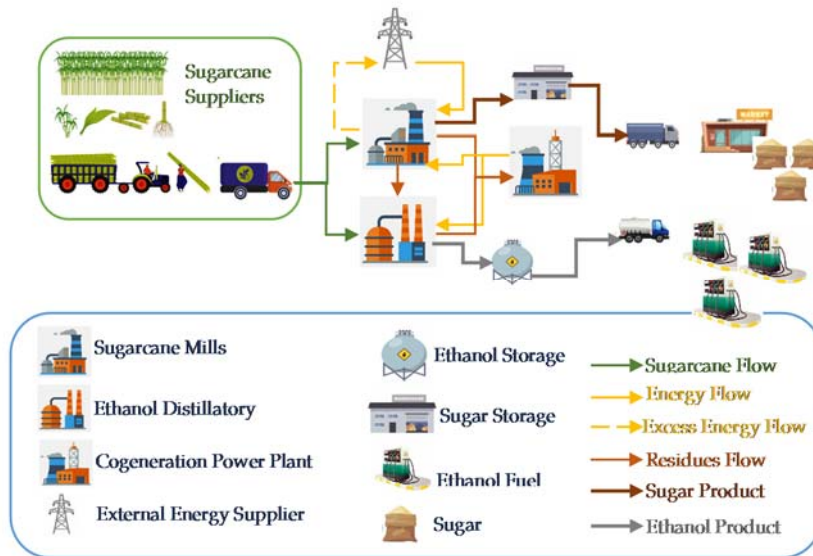


Fig. 4. 2. Sugar/Ethanol SC Network with the integrated cogeneration power plant.

#### 4.4.1. Cogeneration power plant

Cogeneration plants are utility sections to respond to the need of process steam demand or/and power demand. In the sugarcane industry, steam is the base utility, and electrical power is a byproduct. Hence, the bagasse-based cogeneration plant has been considered as the single renewable energy generation to provide process steam and generate possible excess power.

##### 4.4.1.1. Modeling of cogeneration power plants

In this contribution, the cogeneration power plant is considered the integrated energy generation part and modeled based on (Illukpitiya, Yanagida, Ogoshi, & Uehara, 2013). Since sugarcane residues such as bagasse generate energy (heat and electricity), a cogeneration power plant can

be considered a renewable energy generator. Here,  $EnIG_{g,t}$  represents the energy that is generated in the cogeneration power plant.

$$EnIG_{g,t} = P_{eg} \times SL \times W_{i,g,t} \quad \forall i, g, t \quad (4.59)$$

where  $P_{eg}$  denotes the power generated by the cogeneration per ton of biomass; its quantity depends on the cogeneration thermodynamic and design data. Hence, in the following, the cogeneration plant adopted to the general model is introduced.

#### Anderson Power Cycle

While the energy provided by conventional technologies is limited to the crushing season, the Anderson power cycle with the back-pressure turbine lets the sugar/distillery complex send power to the grid all year round. Besides, conventional technologies suffer from the lack of ability to provide zero pollution. By adopting Anderson flue gas coolers, the wasted heat in flue gases is wholly recovered and cleaned. Also, a multi-effect evaporator can evaporate distillery spent-wash, and the concentrated effluent is burnt in a boiler with the bagasse to generate more power (Kamate & Gangavati, 2009).

In this line, several innovative biomass-based carbon-negative power generation systems have been developed during recent decades. (Yan, Wang, Wang, Cao, & He, 2021) have compared three biomass-based carbon-negative power generation systems. These three models are validated thermodynamically and economically (see Table. 4.1.).

Table. 4. 1. Thermodynamic and economic data of Bioenergy models.

	Efficiency %	Electric costs \$/kWh	CO <sub>2</sub> mitigations kg/kWh
BFPP	30.7	0.0584	0.943
BIGCC	44.5	0.0497	0.629
BIGFC	50.5	0.0493	0.567

Regarding the system retrofitting strategies and have more efficient and adaptable to the sugarcane industry, the industries have replaced biomass integrated gasification with fuel cells (BIGFC) power plant with the conventional gas turbine. The advantages of utilizing the BIGFC, studied by (Lobachyov & Richter, 1998), are as below:

- A simple feeding system and non-required pressurized vessels;
- Being functional at low pressures;
- No need for an additional gas cooler nor a high calorific value gas;

Molten carbonate fuel cells (MCFC) are the more convenient technological choice because of the following reasons (Bocci et al., 2009):

- Allowable use of carbon monoxide and hydrogen;
- Possibility to reform the remaining hydrocarbons;

- Possibility of using the anode-exhausted gas and the outgoing cathode gas (mainly contains CO<sub>2</sub>) as fuel for the combustion chamber;
- Contribution of high-temperature heat to generate the steam for gasification chamber, sugar production, and a combined steam cycle;

The BIGFC plant, showed in Fig. 4.3., consists of an atmospheric pressure indirectly heated fluidized bed gasifier, hot gas conditioning system, and MCFC power generation unit.

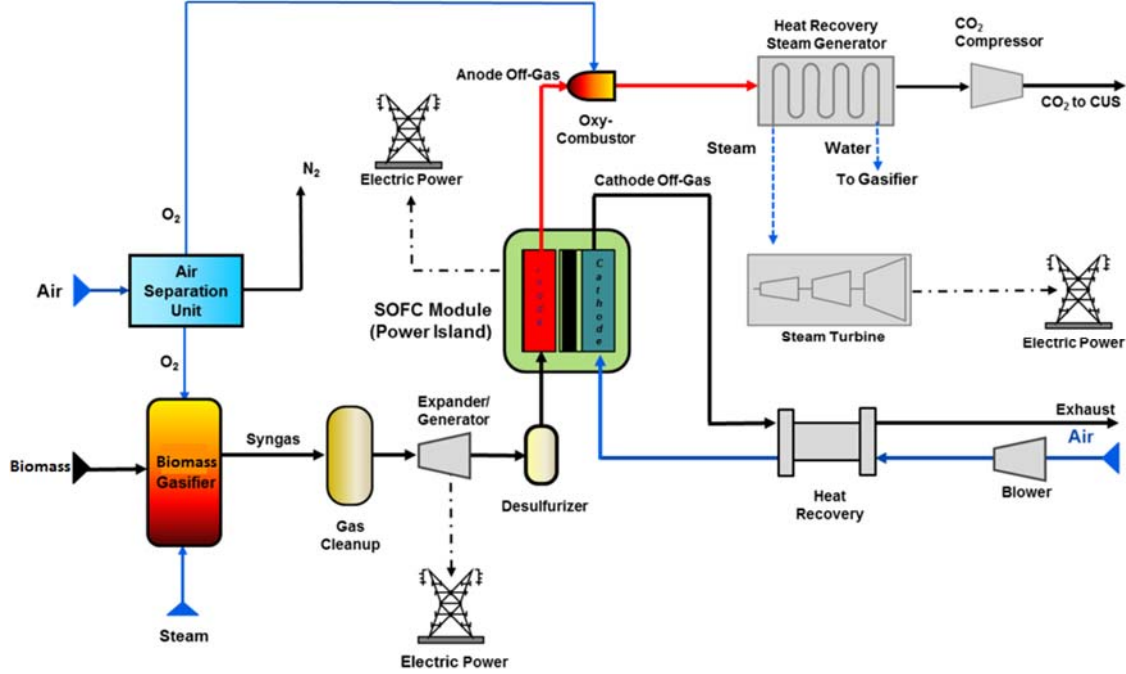


Fig. 4. 3. Simplified Process Diagram of Integrated Gasification Fuel Cell Power Cycle at Atmospheric Pressure ("Integrated gasification fuel cell cycle - Wikiwand").

The overall energy efficiency of the plant is measured based on the net amount of electric power generated per unit of biomass (Yan et al., 2021):

$$\eta = \frac{\sum P_{eg} - \sum P_{ec}}{m_{bio}LHV} \quad (4.60)$$

Where,  $P_{eg}$  and  $P_{ec}$  are the power generated and consumed, respectively.  $m_{bio}$  is the biomass flow rate, and  $LHV$  is the lower heating value of the material in its original form(including ash and moisture). The electric power generated  $P_{eg}$  is calculated using the following equation(Bocci et al., 2009):

$$P_{eg} = m_g c_p (T_3 - T_2) \eta_t \eta_{mT} \eta_{aux} \eta_{alt} \quad (4.61)$$

Where  $m_g$  represents the mass flow rate of the gas (the gasifier efficiency is assumed 90%);  $c_p$  is specific heat;  $\eta_t$ ,  $\eta_{mT}$ ,  $\eta_{aux}$  and  $\eta_{alt}$  are efficiencies related to the turbine. This contribution has chosen the Direct Brayton cycle as the thermodynamic cycle, and the turbine thermodynamic efficiency equation is as below (Bocci et al., 2009):

$$\eta_t = \frac{(h_3 - h_4) - (h_2 - h_1)}{h_3 - h_2} \quad (4.62)$$

By MCFC overall efficiency 40% (gasifier efficiency of 90%), the heat balance proposed by (Lobachyov & Richter, 1998) and using Design parameters are provided in Appendix section B.1 (Table. B.1), global power of 50 MW with an electricity efficiency of 41% is obtained. Assumed nominal capacity of the power plant is 8.33 MW. The power generation is available continuously for at least 7800 h annually (Illukpitiya et al., 2013). Thermal consumptions are assumed 307 kWh/t and, the estimated total electricity requirement for internal use in the processing plants is 45 kWh per t of cane (Bocci et al., 2009; Illukpitiya et al., 2013).

The model optimizes the retrofitting of the SC network. For comparison purposes, the problem is first solved following a standard MOO approach and then compared to the basic model proposed by (Mele et al., 2011) to illustrate its advantages.

#### 4.5. Multi-Objective solving approach

This contribution has used the  $\epsilon$ -constraint method to produce a set of Pareto solutions in the space of the two original objectives, NPV and DAM (Ehrgott, 2005). MO-MILP form of the model (M), implemented in GAMS 28.2.0 and solved CPLEX 12.4 on a Windows XP computer with Intel® Core™ i7-3770 CPU (920) 3.90GHz processor with 8.00GB of RAM. It takes approximately 1200 seconds to identify the global optimum in every instance. The solver generated 12 Pareto points, as shown in Fig. 4.4, including nadir and utopia points.

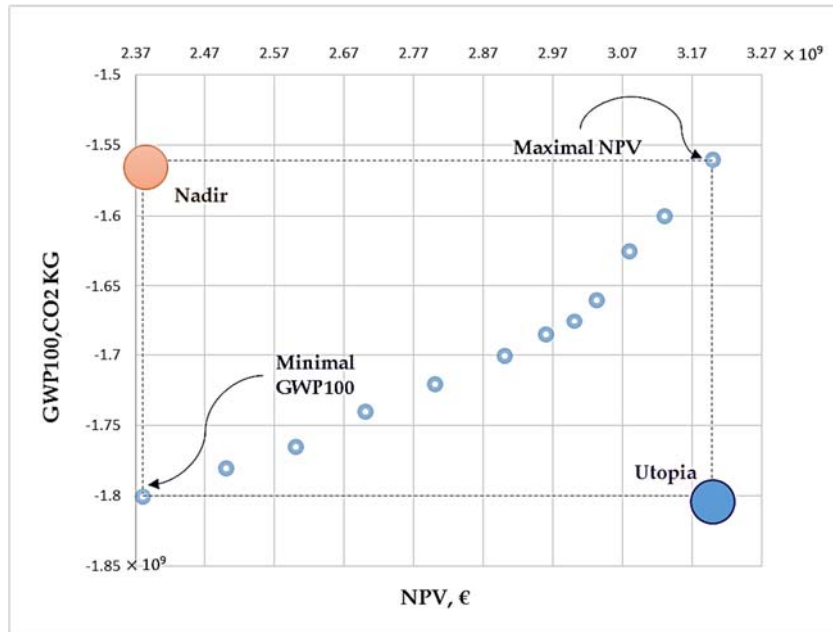


Fig. 4. 4. Pareto set of solutions NPV vs. GWP100.

In general, Fig. 4.4 depicts that the amount of  $CO_2$  decreases at the expense of compromising the NPV performance. Within the  $GWP100, CO_2$  range, the NPV varies about  $\text{€}8.20 \times 10^8$  (increases from  $\text{€}2.380 \times 10^9$  to  $\text{€}3.20 \times 10^9$ ), whereas GWP100 drops  $2.40 \times 10^8 CO_2 kg$  (from  $1.56 \times$



$10^9 CO_2 \text{ kg}$  to  $1.80 \times 10^9 CO_2 \text{ kg}$ ). The previous work (Morakabatchiankar, Hjaila, Graells, & Espuña, 2017) discussed the extreme solutions. In effect, to obtain the optimum environmental impact and economic benefit, it is required to retrofit the sugar plants of 5 regions (regions with sugarcane plantations) with the cogeneration power plants (upper bound according to the problem formulation) in the **maximal NPV** solution, whereas, the **minimal GWP100** up to 9 regions, can be retrofitted with the cogeneration power plants. Table 4.2 mentions the design solutions for both extreme cases.

Table. 4. 2. Output data for the two extreme solutions.

	NPV, €	GWP100, $CO_2, \text{kg}$	Retrofitted Regions	Non Retrofitted Regions	Distillery Production Technology	Sugar Mill Production Technology
<b>Maximal NPV</b>	$3.20 \times 10^9$	$-1.56 \times 10^9$	5	4	T3, T4	T1, T2
<b>Minimal GWP100</b>	$2.380 \times 10^9$	$-1.8 \times 10^9$	9	0	T3, T4, T5	T1, T2

Comparing to the base model (the model without considering cogeneration units), the extended model has resulted in a more expanded solution area. Mathematically, changing the boundaries of the constraints increases the opportunity of finding more optimum solutions. Fig. 4.5 illustrates the effect of retrofitting on the results. Note that in both GWP100 and the NPV, there is a broader range of solutions.

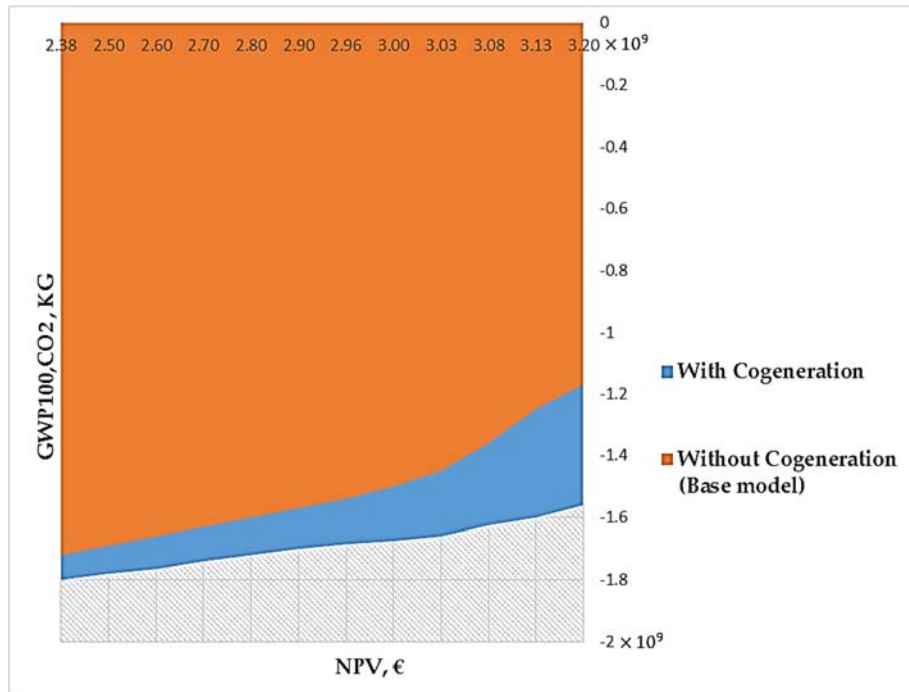


Fig. 4. 5. Solutions Area comparison between a network with and without cogeneration.

Analyzing the results approves that in the **minimal GWP100** case, integrating cogeneration technology with negative- $CO_2$  emissions decrease 4.65% in GWP100 at the same NPV ( $\text{€}2.380 \times 10^9$ ) comparing to the model without considering the cogeneration unit. It means that although

feeding residues (bagasse and distillery spent wash) to the cogeneration plant results in a 4% reduction in disposal costs in addition to the revenues obtained by selling excess electricity to the grid, there is a break-even point between the installation and operational costs and the revenue. Thus, the high transportation costs and many storage tanks/warehouses deteriorate the network performance in both the NPV and DAM objectives.

On the other extreme, evaluating the **maximal NPV** solution shows an improvement in the overall economic performance of the network compared to the non-retrofitted model. The NPV is increased by 3.6%. As mentioned before, the solution space (decision variables space) is loosened so that there are more possibilities to find more optimum solutions.

From the mathematical perspective, while the number of economic constraints is significantly more than environmental impact constraints, the DAM objective is minimized subjected to numerous operation and design constraints (i.e., the tight feasible solution space). On the other side, a limited number of environmental impact constraints and the economic objective are maximized with fewer constraints.

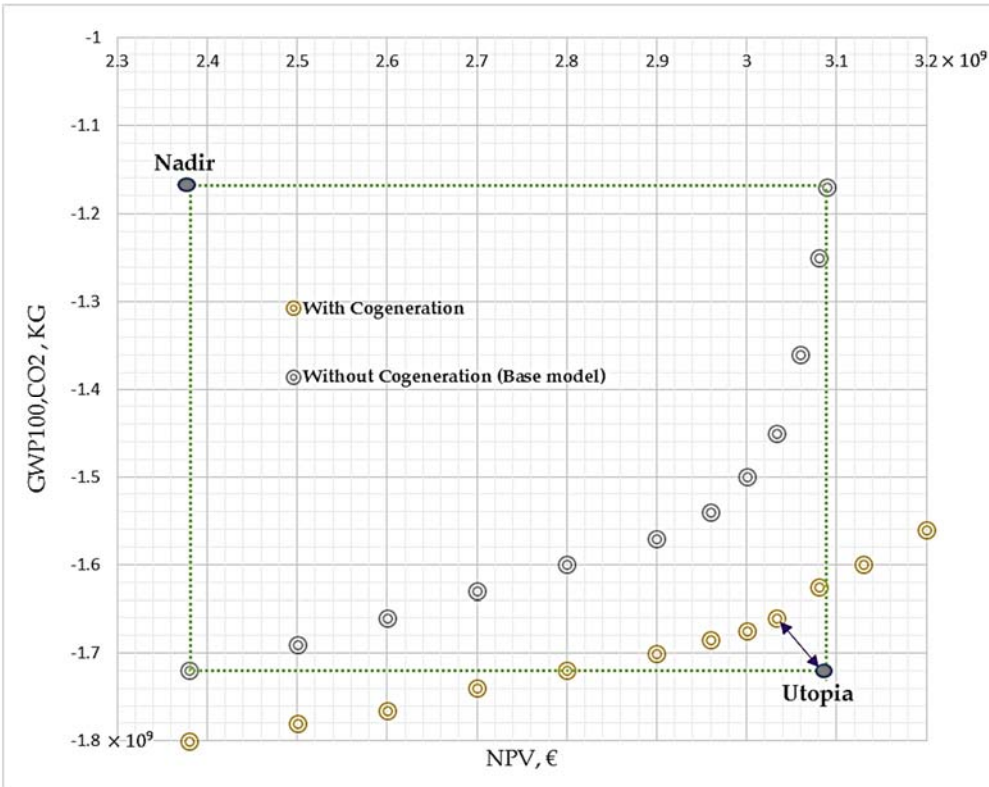


Fig. 4. 6. Pareto Sets of Solutions in two cases.

Nevertheless, the most important result is that all the solutions obtained by the extended model are in the Utopia zone of the base (non-retrofitted) model. The deduction is that, by retrofitting the base model, the possibility of achieving more optimum solutions will increase, particularly as pointed in the graph (see Fig. 4.6), the solution that has the minimum distance with the utopia

point can be considered a desirable one (at  $(NPV, GWP100) = (\text{€}3.03 \times 10^9, -1.66 \times 10^9 \text{ kg } CO_2)$ ) and this contribution considers it as a reference solution for comparison purposes.

The Maximum NPV solution attains  $\text{€}3.20 \times 10^6$  for the NPV and  $-1.56 \times 10^9 \text{ kg } CO_2$  for the DAM objective and 6% variation (in both the NPV and DAM) from the reference solution. Therefore, this point can also be another desirable solution for the decision-maker. The design configuration of the maximum NPV solution is visible in Fig. 4.7; the solution has classified the country regions into three main parts, the industrial regions with and without sugarcane plantations (5 and 4 provinces, respectively) and the nonindustrial ones. Both industrial regions contain sugar mills and distilleries, while the sugar mills and distilleries installed in regions with sugarcane plantations are retrofitted with cogeneration power plants. The network overall provides the required process energy, and the industry markets the excess to the grid. The feedstock availability and fewer transportation costs, and less carbon dioxide emissions cause a simultaneous improvement in economic and environmental impacts. The other industrial regions supply their required energy from the external resources, as is shown in the figure.

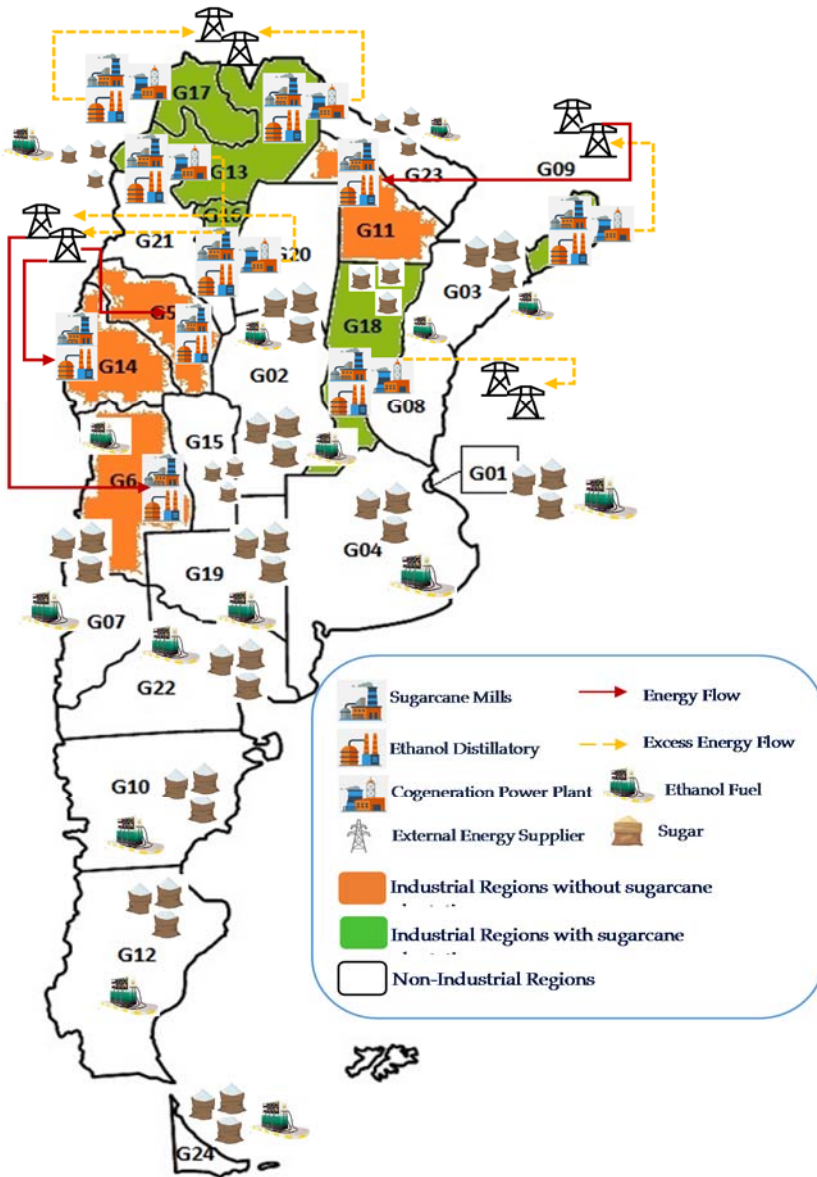


Fig. 4. 7. Configuration of solution with the maximum NPV value.

Comparing the optimum design of retrofitted and non-retrofitted network configurations (Maximal NPV in both cases) can highlight some differences. First, in retrofitted cases, the production process involves more regions, and more production technologies are in use. The production process diagram, including the associated technologies, is illustrated in Fig. 4.8. Five production technologies are corresponding to sugar and ethanol productions, while two technologies ( $T_1$  and  $T_2$ ) are available for producing raw and white sugar, three technologies ( $T_3$ ,  $T_4$ , and  $T_5$ ) are used to produced ethanol. In the non-retrofitted case, just one sugar production technology ( $T_1$  in minimal GWP100 and  $T_2$  in maximal NPV) is utilized, while the current contribution allows taking advantage of both technology types ( $T_1$ ,  $T_2$ ) in both optimum solutions. Similarly, in a non-retrofitted design, it is only used  $T_5$  in maximal NPV solution and

$T_3$  in minimal GWP100 solution to produce ethanol. However, in the retrofitted design, all three types of distillery technologies are utilized for producing bioethanol. Table 4.3 depicts more details about the number of industrial regions, technologies in use, and cogeneration capacity.

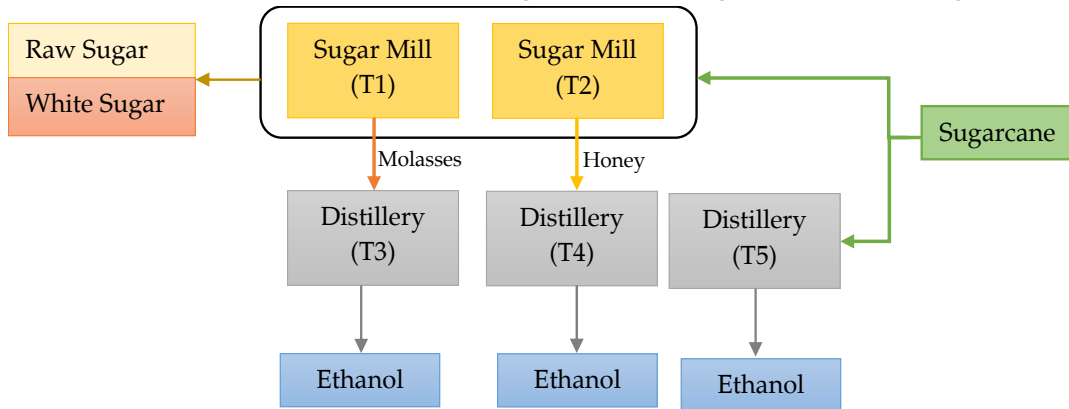


Fig. 4. 8. Schematic representation of the five production technologies.

As a result, integrating the alternative energy resources (cogeneration as a particular case) reduces the environmental impact at the expense of increasing the installation and operation costs. Fig. 4.9 illustrates the amount of  $CO_2$  emissions of each level of the network.

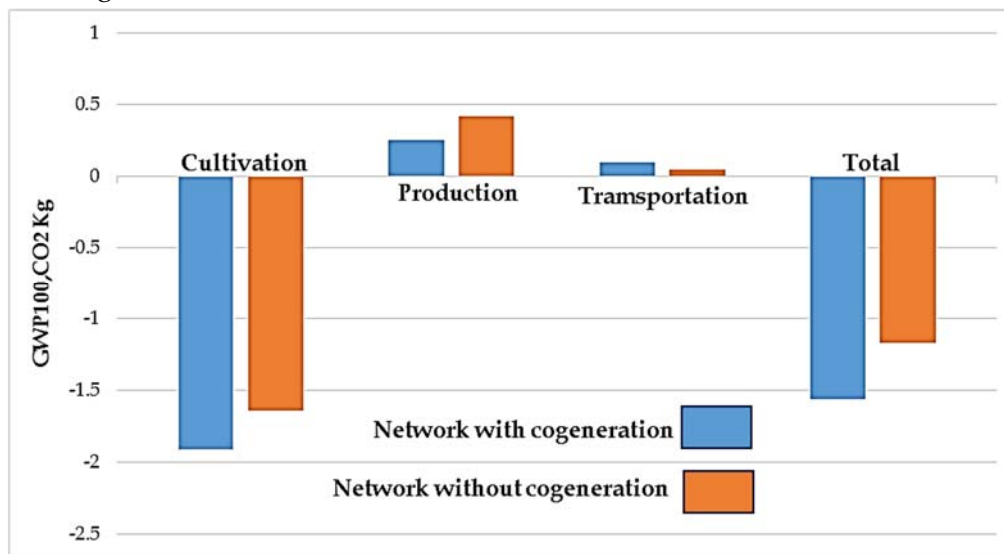




























Fig. 4. 9. Contribution of different SC stages to the GWP100 for the non-retrofitted and retrofitted networks in Maximal NPV.

It shows the contribution of each source of impact (i.e., cultivation, production, and transportation) to the GWP100 for the Maximal NPV among Pareto solutions. The cultivation of sugar cane shows in both cases an immense contribution to the total impact. Note that sugar cane cultivation has a considerable negative GWP100 that offsets the positive impacts of transportation and production tasks. Hence, in minimal GWP100 design, retrofitted regions are confined to those with the sugarcane plantations. In this way, fewer transportations happen that leads to  $CO_2$

emissions reduction. Besides, the energy generated in this case is enough to supply internal energy demand, so that it is not required to purchase it from external resources. Note that the integrated cogeneration in the process industry reduces  $CO_2$  emissions while the utilized cogeneration is  $CO_2$  negative technology. Study the effects of carbon dioxide-negative is out of the scope of this thesis.

Table. 4. 3. Comparing optimum design network configurations for non-retrofitted and retrofitted cases.

Region	Non-retrofitted Case		Retrofitted Case	
	Max NPV (€)	Min GWP100 (kgCO <sub>2</sub> )	Max NPV (€)	Min GWP100 (kgCO <sub>2</sub> )
	$3.09 \times 10^9$	$-1.56 \times 10^9$	$3.2 \times 10^9$	$-1.8 \times 10^9$
Region	Technology		Technology/cogeneration	
La Rioja ( $g_5$ )	-	-	 $T_1, T_2, T_3, T_4$	 $T_1, T_2, T_3, T_5$ 50MW
Mendoza ( $g_6$ )	-	-	 $T_1, T_2, T_3, T_4$	 $T_1, T_2, T_3, T_5$ 50MW
Misiones ( $g_9$ )	-	 $T_1, T_3$	 $T_1, T_2, T_3, T_4$ 50MW	 $T_1, T_2, T_3, T_5$ 50MW
Chaco ( $g_{11}$ )	-	-	 $T_1, T_2, T_3, T_4$	 $T_3, T_5$ 50MW
Salta ( $g_{13}$ )	 $T_5$	 $T_1, T_3, T_5$	 $T_1, T_2, T_3, T_4$ 50MW	 $T_1, T_2, T_3, T_5$ 50MW
San Juan ( $g_{14}$ )	-	-	 $T_3, T_5$	 $T_3, T_5$ 50MW
Tucumán ( $g_{16}$ )	 $T_2, T_4, T_5$	 $T_1, T_3, T_5$	 $T_1, T_2, T_3, T_4$ 50MW	 $T_1, T_2, T_3, T_5$ 50MW
Jujuy ( $g_{17}$ )	 $T_5$	 $T_1, T_2, T_5$	 $T_1, T_2, T_3, T_4$ 50MW	 $T_1, T_2, T_3, T_5$ 50MW
Santa Fe ( $g_{18}$ )	-	 $T_1, T_3, T_5$	 $T_1, T_2, T_3, T_4$ 50MW	 $T_1, T_2, T_3, T_5$ 50MW



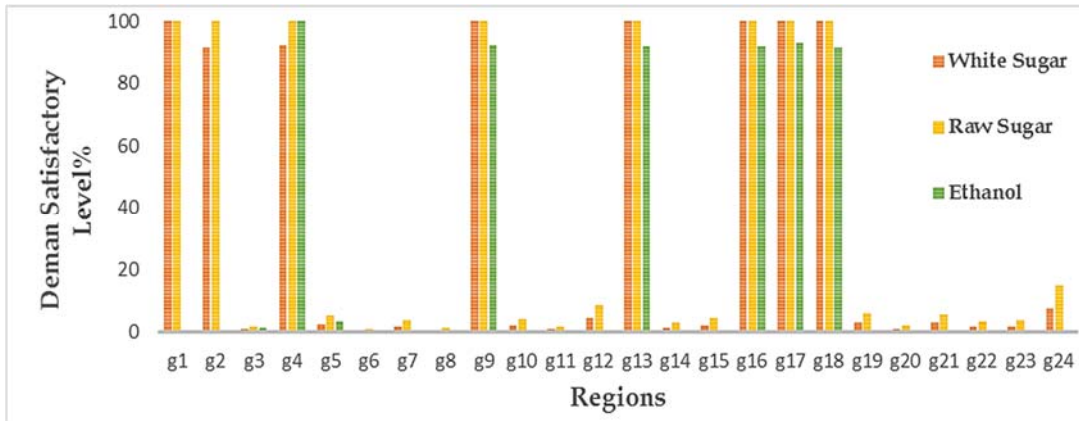


Fig. 4. 10. Demand satisfaction level associated with the maximum NPV solution.

It results in an approximate enhancement of 30% in production capacity reflected in satisfactory demand level as shown in Fig. 4.10. It means, in this case, more demand sites are covered comparing to the non-retrofitted network.

#### 4.6. Concluding remarks

A MILP model addressing the SC retrofitting in the process industry was presented, whose main contribution is to propose a novel model applicable for integrated energy/material SC networks to obtain optimal solutions. The problem is formulated as a bi-criterion MILP that simultaneously optimizes the network's NPV and environmental impact performance. The environmental impact was measured over the entire life cycle of the process by applying two LCA-based methodologies. The capabilities of the proposed model were validated through the retrofitting of a large-scale SC management system on a country-size problem (sugar/distillery industry in Argentina). The case study accounts for a bio-based cogeneration power plant to satisfy internal energy demand and possibly sell the excess to the external market (the grid). Notably, the results have clearly shown how significant environmental and economic benefits can be attained by adequately retrofitting the process industry.

Numerical results show that in the retrofitted network, the  $CO_2$  emissions amount is reduced notably along with an improvement in the economic performance of the system. Altogether, the identified solutions indicate an improvement in the economic objective, NPV, and a reduction in environmental impacts, reinforcing the idea that utilizing more energy resource alternatives are promising and feasible options to reduce the expenses of purchasing energy from external resources.

This chapter provided valuable insight into the strategic and tactical decision-making of sustainable production and bioenergy generation supply chains.

## 4.7. Nomenclature

### Abbreviations

BFPP	Biomass-Fired Power Plant
BIGCC	Biomass-Fueled Integrated Gasification Combined Cycle
BIGFC	Biomass Integrated Gasification with Fuel Cells
BPT	Back Pressure Turbine
GHG	Greenhouse Gas
LCA	Life Cycle Assessment
MCFC	Molten Carbonate Fuel Cells
MILP	Mixed Integer Linear Programming
MOO	Multi-Objective Optimization
NPV	Net Present Value
PSE	Process System Engineering
SC	Supply Chain
SSC	Sustainable Supply Chain
SSCM	Sustainable Supply Chain Management

### Index

$e$	Set for Energy types ( $e e = 1, \dots, E$ )
$g$	Set for Regions ( $g g = 1, \dots, G$ )
$i$	Set for Material types ( $i i = 1, \dots, I$ )
$l$	Set for Transportation modes ( $l l = 1, \dots, L$ )
$p$	Set for Production technologies ( $p p = 1, \dots, P$ )
$s$	Set for Storage technologies ( $s s = 1, \dots, S$ )
$t$	Set for Planning periods ( $t t = 1, \dots, T$ )
$x$	Set for External energy suppliers ( $x x = 1, \dots, X$ )

### Sets

EX( $e, x$ )	Subset of ordered pairs that link energy types $e$ to external resource $x$
IL( $i, l$ )	Subset of ordered pairs that link materials $i$ to transport modes $l$
IM( $i, p$ )	Subset of ordered pairs that link main products $i$ to technologies $p$
IS( $i, s$ )	Subset of ordered pairs that link materials $i$ to storage technologies $s$
SEP( $i$ )	Subset of final products $i$

### Parameters

$\alpha_{p,g,t}^{Pr}$	Fixed investment coefficient for technology $p$
$\alpha_{s,g,t}^{St}$	Fixed investment coefficient for storage technology $s$
$\beta_{p,g,t}^{Pr}$	Variable investment coefficient for production technology $p$
$\beta_{s,g,t}^{St}$	Variable investment coefficient for storage technology $s$
$\varepsilon$	Auxiliary boundary for the $\varepsilon$ -constraint method
$\rho_{p,i}$	Material balance coefficient associated with material $i$ and technology $p$
$\eta$	Net cogeneration efficiency



$\eta_{alt}$	Alternator efficiency
$\eta_{aux}$	Auxiliary devices (pumps, cooling towers, and other components) efficiency
$\eta_{mT}$	Mechanical turbine efficiency
$\eta_t$	Turbine thermodynamic efficiency
$\sigma$	Storage period
$\tau$	Minimum desired percentage of the available installed capacity
$\varphi$	Tax rate
$\omega_p^{Pr}$	Life cycle environmental burden associated with production technology $p$
$\omega_i^{PU}$	Life cycle environmental burden associated with purchasing material $i$
$\omega_l^{Tr}$	Life cycle environmental burden associated with transportation mode $l$
$avl_l$	Availability of transportation mode $l$
$CapCrop_{g,t}$	Total capacity of raw material production (sugar cane plantations) in region $g$ in period $t$
$c_p$	specific heat
$Demand_{g,t}$	energy demand needed per unit of raw material $i$
$DW_{l,t}$	Driver wage of transportation mode $l$ in period $t$
$EfIJ_e$	Conversion efficiency between internal energy resource type $e$ and the process plant $i$
$EfIX_{e,x}$	Conversion efficiency of the excess energy type $e$ sent to the external energy generation resource $x$
$EfXJ_{e,x}$	Conversion efficiency between external resource $x$ energy type $e$ and the process plant $i$
$EL_{g,g'}$	Distance between $g$ and $g'$
$\overline{FIC}$	Upper limit on the capital investment
$FE_l$	Fuel consumption of transportation mode $l$
$FP_{l,t}$	Fuel Price of transportation mode $l$ in period $t$
$GE_{l,t}$	General expenses of transportation mode $l$ in period $t$
$GHGEnI_e$	Emissions per unit of energy generated for each type $e$
$GHGMax$	Maximum allowable emissions amount
$GHGPr$	Price of GHG emissions $kg CO_2$ equivalent
$GHGPwl$	Emissions per unit of power
$h$	Enthalpy
$ir$	Interest rate
$LHV$	Lower heating value
$LT_{i,g,t}$	Landfill tax in period $t$
$LUT_l$	Loading/unloading time of transportation mode $l$
$m_{bio}$	Biomass flow rate
$m_g$	Mass flow rate of the gas
$ME_l$	Maintenance expenses of transportation mode $l$
$MinPgCO$	Minimum power generation coefficient
$P_{ec}$	power consumed inside the production process

$P_{eg}$	Power generated by the cogeneration per ton of biomass
$\overline{PCap}_p$	Maximum capacity of technology $p$
$\underline{PCap}_p$	Minimum capacity of technology $p$
$PR_{i,g,t}$	Prices of final products $i$
$PrEnI_e$	Price of energy type $e$
$PrEnP_{e,x}$	Purchase price of external energy type $e$ source $x$
$PrEnS_{e,x}$	Selling price of energy type $e$ to external source $x$
$PrPwI$	Installation power cost
$PwIMax$	the maximum power to be installed
$\overline{Q}_l$	Maximum capacity of transportation mode $l$
$\underline{Q}_l$	Minimum capacity of transportation mode $l$
$\overline{SCap}_s$	Maximum capacity of storage technology $s$
$\underline{SCap}_s$	Minimum capacity of storage technology $s$
$SD_{i,g,t}$	Demand of product $i$ in region $g$ in period $t$
$SL$	Slot length
$SP_l$	Average speed of transportation mode $l$
$SurfPwI$	Surface occupied per unit power
$SurfTMax$	Maximum available surface
$sv$	Salvage value
$T$	Number of time intervals
$TCap_l$	Capacity of transportation mode $l$
$TMC_{l,t}$	Cost of establishing transportation mode $l$ in period $t$
$UPC_{i,p,g,t}$	Unit production cost of product $i$ in region $g$ in period $t$
$USC_{i,s,g,t}$	unit storage cost of product $i$ in region $g$ in period $t$
<b>Variables</b>	
$AIL_{i,g,t}$	Average inventory level of product $i$ in region $g$ in period $t$
$CF_t$	Cash flow in period $t$
$CIns$	Total cost of installation of all renewable power plants
$COP_t$	Operation cost of all renewable power plants in period $t$
$DAM$	Environmental metric to be optimized
$DC_t$	Disposal cost in period $t$
$DEP_t$	Depreciation in period $t$
$DTS_{i,g,t}$	Amount of material $i$ delivered in region $g$ and period $t$
$EnIG_{e,g,t}$	Energy type $e$ generated in region $g$ and period $t$
$EnIJ_{e,g,t}$	Energy flux type $e$ between renewable source and demand of region $g$ in period $t$
$EnIX_{e,x,g,t}$	Energy flux type $e$ between renewable source and external source $x$ region $g$ in period $t$
$EnXJ_{e,x,g,t}$	Energy flux type $e$ between external source $x$ and demand of region $g$ in period $t$
$EnXP_{e,x,g,t}$	Energy type $e$ purchased from external source $x$ in period $t$
$EnXS_{e,x,g,t}$	Energy type $e$ sales to external source $x$ in period $t$
$FC_t$	Fuel cost in period $t$
$FCI$	Fixed capital investment

$FOC_t$	Facility operating cost in period $t$
$Fuel\ Usage_{i,l,g,g',t}$	Fuel consumption for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$
$GC_t$	General cost in period $t$
$GHGCOP_t$	Total GHG operational emissions $kg\ CO_2$ equivalent in period $t$
$GHGIns$	Total GHG Installation emissions $kg\ CO_2$ equivalent for all renewable power plants
$GWPCul$	GWP100 amount in the cultivation process
$GWPPr$	GWP100 amount in the production process
$GWPPQ$	GWP100 amount in the transportation process
$LC_t$	Labor cost in period $t$
$MC_t$	Maintenance cost in period $t$
$NE_t$	Net earnings in period $t$
$NPV$	Net Present Value
$NP_{p,g,t}$	Number of plants with technology $p$ established in region $g$ and period $t$
$NS_{s,g,t}$	Number of storages with storage technology $s$ established in region $g$ and period $t$
$NT_{l,t}$	Number of transportation units $l$ in period $t$
$PE_{i,p,g,t}$	Production rate of material $i$ associated with technology $p$ established in region $g$ and period $t$
$PCap_{p,g,t}$	Existing capacity of technology $p$ in region $g$ and period $t$
$PCapE_{p,g,t}$	Capacity expansion of technology $p$ in region $g$ and period $t$
$PT_{i,g,t}$	Total production rate of material $i$ in region $g$ and period $t$
$PU_{i,g,t}$	Purchases of material $i$ in region $g$ and period $t$
$PwI_g$	Power to install at own source in region $g$
$PwIG_{g,t}$	Power to generate by a renewable source, in each region $g$ , each period $t$
$PwIGMax_{g,t}$	Maximum power to generate by renewable source in each region $g$ and period $t$
$PwIGMin_{g,t}$	Minimum power to generate by renewable source in each region $g$ and period $t$
$PwXP_{e,x,g,t}$	Power purchased from external source $x$ in period $t$
$PwXS_{x,g,t}$	Power selling to external source $x$ in period $t$
$Q_{i,l,g,g',t}$	Flow rate of material $i$ transported by mode $l$ from region $g$ to region $g'$ in period $t$
$Rev_t$	Revenue in period $t$
$SCap_{s,g,t}$	Existing capacity of storage $s$ in region $g$ and period $t$
$SCapE_{s,g,t}$	Capacity expansion of storage $s$ in region $g$ and period $t$
$ST_{i,s,g,t}$	Total inventory of material $i$ in region $g$ stored by technology $s$ in period $t$
$TOC_t$	Transport operating cost in period $t$
$TOTAL_t$	total depreciable capital during period $t$
$Total\ Delivery\ time_{i,l,g,g',t}$	Delivery time for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$

Chapter 4. Simplified targeting models for SC retrofitting

$TotalDemand_{g,t}$

Energy demand of region  $g$  and period  $t$

$W_{i,g,t}$

Amount of wastes of  $i$  generated in region  $g$  and period  $t$

**Binary Variables**

$Gn_{g,t}$

Per the Big-M method, the local binary variable to define lower and higher generation limits

$X_{l,g,g',t}$

1 if a transportation link established between regions  $g$  and  $g'$ , otherwise 0

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## SC RETROFITTING UNDER UNCERTAINTY

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Regarding efficient management, the process sustainability depends on reducing the outsources contingency factors effects, which are subject to different variations, for instance, quality/quantity conditions of raw material resources, climatic conditions, and market demand. Analyzing the effects of these uncertain conditions is a serious challenge. It has to be addressed along with a multi-objective evaluation, seeking for the process sustainability. Therefore, there is a need for integrating strategies that consider multi-objective and uncertainty management approaches simultaneously. Hence, regarding the development of the model (the general model proposed in the previous chapter), the individual challenges associated with uncertainty management should be considered. Therefore, the core of this chapter addresses the efficient definition of the number of scenarios required to represent uncontrollable parameters.

Thus, this chapter, it is addressed the uncertainty management issue in SSC retrofitting process. The proposed approach is based on the previous energy integration multi-objective model to optimize a retrofitted network in the presence of uncertainty. Such a strategy can produce a robust set of solutions while considering products demand uncertainty. The result consists of dominant and feasible solutions set. This contribution has utilized a case study to validate the proposed model and demonstrate details.

### 5.1. Representation of uncertain process conditions

The applied development of sustainable industrial processes has highly motivated researchers to propose approaches. These approaches aim to tackle problems present multidisciplinary challenges at multi scientific levels, which lead to integrated solution strategies. Hence, the optimization strategies should be improved. As commented in Chapter 2, there are two main challenges while addressing sustainability problems; the limitation fundamental to any MO problem (Mele et al., 2011) and the high complexity associated with the uncertainty (Grossmann, Apap, Calfa, Garcia-Herreros, & Zhang, 2015).

While there are not capable models to systematically address these challenges simultaneously, a significant bias is identified in the solutions obtained by the current strategies. Therefore, it is necessary to develop models leading to robust and capable methods to address them. Studies in the PSE literature have predominantly focused on the uncertainty effects representation on processes. These studies primarily have utilized the reactive and proactive approaches (explained sufficiently in Chapter 3).

Comparing the two approaches, the proactive is more reliable and assures the robustness of the solution by cause of pre-description of uncertainty. Applying to SCM, the recent contribution (Elluru, Gupta, Kaur, & Singh, 2019) has mentioned these strategies' strengths and weaknesses. Here, the strategies such as robust optimization (Govindan & Fattahi, 2017; Z. Li & Ierapetritou, 2008; Q. Zhang et al., 2016), two-stage stochastic programming (You et al., 2009), and chance constraint optimization (Guillén-Gosálbez & Grossmann, 2010) are commonly used as methods to model the effect of uncertain parameters over a network. Despite the idea that says the larger the number of scenarios better the uncertainty representation, it leads to complex situations due to computational limitations, which turns to be a severe problem when addressing more complex systems. Hence, finding an optimal size of the uncertainty set still remains like a critical challenge (Moret et al., 2017, 2016). Thus, managing the large number of scenarios defining the uncertainty space has remained one of the deficiencies for uncertainty management approaches. In this line, scenario reduction approaches are prevalent as the methods allow selecting a representative number of scenarios from the original set (Z. Li & Floudas, 2014, 2016). Despite the successful use of these methods to several contributions, their application is limited to finite numbers of approaches and, a general framework needs development to apply to large-scale multi-objective SC retrofitting problems.

In this chapter, a scenario reduction method is used within an  $\epsilon$ -constraint method to optimize the retrofitting of material/energy supply chains under uncertainty. For this purpose, the presented model in this chapter is a modified model of the previous chapter by considering product demand as an uncertain parameter.

### 5.1.1. Management of alternative energy resources

Recently, bio-based energy integration has become an effective alternative for providing energy to solve at least two problems simultaneously: improving the economic performance of the system by reducing the energy costs (while the fossil-based energies are expensive) as well as reducing environmental impact (particularly  $CO_2$  emissions). In this regard, several studies have proposed different models to optimize the retrofitting, design, and planning of bio-energy SCs. Due to the complexity of the problem, and as discussed in Chapter 2, applying multi-objective optimization approaches to sustainable networks has been very common in recent studies, particularly biomass to energy systems. In this line, Yue, You, & Snyder (2014) have proposed a profound overview to describe the key challenges and opportunities in modeling and biomass-to-bioenergy supply chains optimization.

Researchers have conducted several extensive studies in the last decade regarding uncertainty management in biomass supply chains. In these studies, they commonly have applied uncertainty management approaches. As a remarkable instance, a recent novel model has been proposed by (Medina-González et al., 2020) in which a multi-objective model has been applied to the bio-based

energy supply chain network, subjected to multiple sources of uncertainty. However, the studies have not targeted the demand uncertainty in integrated energy/material SCs.

Accordingly, in this chapter, the proposed approach is to merge generic SCs with biomass SCs and develop bio-based closed-loop energy integrated MOO model considering demand uncertainty to optimize the strategic and tactical decisions of large-scale SCs in the presence of conflicting objectives.

## 5.2. Problem statement

Regarding the approach mentioned in the previous section, the proposed model determines the development of the general material/energy integration SC network introduced in the previous chapter (**Chapter 4**). It aims to determine optimal configurations of the retrofitted SC under uncertainty. Obtained solutions propose optimum network configurations, including the number, locations, and capacities of the process plants with the associated production technologies and their capacity expansion policy.

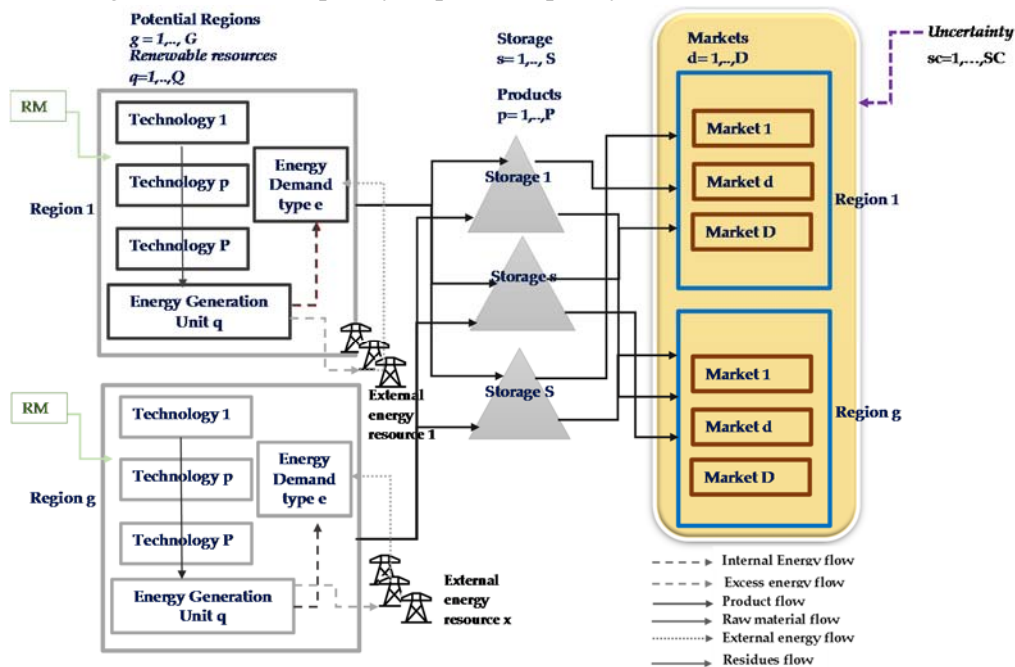


Fig. 5. 1. Schematic representation of integrated material/energy SC under uncertainty.

The single integrated energy resource (particular case is bio-based energy generation) SC subject to product demand uncertainty, as schematized in Fig. 5.1, is used from the previous chapter (**Chapter 4**) as a paradigmatic example of the problem to be addressed.

A modified version of the case study (Kostin, Guillén-Gosálbez, Mele, Bagajewicz, & Jiménez, 2012) applies to the contribution, aimed to test the viability. The objectives consider the expected net present value as an economic metric and GWP100 as the expected environmental impact of

the entire SC. Remarkably, the following subsection details the most relevant mass and energy balances and the associated constraints that describe the technologies involved.

### 5.3. Mathematical formulation: Stochastic model

This section describes how the stochastic model was obtained from the deterministic one. The stochastic model is a slight modification of the deterministic MILP described in the previous chapter. More precisely, equations describing the design of the process plants and energy generation units remain unaffected. Note that the source of uncertainty affects both the economic and environmental impact objective functions.

Since the equations are the extension of the formulation in Chapter 4, they are provided in Appendix B.2. The equations are classified into four main blocks: mass balance equations and capacity constraints of the production process section, mass/energy balance equations and capacity constraints of the energy cogeneration section, and objective function equations.

#### 5.3.1. Objective functions

The model aims to optimize the economic and environmental performance of the process network simultaneously and under uncertainty. Below is described how to quantify these performance criteria.

Since the model shows different performances in each scenario, one goal of the mathematical formulation is to maximize the expected value of the resulting NPV distribution versus environmental impact minimization. Definite risk measures are also conjoint to the formulation to control the possibility of unfavorable scenarios with low NPV values. The following sections describe how to determine these metrics.

##### 5.3.1.1. Expected NPV

One of the objectives of the model is to maximize the expected NPV. This metric is defined as below:

$$E[NPV] = \sum_{sc} Prob_{sc} NPV_{sc} \quad (5.1)$$

Where  $Prob_{sc}$  is the probability of scenario  $sc$ , and  $NPV_{sc}$  represents the net present value attained in the same scenario.

##### 5.3.1.2. Environmental objective

The environmental impact, as an objective function, is defined through the expected  $DAM$  as an environmental metric to be minimized.

$$E[DAM] = \sum_{sc} Prob_{sc} \times DAM_{sc} \quad (5.2)$$



### 5.3.1.3. The probabilistic constraint for financial risk management

A set of constraints that measure the probability of not achieving a predefined target value  $\Omega$  can control the variability of the objective function. Hence, it is needed to define the binary variable  $Z_{sc}$ . This variable takes the value of 1 if the NPV attained in scenario  $sc$  is below the target level  $\Omega$ , and it is 0 otherwise. The following constraints (Kostin et al., 2012) enforce the definition of such a variable:

$$NPV_{sc} \leq \Omega + M(1 - Z_{sc}) \quad \forall sc \quad (5.3)$$

$$NPV_{sc} \geq \Omega - MZ_{sc} \quad \forall sc \quad (5.4)$$

The probability of having an NPV below  $\Omega$  is defined as follows:

$$Pro[NPV \leq \Omega_k] = \sum_{sc} prob_{sc} Z_{sc} \quad (5.5)$$

The following section proposes the results of these probabilistic metrics in a particular case.

### 5.3.1.4. The probabilistic constraint for environmental impact risk management

The goal of risk analysis is to identify robust solutions with low probabilities of significant impacts. This section attempts to adopt stochastic metrics borrowed from financial risk management to present a model that controls the risk. Hence, rather than minimizing the expected value of the impact distribution (which is the standard approach in stochastic programming), we propose to minimize the probability of exceeding a given target value. This probability can be quantified employing the following equation:

$$Pro\{DAM \geq \Omega'\} \leq k \quad (5.6)$$

The probability of violation of the uncertain inequality in Eq. (5.6) (i.e., the left side representing the stochastic influence exceeds the right side reflecting the desired target limit) is maximum  $k$ . Here, DAM denotes the “true” value of the impact, and  $k$  represents the probability of violation of the constraint. A  $k$  value of zero indicates no chance of constraint violation, yielding the most conservative solution.

Equation (5.6) is a probabilistic or chance-constraint widely used in robust optimization (Ben-Tal & Nemirovski, 1998). This section, inspired by (Sabio et al., 2014), addresses the environmental impact risk issue by discretizing the probabilistic constraints. Eq. (5.7) is, therefore, approximated via the following constraint:

$$Pro[DAM \geq \Omega'_k] = \sum_{sc} prob_{sc} Z'_{sc} \quad (5.7)$$

where  $prob_{sc}$  as explained before, is a parameter representing the probability of occurrence of scenario  $sc$ , whereas  $Z'_{sc}$  is a binary variable that takes the value of 1 if the environmental impact exceeds the target limit in scenario  $sc$  and 0 otherwise. The following constraints enforce the definition of this binary variable. Here,  $M$  is a sufficiently large parameter.

$$DAM_{sc} \geq \Omega' - M(1 - Z'_{sc}) \quad \forall sc \quad (5.8)$$

$$DAM_{sc} \leq \Omega' + MZ'_{sc} \quad \forall sc \quad (5.9)$$

### 5.3.1.5. Multi-objective equations

The proposed approach relies on an  $\varepsilon$ -constraint method applied to the mixed-integer linear programming (MILP) to incorporate the uncertainty associated with demand. This method, as explained before, is based on maximizing one of the objective functions and considering the other ones as constraints bounded by levels of  $\varepsilon$ . Then, the levels of  $\varepsilon$  can be changed to generate the entire Pareto optimal set. Thus, the following MILP optimization formulation aims to obtain the Pareto solutions.

Here, the mathematical model seeks to optimize simultaneously the  $E[NPV]$  and  $E[DAM]$  objectives described in the bi-dimensional objective function as presented in model  $M$ . The overall bi-MILP formulation is expressed briefly, as follow:

$$(M) \quad \min_{x,X,N} \{-E[NPV(x, X, N)]; E[DAM(x, X, N)]\}$$

s.t. constraints (5.1)-(5.9) and the equations provided in Appendix B.2

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

Here,  $x$  represents the continuous variables such as capacities, production rates, inventory levels, and materials flows,  $X$  denotes the binary variables (i.e., the transportation links), and  $N$  refers to the integer variables like the number of plants, storage facilities, and transportation units of each selected mode.

$$(M1) \quad \min_{x,X,N} \{-E[NPV(x, X, N)]\}$$

s.t. constraints (5.1)-(5.9) and the equations provided in Appendix B.2

$$E[DAM(x, X, N)] \leq \varepsilon$$

$$\underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon}$$

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

Where the lower and upper limits are obtained from the optimization of each scalar objective separately:

$$(M1a) \quad (\bar{x}, \bar{X}, \bar{N}) = \arg \min_{x,X,N} \{E[DAM(x, X, N)]\}$$

s.t. constraints (5.1)-(5.9) and the equations provided in Appendix B.2

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

which defines the lower bound of the epsilon parameter, i.e.,  $\underline{\varepsilon} = DAM(\bar{x}, \bar{X}, \bar{N})$  and

$$(M1b) \quad (\hat{x}, \hat{X}, \hat{N}) = \arg \min_{x,X,N} \{-E[NPV(x, X, N)]\}$$

s.t. constraints (5.1)-(5.9) and the equations provided in Appendix B.2

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

defines the upper bound of the epsilon parameter, i.e.  $\bar{\epsilon} = DAM(\hat{x}, \hat{X}, \hat{N})$ . Considering uncertainty creates more opportunities to control the variability and make more flexibility in the decision-making process.

Standard stochastic optimization models try to identify robust solutions by optimizing the expected value of the objective distribution. This strategy ensures the best average performance but provides no control over its variability. Hence, the number of scenarios and their representativeness is the crucial factor for obtaining robust solutions.

#### 5.4. Methodology

This section introduces a novel optimization-based method for scenario reduction. This method applies multiple standards, not only can quantify the difference in the spatial distribution of parameter inputs but also quantify the difference in system output. The following subsections will describe the methods in detail according to different standards, and finally, the overall optimization model will be summarized.

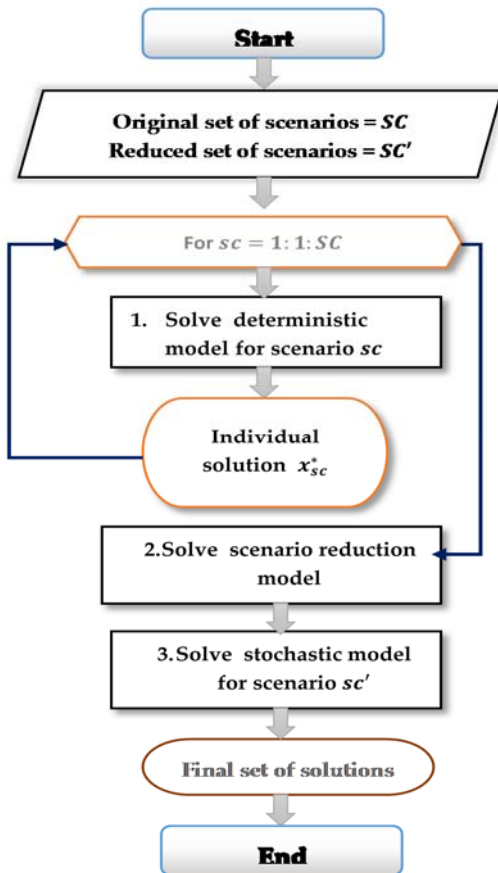


Fig. 5. 2. Schematic representation of a detailed description of the solution strategy proposed.

Here, the proposed model adopts the form of a general mixed-integer programming-based scenario described by (Z. Li & Floudas, 2014), and the next presents a brief description of such a formulation. The proposed solution strategy includes three steps: deterministic optimization for

the nominal scenario, scenario reduction, stochastic optimization for reduced sets to obtain final solutions. Figure 5.2 shows the general algorithm of the proposed solution strategy of step one.

#### 5.4.1. Scenario reduction algorithm

Given a set of scenarios  $SC$ , a subset of scenarios  $R$  is to be removed, and  $SC'$  is the subset of scenarios  $SC' = SC - R$  (reduced set), the following two discrete distributions are:

- i) The original distribution which contains all scenarios in set  $SC$  and each scenario  $sc$  has the probability  $prob_{sc}^{orig}$  that  $\sum_{sc \in SC} prob_{sc}^{orig} = 1$
- ii) The reduced distribution represented by all scenarios  $SC'$  and each scenario  $sc'$  has the probability  $prob_{sc'}^{new}$  that  $\sum_{sc' \in SC'} prob_{sc'}^{new} = 1$

The Kantorovich distance between discrete distributions is defined by the optimal objective value of the following linear problem:

$$\min_{n_{sc,sc'}} \sum_{sc} \sum_{sc'} n_{sc,sc'} C_{sc,sc'} + f_{exp}^{err} \quad (5.10)$$

$$\text{s.t.} \quad \sum_{sc \in SC} n_{sc,sc'} = prob_{sc'}^{new} \quad (5.11)$$

$$\sum_{sc' \in SC'} n_{sc,sc'} = prob_{sc}^{orig} \quad (5.12)$$

$$n_{sc,sc'} \geq 0, \quad \forall sc \in SC, \quad \forall sc' \in SC'$$

Where  $sc$  and  $sc'$  are scenarios;  $prob_{sc'}^{new}$  and  $prob_{sc}^{orig}$  represent the probability of scenario  $sc'$  in the new distribution and scenario  $sc$  in the original distribution;  $n_{sc,sc'}$  is the probability displacement between scenarios;

One of the critical parameters is  $C_{sc,sc'}$  which defines the distance between two scenarios that the following equation can model:

$$C_{sc,sc'} = \sum_{d=1}^D |\theta_{sc}^d - \theta_{sc'}^d| + |f_{sc}^* - f_{sc'}^*| \quad \forall sc, sc' \quad (5.13)$$

Note that  $\theta_{sc}^d$  and  $\theta_{sc'}^d$  are the realization of the uncertain parameters  $d$  in scenarios  $sc$  and  $sc'$ , respectively;  $f_{sc}^*$  and  $f_{sc'}^*$  are the optimal objective value under scenarios  $sc$  and  $sc'$ .

$$prob_{sc'}^{new} = (1 - y_{sc'}) \times prob_{sc'}^{orig} + \sum_{sc \in SC} v_{sc,sc'} \times prob_{sc}^{orig} \quad \forall sc', y_{sc} \in \{0,1\} \quad (5.14)$$

Where continuous variable  $v_{sc,sc'}$  denotes if a scenario  $sc$  is removed and assigned to scenario  $sc'$  or not; binary variable  $y_{sc}$  denotes whether a scenario is removed ( $y_{sc} = 1$ ) or not ( $y_{sc} = 0$ ). Note that if  $prob_{sc'}^{new} = 0$ , it means scenario  $sc$  is removed.

$$\sum_{sc \in SC} y_{sc} = N \quad (5.15)$$

$$\sum_{sc' \in SC} v_{sc,sc'} \geq y_{sc} \quad \forall sc \quad (5.16)$$

$$0 \leq v_{sc,sc'} \leq 1 - y_{sc} \quad \forall sc, sc' \in SC \quad (5.17)$$

One of the most significant features of the proposed model is its capability to minimize the probabilistic distance in both parameter and output spaces, which means the objective value's expected performance. To modeling this feature, it is necessary to add the difference between the expected value obtained by the original and reduced sets of scenarios ( $f_{exp}^{err} = |f_{exp}^{orig} - f_{exp}^{new}|$ ) to the primary objective function of the scenario reduction algorithm (Eq. (5.10)). Here,  $f_{exp}^{orig} = \sum_{sc} prob_{sc}^{orig} \times f_{sc}^*$  and  $f_{exp}^{new} = \sum_{sc'} prob_{sc'}^{new} \times f_{sc'}^*$ . Here is the point that the performance of the deterministic optimization in the first step becomes relevant. Note that  $f_{sc}^*$  is the objective value obtained by scenario  $sc$ .

$$f_{exp}^{err} \geq -\sum_{sc'} prob_{sc'}^{new} \times f_{sc'}^* + \sum_{sc} prob_{sc}^{orig} \times f_{sc}^* \quad (5.18)$$

$$f_{exp}^{err} \geq \sum_{sc'} prob_{sc'}^{new} \times f_{sc'}^* - \sum_{sc} prob_{sc}^{orig} \times f_{sc}^* \quad (5.19)$$

For minimizing the differences between the worst and best performance, the error between the minimum (or maximum) objective values can incorporate into the scenario reduction model. More details about this model are perfectly explained in the contribution proposed by (Z. Li & Floudas, 2014).

### 5.5. Case study: Retrofitting of integrated biomass-based SCs under uncertainty

This contribution has used a real-life case study previously studied by (Kostin et al., 2012) to illustrate the proposed procedures application. This case study has addressed optimal retrofitting of existing bioethanol and the sugar production industry established in Argentina under demand uncertainty. In this problem, three different products (i.e., white sugar  $D_1$ , raw sugar  $D_2$ , and ethanol  $D_3$ ) are produced from 3 raw materials (sugarcane  $RM_1$ ) and by-products (molasses  $RM_2$  and honey  $RM_3$ ) by five different production technologies (sugar mills  $T_1$  and  $T_2$ , distilleries  $T_3$ ,  $T_4$  and  $T_5$ ) through the process network shown in Fig. 5.3.

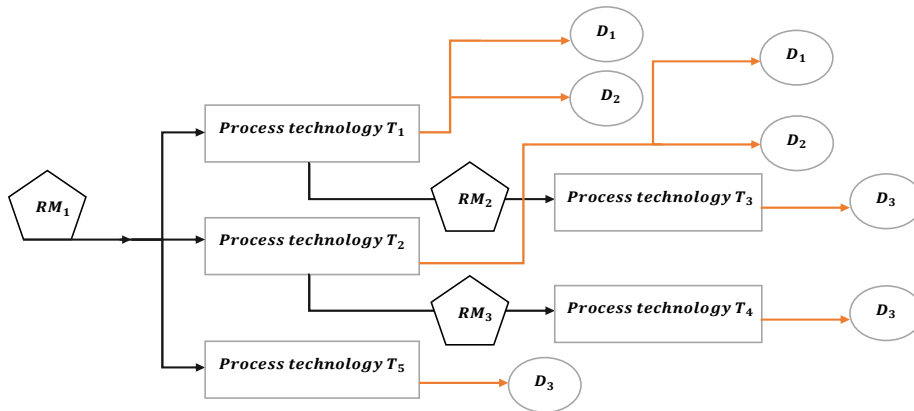


Fig. 5. 3. Production process network.

The nominal capacity of the sugar mill and distillery plants are 350 and 300 thousand tons annually, respectively. Cogeneration power capacity has been calculated in the previous chapter

(section 4.4.1, Chapter 4), which is 50 MW with 41% of electricity efficiency. A time horizon of 4 years is assumed and divided into yearly periods, and a specific geographic area is divided into a set of 24 sub-regions  $g$  where the facilities of the SC can be configured and may play the role of biomass producers, energy generators, and consumers.

Assume that the products' demand parameters  $SD_{i,g}$  are subject to uncertainty, while the rest of the parameters are deterministic (take the nominal values). Nominal parameter data for this problem are provided in Table 5.1.

Table 5. 1. Products nominal demand.

Region	Associated sub region	Product demand ( $10^3\text{t/yr}$ )		
		White sugar	Raw sugar	Ethanol
(Buenos Aires)	$g_1$	76.61	38.31	84.28
(Córdoba)	$g_2$	84.13	42.06	92.54
(Corrientes)	$g_3$	25.44	12.72	27.98
(La Plata)	$g_4$	379.3	189.63	417.2
(La Rioja)	$g_5$	9.714	4.857	10.69
(Mendoza)	$g_6$	43.56	21.78	47.92
(Neuquén)	$g_7$	13.72	6.86	15.09
(Entre Ríos)	$g_8$	31.55	15.77	34.70
(Misiones)	$g_9$	27.14	13.57	29.85
(Chubut)	$g_{10}$	11.52	5.758	12.67
(Chaco)	$g_{11}$	26.44	13.22	29.08
(Santa Cruz)	$g_{12}$	5.708	2.854	6.279
(Salta)	$g_{13}$	30.75	15.37	33.82
(San Juan)	$g_{14}$	17.53	98.76	19.28
(San Luis)	$g_{15}$	11.02	5.508	12.12
(Tucumán)	$g_{16}$	37.15	18.58	40.87
(Jujuy)	$g_{17}$	17.12	8.562	18.84
(Santa Fe)	$g_{18}$	81.12	40.56	89.23
(La Pampa)	$g_{19}$	8.412	4.206	9.253
(Santiago del Estero)	$g_{20}$	21.73	10.86	23.90
(Catamarca)	$g_{21}$	8.612	4.306	9.474
(Rio Negro)	$g_{22}$	15.02	7.511	16.52
(Formosa)	$g_{23}$	13.52	6.760	14.87
(Tierra del Fuego)	$g_{24}$	3.204	1.602	3.525

The by-products of the production plants (particularly bagasse) are supposed to send to the cogeneration to generate heat and electricity as added-value products. The electricity market price and the operational cost of electricity generation are 0.15€/kWh and 0.08€/kWh respectively. This contribution has aimed to maximize the economic metric (NPV) whereas minimizing the

environmental impacts (GWP100,  $kg, CO_2$ ). The deterministic model of the above retrofitting problem has been solved in **Chapter 4**.

The scope of this chapter is limited to providing an effective strategy to solve the challenges associated with using a large number of solutions to represent the process uncertainty in MOO problems. Therefore, technical challenges such as temporary power supply (e.g., power storage, switching on/off the transmission grid, and power supply during certain hours of the day) are not within this scope. Other research is needed to expand this formulation and solve the power supply problem to explore the solutions' economic, environmental, and social performance differences.

The objective is to select the optimum configuration (including their capacities and locations) and the best way to interconnect the various supply chain elements (i.e., providers, intermediates, and consumers).

In the following, scenario reduction studies are performed assuming different sets of uncertain parameters and different discretization levels. The objective is to generate a different number of a superset of scenarios (from relatively large to small) by factorial design and test the proposed scenario reduction algorithm. The scope of this chapter is limited to address the challenges associated with the uncertainty within the SC problem.

The objective is to select the most suitable configuration (including their capacities and locations), the best way to interconnect the various elements of the supply chain (i.e., feedstock, process plants, external energy provider, and the markets), and adequate storage/transport flows to make the best use of the feedstock. The solution obtained will be compared with deterministic results proposed in the previous chapter to highlight the uncertainty over the overall solution space.

### **5.5.1. Scenario reduction solution**

#### ***Deterministic solution analysis and Scenario reduction***

Chapter 4 illustrated the capabilities of the modeling framework and solution strategy using the process network introduced previously. It described first the results obtained with the deterministic model that shed light on the inherent trade-offs between the economic and environmental performance of the industrial network. This section uses the stochastic formulation to address the uncertainty on the final product demand.

A critical issue in the multi-scenario model is the generation of appropriate values of the uncertain parameters. Therefore, from 72 uncertain parameters corresponding to demand product  $i$  in region  $g$  ( $SD_{i,g}$ ), Monte Carlo simulation using What-If Analysis generated 1500 scenarios with the normal distribution and global and local standard deviations 8% and 3% assuming the mean values in Table 5.1.

This study selected 125 scenarios randomly; then solved the deterministic model of the previous chapter to obtain the design variables and fixed them. Afterward, the 125 scenarios are used to attain 125 solutions. In the next step, the algorithm proposed in **Section 5.4.1** generated a reduced

set of **100** scenarios (**case 1**). Without loss of generality, the size of 100 scenarios was selected to ensure a large set to be sufficiently representative. After the optimization realization and fixing the design variable, the 125 scenarios are applied to the model. To check the viability of the model, in the next step, the stochastic optimization is done for reduced sets of **50** (**case 2**), **20** (**case 3**), **10** (**case 4**), and **1** (**case 6**) scenarios, obtained through the algorithm described in **Section 5.4.1**, and 3 scenarios (**case 5**) that explained how to attain in the following. Then the expected values of the economic performance are obtained. Fig. 5.4 illustrates the deterministic solutions against the stochastic solutions obtained by the reduced sets of scenarios, while Table 5.2 shows the max, min, and expected values of the maximized economic objective for the reduced set.

Table. 5. 2. Statistics on scenario reduction results for economic performance maximization.

	Size	Optimization NPV (€(GAMS))	Design	Investment cost	Max NPV(€)	Min NPV(€)	Exp NPV(€)
<b>Deterministic</b>		$3.202 \times 10^9$	50MW	$9.530 \times 10^9$	$3.200 \times 10^9$	$1.182 \times 10^9$	$2.360 \times 10^9$
<b>Stochastic</b>							
<b>Case6</b>	1	$3.195 \times 10^9$	50MW	$9.530 \times 10^9$	$3.190 \times 10^9$	$1.510 \times 10^9$	$2.361 \times 10^9$
<b>Case5*</b>	3	$3.185 \times 10^9$	58MW	$9.610 \times 10^9$	$3.181 \times 10^9$	$1.152 \times 10^9$	$2.362 \times 10^9$
<b>Case4</b>	10	$2.90 \times 10^9$	80MW	$9.860 \times 10^9$	$3.062 \times 10^9$	$1.695 \times 10^9$	$2.400 \times 10^9$
<b>Case3</b>	20	$2.75 \times 10^9$	81MW	$10.000 \times 10^9$	$2.580 \times 10^9$	$1.799 \times 10^9$	$2.449 \times 10^9$
<b>Case2</b>	50	$2.60 \times 10^9$	83MW	$10.150 \times 10^9$	$2.598 \times 10^9$	$1.875 \times 10^9$	$2.485 \times 10^9$
<b>Case1</b>	100	$2.56 \times 10^9$	85MW	$10.170 \times 10^9$	$2.899 \times 10^9$	$1.895 \times 10^9$	$2.726 \times 10^9$

\*in case5, the set size is not obtained by the scenario reduction algorithm.

In other words, Fig. 5.4 is used to visualize the relationships between the deterministic and the stochastic model solved by reduced sets of scenarios for the uncertain parameters.

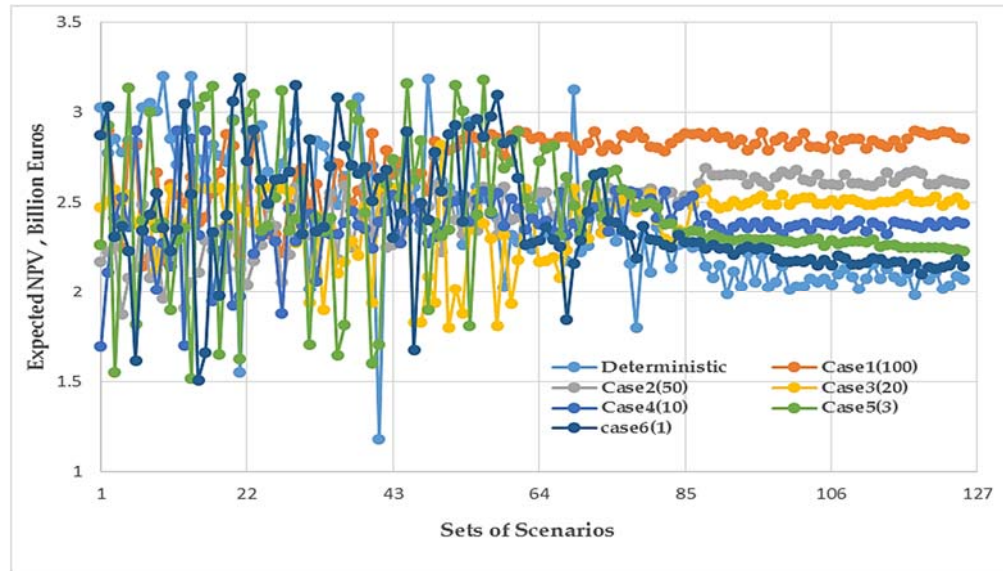


Fig. 5. 4. Expected NPV objective values for 125 scenarios.

After the deterministic design optimization procedure, 125 solutions were obtained. Individually, the results achieved by the reduced sets with fewer numbers of scenarios represent a poor



approximation for the global problem; however, they are used to evaluate the “similarity” among different sizes of scenario sets. Notice that the scenario reduction produces a well-balanced distribution considering the 72 uncertain parameters. Besides, stochastic cases with larger sizes of scenarios show more flexibility in response to various probabilities. For instance, **case 1** (100 scenarios-case) can manage the result variations compared to deterministic and other stochastic cases.

Testing different sets of scenarios, the plot below (Fig. 5.5) demonstrates exponential behavior that any increment in the size of scenarios (scenarios > 50) leads to a few variations in the final solution (less than 1%) while lowering the number of scenarios increases such a difference exponentially.

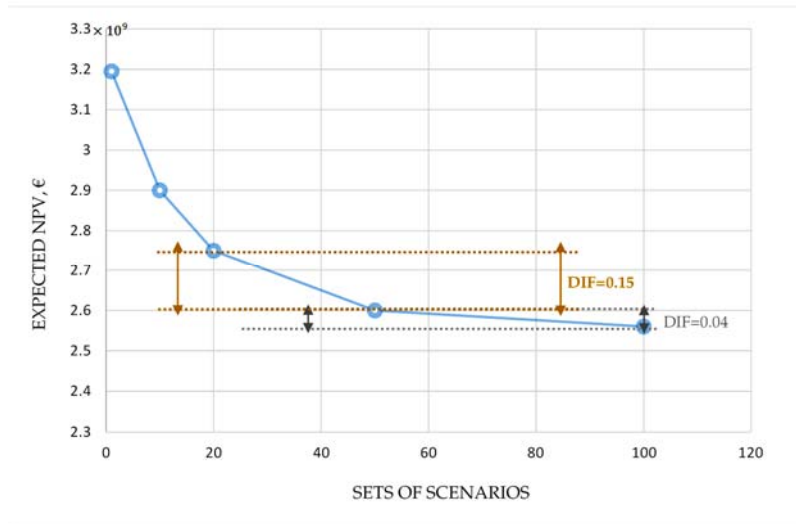


Fig. 5. 5. NPV performance for each size of scenarios.

Furthermore, note that the scenarios represent better input (uncertain conditions) and output (expected economic performance) data. Accordingly, the deduction is that using sets containing at least 100 scenarios is more viable.

### 5.5.2. Financial risk management

In the following, Fig. 5.6 represents the cumulative probability profile of each set and **Deterministic case**. The cumulative probability distribution chart shows that the probability of the NPV is less than or equal to a particular value for each alternative.

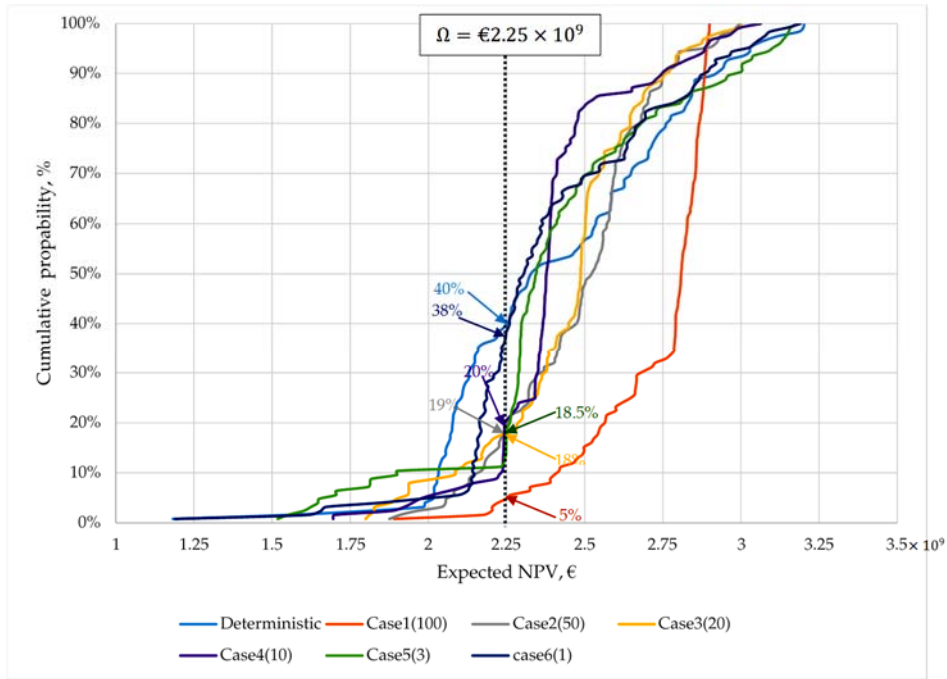


Fig. 5. 6. Cumulative probability profiles for reduced sets of scenarios and deterministic cases.

Regarding probabilistic metrics, defined in **section 5.3.3.3**, Fig. 5.6 depicts the cumulative probability curves associated with given SC designs. It is considered stochastic and deterministic formulations with 125 scenarios and, each one corresponding to a different materialization of the uncertain parameters. Assume that the target value  $\Omega$  is equal to  $\text{€}2.25 \times 10^9$ . For **Case 1**, there are five scenarios out of 125 with an NPV below this target value (i.e., the probability of not exceeding the target value is 5%) comparing to the deterministic case, not exceeding probability raises to 40%. In other words, **Case 1** shows a significantly lower probability of small and high NPVs (comparing to the other cases), which would make it appealing for risk-averse decision-makers. On the other hand, the deterministic case might be the preferred alternative for risk-takers decision-makers, as it leads to larger probabilities of high NPVs at the expense of increasing along with the probability of low benefit.

Values at risk (VaR) is the most common metric that defines the difference between the expected NPV and the NPV value corresponding to a certain level of risk. Here is assumed that this level is 5%. The symmetrically opposite measure of risk is the opportunity value (OV) or upside potential, which was discussed by (Aseri & Bagajewicz, 2004), which defines the difference between the NPV at 95% risk and  $E[\text{NPV}]$  value. Fig. 5.7 presents the calculation of VaR and OV for the risk-averse and risk-taker cumulative probability curves.

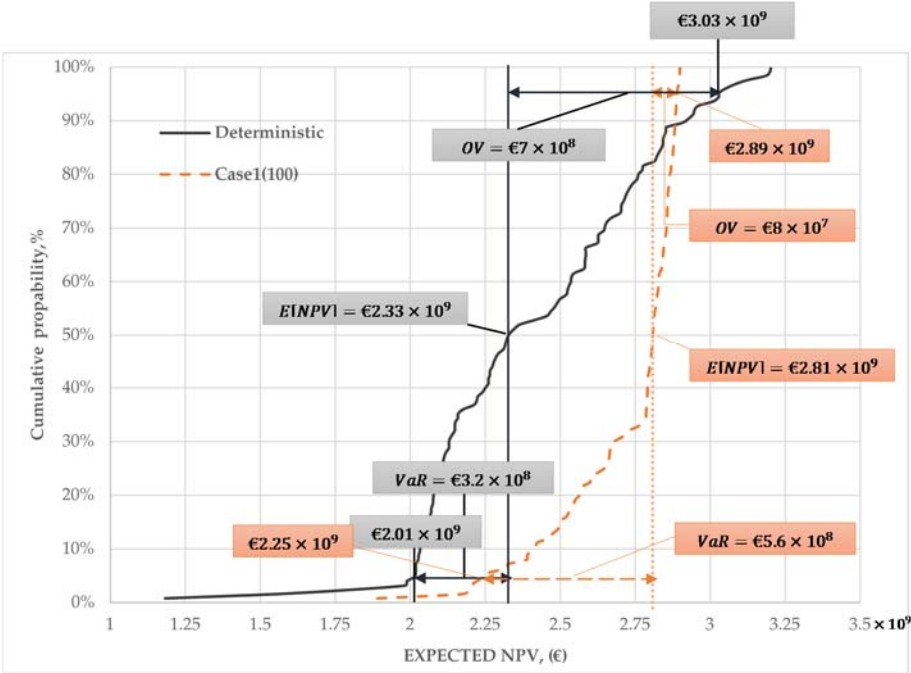


Fig. 5. 7. Value at Risk (VaR) vs. opportunity value (OV).

Remarkably, the strategy can adjust the probability of occurrence as a function of the number of scenarios belonging to the new subset. Such an adjustable probability provides the required flexibility to mimic the original uncertainty distribution accurately.

Note that **case 5** deals with the scenario simplification approach; all uncertain parameters are classified into three scenarios as max, mid, and min  $(-\delta, D_i, +\delta)$  while  $\pm\delta = \pm 10\%$ , and tested with all possible ordered triples (4851 ordered triples contain discrete numbers between 1 and 98 obtained by Gauss' formula. Note that the probabilities 0% and 100% are not considered).

$$\begin{array}{ll}
 sc_1: \{D_1^{max} \dots D_{72}^{max}\} & \text{Ordered triple} \\
 sc_2: \{\bar{D}_1 \dots \bar{D}_{72}\} & \text{With probability } Prob_j(p_{min}, p_{mid}, p_{max}) \\
 sc_3: \{D_1^{min} \dots D_{72}^{min}\} & j = 1, \dots, 4851
 \end{array}$$

Fig 5.8 illustrates all possible results obtained by this approach. The graph has constituted from 4851 points that each point represents a solution obtained by a particular ordered triple of probabilities. Remarkably, the majority of the results locate between  $\text{€}3 \times 10^9$  and  $\text{€}3.5 \times 10^9$ . It means the model mimes the deterministic model.

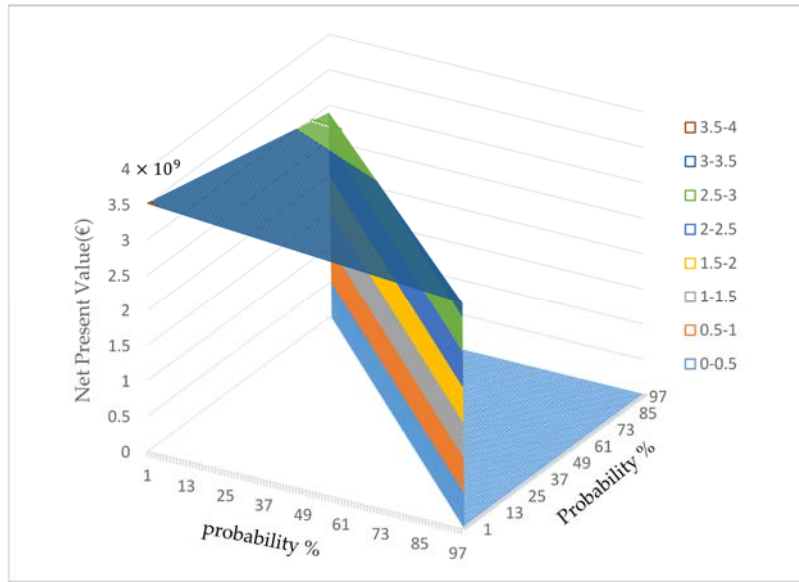


Fig. 5. 8. Results corresponding to scenario simplification approach.

Case 5 is a particular case with ordered triple probability (25%, 50%, 25%) that its behavior was explained in the previous section. Therefore, the deduction is that although the simplification approach is needed less computational effort, it cannot afford the flexibility required for managing this problem addressed in this thesis.

### 5.5.3. Environmental impact risk management

The previous section sat to solve the stochastic MILP to maximize the economic performance of the network. Here, it targets to minimize the environmental impact and analyze the corresponding results. First, the deterministic and stochastic problems in the multi-scenario MILP (considering the same reduced sets of scenarios from the previous section) were solved, the values of the design decision variables got fixed. Then, the viability of each case was examined for the 125 scenarios. Table. 5.3 shows the obtained results in detail.

Table. 5. 3. Statistics on scenario reduction results for the environmental impact minimization.

	Size	Optimization DAM (GWP100,kg,CO <sub>2</sub> × 10 <sup>9</sup> ) (GAMS)	Design	Investment cost	Min DAM	Max DAM	Exp DAM
					GWP100 (kg,CO <sub>2</sub> ) × 10 <sup>9</sup>		
<b>Deterministic</b>		-1.8	65MW	1.030 × 10 <sup>10</sup>	-1.790	-0.8155	-1.292
<b>Stochastic</b>							
Case6	1	-1.79	65MW	1.031 × 10 <sup>10</sup>	-1.783	-0.8150	-1.286
Case5*	3	-1.79	68MW	1.610 × 10 <sup>10</sup>	-1.779	-0.8225	-1.330
Case4	10	-1.77	75MW	1.860 × 10 <sup>10</sup>	-1.778	-0.8340	-1.336
Case3	20	-1.76	90MW	1.900 × 10 <sup>10</sup>	-1.759	-0.8343	-1.396
Case2	50	-1.75	93MW	1.950 × 10 <sup>10</sup>	-1.749	-0.8346	-1.450
Case1	100	-1.74	95MW	1.970 × 10 <sup>10</sup>	-1.740	-0.845	-1.516

\*in case5, the set size is not obtained by the scenario reduction algorithm.

The results show that by increasing the number of scenarios, the difference between the value of the optimized solution (obtained by GAMS) and the expected value is reduced. It is deduced that

using more significant size scenarios can control the variations, indicating the robustness of the solutions obtained. Fig. 5.9 illustrates this explanation.

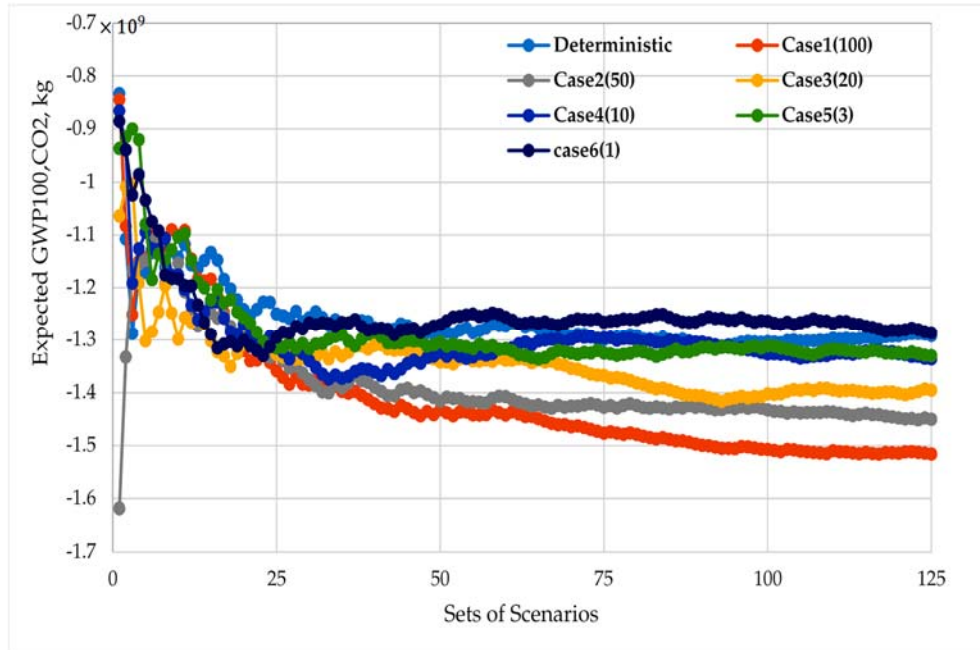


Fig. 5. 9. Expected DAM objective values for 125 scenarios.

Compared to Fig. 5.4, fewer solution variations are observed because fewer uncertainty-affected variables are involved for minimizing the DAM objective.

Fig. 5.10 shows the cumulative probability curves for the environmental impact of the deterministic and stochastic solutions. The figure shows the probability of a value of GWP100 when the expected DAM objective is minimized. The solving process first minimizes the impact in the most likely scenario (i.e., considering the mean values of the uncertain parameters) and then recalculating the objective function by fixing the values of the decision variables in the stochastic MILP. It is worthwhile to mention that the same solution could be ideally obtained by minimizing the expected impact in the stochastic MILP for an infinite number (or large sizes) of scenarios. Case 1 (100 scenarios) approves it; in the environmental performance target  $\Omega' = -1.3 \times 10^9 \text{ kg CO}_2$ , there is only a 24% probability of not achieving the goal, while in the deterministic case, this failure probability raises to 50%.

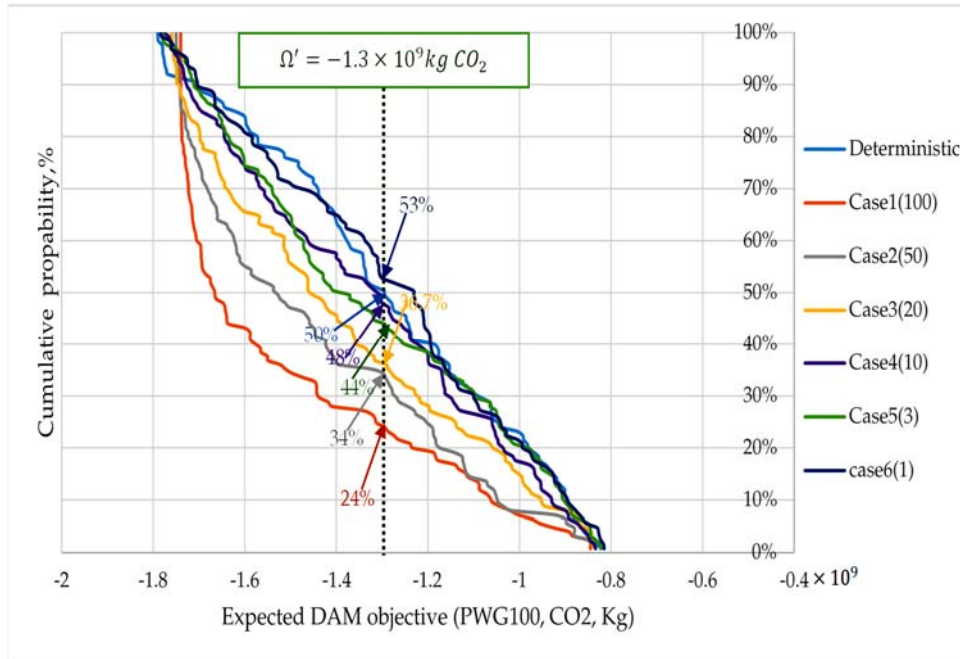


Fig. 5. 10. Cumulative probability profiles for stochastic and deterministic cases.









































































































































In the following section, the design configuration and planning solutions of deterministic and stochastic cases are explained. Note that the network configuration of the environmental impact minimization is very similar to the maximum economic performance solutions. Hence, the following section is just discussing the NPV maximal solution performance of different cases.

**Design and Planning comparison for deterministic and stochastic cases**

Here, the design solutions were obtained by solving the stochastic model for different reduced sets of scenarios. These solutions were compared to validate the reduced set representativeness. Table 5.4 illustrates three SC configurations (location and capacities of the different nodes expressed in thousand metric ton per year for production plants and MW for energy generation unit) which correspond to the three scenario size cases and happen in the maximal NPV. The capacities are the **maximum** ones.

It expects that networks with larger capacities and more technologies guarantee higher demand satisfaction levels due to covering more demand. For instance, the design which corresponds to **case 1** involves the technology establishment  $T_5$  moreover, larger energy generation capacity compared to the other cases. Note that the material flows are not mentioned in the table, while in stochastic case, there are more regions interconnected, which caused more demand satisfaction and an increase in the environmental damage factors.

Table. 5. 4. Design for the optimum network configurations obtained for the different sets of scenarios.

	Case4 Size 10	Case2 Size 50	Case1 Size 100
<b>Max PV(€)</b>	$2.90 \times 10^9$	$2.60 \times 10^9$	$2.56 \times 10^9$
<b>Region</b>			
<b>La Rioja (<math>g_5</math>)</b>	 350  350  300  300	 350  350  300  300	 350  350  300  300
<b>Mendoza (<math>g_6</math>)</b>	 350  350  300  300	 350  350  300  300	 350  350  300  300
<b>Misiones (<math>g_9</math>)</b>	 350  350  80  300  300	 350  350  83  300  300	 350  350  85  300  300  300
<b>Chaco (<math>g_{11}</math>)</b>	 350  350  300  300	 350  350  300  300	 350  350  300  300  300
<b>Salta (<math>g_{13}</math>)</b>	 350  350  80  300  300	 350  350  83  300  300	 350  350  85  300  300  300
<b>San Juan (<math>g_{14}</math>)</b>	 350  350  300  300	 350  350  300  300	 350  350  300  300  300
<b>Tucumán (<math>g_{16}</math>)</b>	 350  350  80  300  300	 350  350  83  300  300	 350  350  85  300  300  300
<b>Jujuy (<math>g_{17}</math>)</b>	 350  350  80  300  300	 350  350  83  300  300	 350  350  85  300  300  300
<b>Santa Fe (<math>g_{18}</math>)</b>	 350  350  80  300  300	 350  350  83  300  300	 350  350  85  300  300  300
	 $T_1$  $T_2$  $T_3$  $T_4$  $T_5$ ( $\times 10^3 MTPY$ )  Cogeneration unit (MW)	$T_1$ and $T_2$ : Sugar mill $T_3$ , $T_4$ , and $T_5$ : Distillery	



Focusing on Case 1 as the reference case, the corresponding Pareto curve illustrates the trade-off between environmental impact minimization and NPV maximization (see Fig. 5.9). Note that each point represents a network configuration and the design proposed in Table 5.3 reveals what is behind the maximal NPV point in the Pareto curve.

Similarly, in the environmental impact minimum cases, the model decides to replace production technologies  $T_3$  and  $T_4$  by  $T_5$  (because the feedstock used in these technologies is sugarcane). The industrial regions are retrofitted with cogeneration units (due to baggage availability) to reduce environmental impact under uncertainty.

Since Case 1 (100 scenarios) shows the best representativeness in both Minimal DAM and Maximal NPV objectives, Fig. 5.11 represents the Pareto set of solutions for this case.

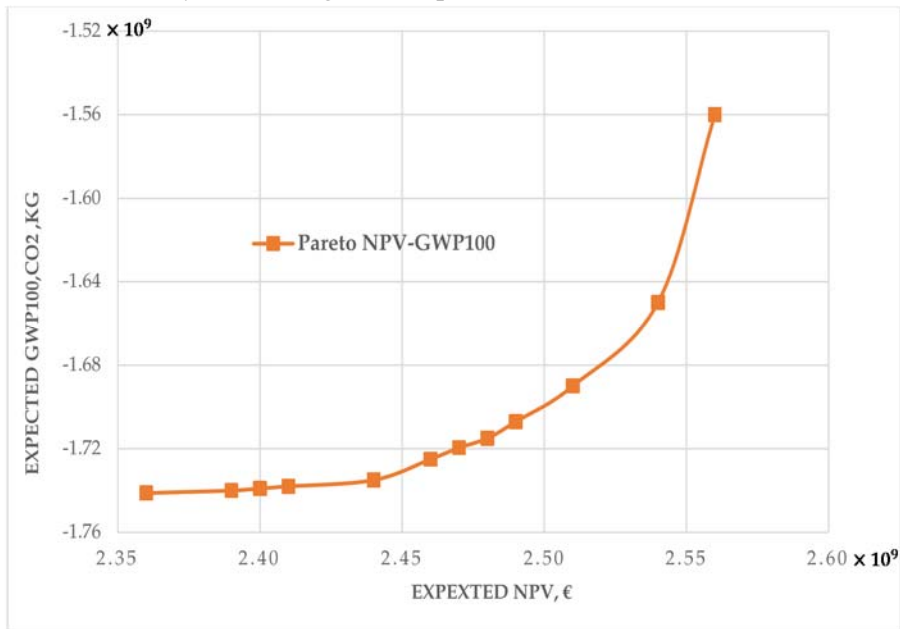


Fig. 5. 11. Pareto set of solutions GWP100 vs. NPV for Case 1.

As mentioned before, the minimal GWP100 solution allows operating at most for energy demand so that it leads to involve more regions in generating bio-based energy and using residues as bioenergy resources (reflecting in Fig. 5.12). In other words, the cogenerated energy in the whole SC meets the internal energy demand, and the excess energy can be marketed to increase renewable energy generation by 20% compared to Maximal NPV solution.



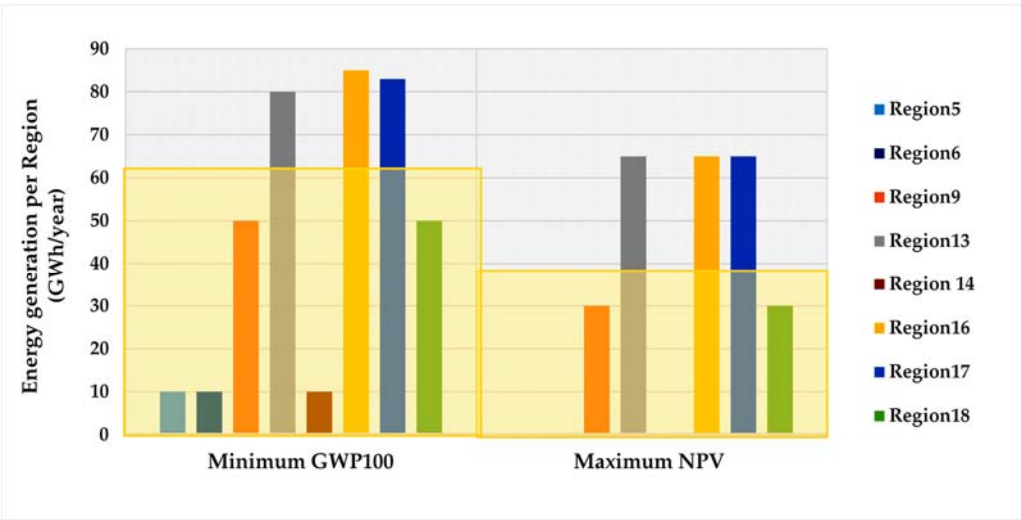


Fig. 5.12. Energy generation per Region in Minimal GWP100 and Maximal NPV (Case 1).

Here, the pie charts (Fig. 5.13) represent the percentage share of Maximal NPV and Minimal GWP100. Bioethanol has a larger share in the minimum GWP100 case while the sugar production decreases almost 10%. Therefore, the deduction is that the ethanol demand satisfactory level is improved reasonably.

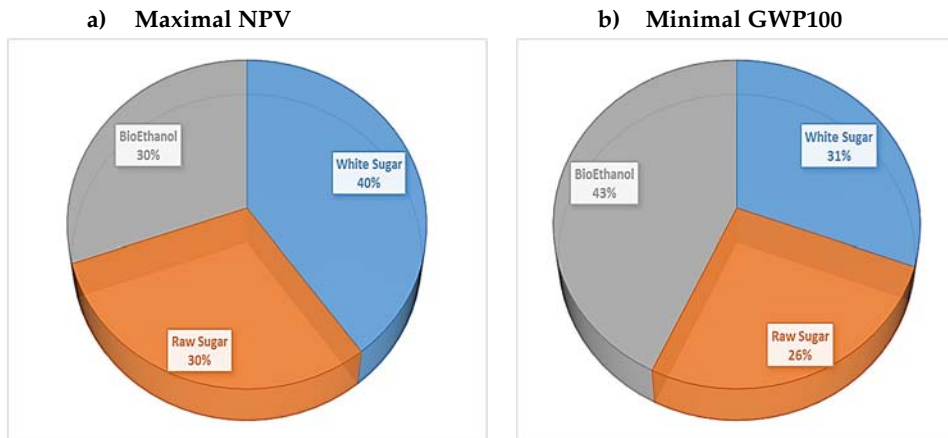


Fig. 5.13. Percentage share of products in a) Maximal NPV and b) Minimal GWP100 and (Case 1).

Finally, the results show (Fig. 5.14) that in the stochastic case, the energy demands lead to an overall decrease of 3.1% in the disposal costs in the stochastic solution. In comparison, only by 12% increase in the purchasing amount of sugar cane the energy demand is satisfied and can be marketed by adding 97.5 Billion Euros to the annual revenue.

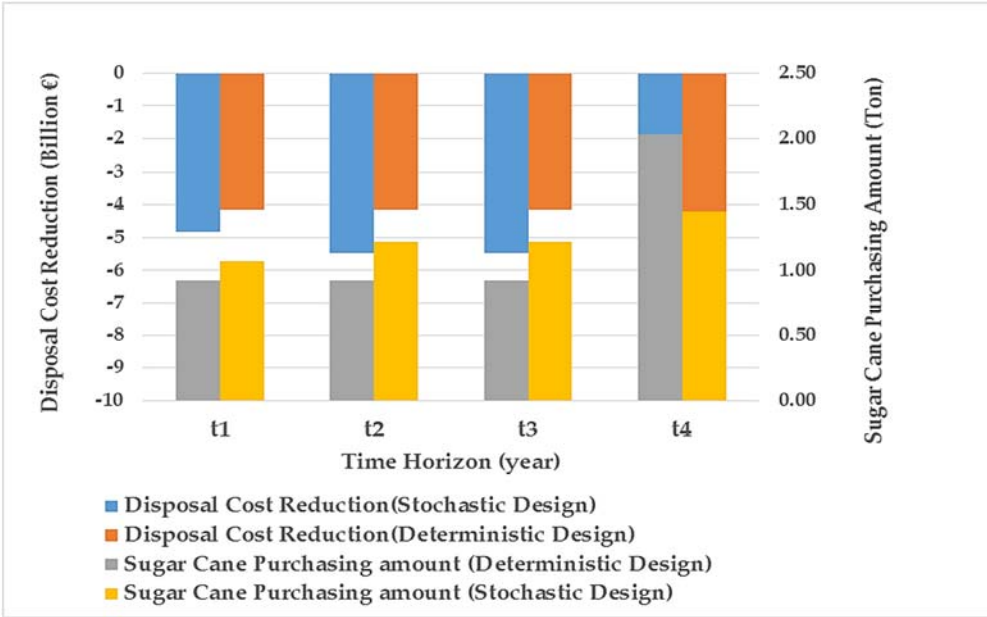


Fig. 5. 14. Disposal Cost Reduction vs. Sugar Cane Purchasing amount.

### 5.6. Conclusions

This chapter has addressed the optimal retrofitting of bio-based energy integrated SC under uncertainty. The problem is mathematically formulated as a multi-objective stochastic MILP aiming to discover further opportunities that account for maximizing the expected NPV and minimizing the environmental impacts (in terms of GWP100). The model was examined with different scenario sizes. The results of each case were analyzed and compared. It is deduced that a larger scenario size shows more representativeness and can control the uncertainty effects. Besides, a risk associated with the NPV quantifies the uncertainty effects, introduced as an additional constraint into the model. Then, this risk can manage to the probability of having low profit. The capabilities of the model were highlighted through its application to a case study. The proposed stochastic approach maximizes the expected NPV while satisfying at the same time a minimum environmental impact. Numerical results show that stochastic solutions improve system flexibility and should be therefore the preferred choice in practice. The optimal solutions are according to the number of residues used in cogeneration energy units directly related to the objectives. The interaction between the design objectives has been shown. This way of generating different possible configurations will help the decision-maker determine the best configuration according to the selected objectives.

Finally, this method allows the management of different material flows within a sustainable way, ensuring energy availability and reducing operational costs and demand satisfaction. Thus, the proposed strategy represents a step forward to overcome problems such as long period forecasting of uncertainty conditions.

## 5.7. Nomenclature

### Abbreviations

<i>MILP</i>	Mixed Integer Linear Programming
<i>MOO</i>	Multi-Objective Optimization
<i>NPV</i>	Net Present Value
<i>OV</i>	Opportunity Value
<i>PSE</i>	Process System Engineering
<i>SC</i>	Supply Chain
<i>SCM</i>	Supply Chain Management
<i>SSC</i>	Sustainable Supply Chain
<i>VaR</i>	Value at Risk

### Index

<i>k</i>	Target value( $k k = 1, \dots, K$ )
<i>sc</i>	Set of scenarios ( $sc sc = 1, \dots, SC$ )

### Parameters

$\varepsilon$	Auxiliary boundary for the $\varepsilon$ -constraint method
$\theta_{sc}^d$	a realization of uncertain parameters in scenario <i>sc</i>
$\Omega_k$	Target level <i>k</i>
$\Omega'_k$	Environmental performance target
$C_{sc,sc'}$	the distance between two scenarios
$f_{sc}^*$	Optimal objective value under scenario <i>sc</i>
<i>M</i>	Big positive number
<i>N</i>	Number of scenarios to be removed
$prob_{sc}$	the probability of scenario <i>sc</i>
$prob_{sc}^{orig}$	the probability of scenario <i>sc</i> in an original discrete distribution
$SD_{i,g}$	Demand of product <i>i</i> in region <i>g</i>

### Variables

$v_{sc,sc'}$	a dual variable which means whether scenario <i>sc</i> is removed and assigned to scenario <i>sc'</i>
$E[DAM]$	Expected environmental damage
$E[NPV]$	Expected net present value
$DAM_{sc}$	Environmental metric to be optimized in scenario <i>sc</i>
$f_{exp}^{err}$	absolute error between the expected performance of original and reduced distribution
$f_{exp}^{orig}$	Expected objective function obtained using the original set of scenarios
$f_{exp}^{new}$	Expected objective function obtained using the reduced set of scenarios
$n_{sc,sc'}$	Probability displacement between scenarios
$NPV_{sc}$	Net Present Value in scenario <i>sc</i>
$prob_{sc}^{new}$	new probability of scenario <i>sc</i> in the reduced distribution

**Binary Variables**

$y_{sc}$	whether scenario $sc$ is removed ( $y_{sc}=1$ ) or not ( $y_{sc}=0$ )
$Z_{sc}$	1 if NPV attained in scenario $sc$ is below the target level $\Omega$ , otherwise 0
$Z'_{sc}$	Binary variable (1 if the impact in scenario $c$ is above the target limit, 0 otherwise)

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## SC RETROFITTING INTEGRATING MULTIPLE RENEWABLE ENERGY RESOURCES

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The recent increase in energy cost, particularly carbon-based fuels, coupled with global concerns related to  $CO_2$  emissions have resulted in serious efforts to redesign the production processes to substitute alternative energy resources. However, energy integration in conventional material supply chains (SC) has experienced a paradigm change, which leads to redesign production processes from a large-scale centralized approach to the in-situ exploitation of renewable sources. Nevertheless, less effort has yet expended in attempting to ensure renewable energy integration comparing to independent industries. However, this aspect creates a new pattern of resource-based energy integrated SCs. Recently, Martín & Grossmann (2017, 2018) evaluate the use of the available renewable resources and the optimal integration of technologies to meet the demand for fuels and power simultaneously. Furthermore, they proposed the most efficient combination of an integrated facility to use renewable sources, solar and wind energy, biodiesel production with no area limitation. Some studies, such as one by Yuan & Chen (2012), presented overviews concerning integration possibilities different renewable resource combinations. Hence, the absence of a holistic model predicting the benefits of renewable integration compared to an energy-independent production system motivated this thesis author to address this issue. Besides, large-scale demand, such as a regional or country-level, requires a model capable of responding to the integration of resources at this large scale. The studies conducted recently have focused on specific technologies and addressed particular cases. Hence, a generic and systematic approach is needed to explore and assess a large set of alternative configurations. Therefore, this chapter proposes various possible combinations of integrated renewable resources, particularly solar and wind energy, in addition to the cogeneration power plant to multi-technology process plants. Afterward, energy integration benefits are evaluated, compared to an individual system. The chapter contains sections as follows. Section 6.1 describes the problem statement. Next, section 6.2 discusses the main model assumptions and solution procedures for formulating multi-objective mixed-integer linear programming MILP models. Afterward, in section 6.3, the model is validated through a case study, and in section 6.4, the results are analyzed and discussed. Finally, in section 6.5, the conclusions are exposed.

### 6.1. Problem Statement

Here, conventional material SC is developed considering several large-scale possible renewable resources, as is depicted in Fig. 6.1.

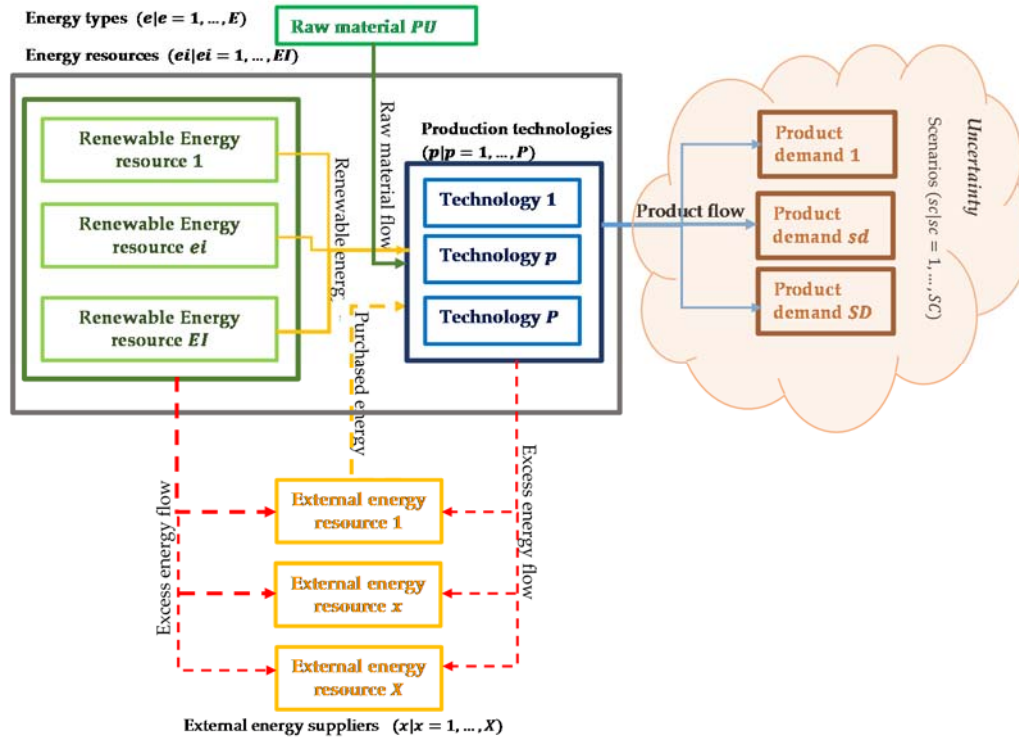


Fig. 6. 1. Renewable-based network integrated into a conventional material SC.

This network includes several potential regions capable of housing a set of plants with available production technologies and product flows to ship them to the associated markets. Assumed each industrial zone has its own sets of energy generation sites such as eco-industrial parks to satisfy production process energy demand.

The problem addressed in this work formally states as follows. Given are:

- A fixed time horizon divided into two sets of periods (months and years),
- A set of potential locations for the material/energy SC facilities, energy generation sites, and energy/material storage technologies
- Capacity limitations associated with these technologies (energy generation and production/storage processes)
- Prices of final products and raw materials and energy to purchase/sell
- Investment and operating costs of the production process/energy generation and environmental data ( $CO_2$  emissions associated with the network operation and a damage assessment model).

The goal of the study is to evaluate the benefits of an energy integration system compared with an individual one and to determine the optimal configuration of the material/energy integrated SC along with the associated planning decision that simultaneously maximizes the expected total net present value (NPV) and minimizes the environmental impact under demand uncertainty. Decisions to be made are of two types: structural and operational. The former include the number, location, and capacity of the plants, warehouses, energy generation technologies to be set up, their capacity expansion policy, and the transportation links between the integrated SC entities. The operational decisions are the production rate at the plants in each period, the flows of materials and energy between plants, energy generation sites, warehouses, energy and product markets, and the sales of final products.

## 6.2. Mathematical Model

In this section, a MILP formulation is presented, based on the model introduced by Mele et al. (2011), which addresses the design and planning of sugar-bioethanol SCs, and further expanded to consider a multi resource-based energy integration. The last was presented initially by Alabert et al. (2016).

The environmental concerns considering  $CO_2$  emissions are included along with the traditional economic objective, giving rise to a bi-criteria decision-making problem. The mathematical formulation considers all possible configurations of the future energy/material SC and all technical aspects associated with the SC performance.

As mentioned above, the specific models' task is to treat each technology's characteristics and translate them into the general model. The input parameters and the results of the previous calculations are transferred to the optimization model to work with global units.

After introducing the specific parameters of each technology, mainly corresponding to prices and technical parameters, they are used in blocks of equations representing the behavior of each particular technology. The outcome of these equations are values applied to the general model. Regarding the specific models of autonomous resources, this configuration varies slightly. The reason is that renewable generation technologies such as solar and wind need to be fed by databases of atmospheric conditions for each period. In this way, Fig. 6.2 shows the general structure of the proposed data flow.

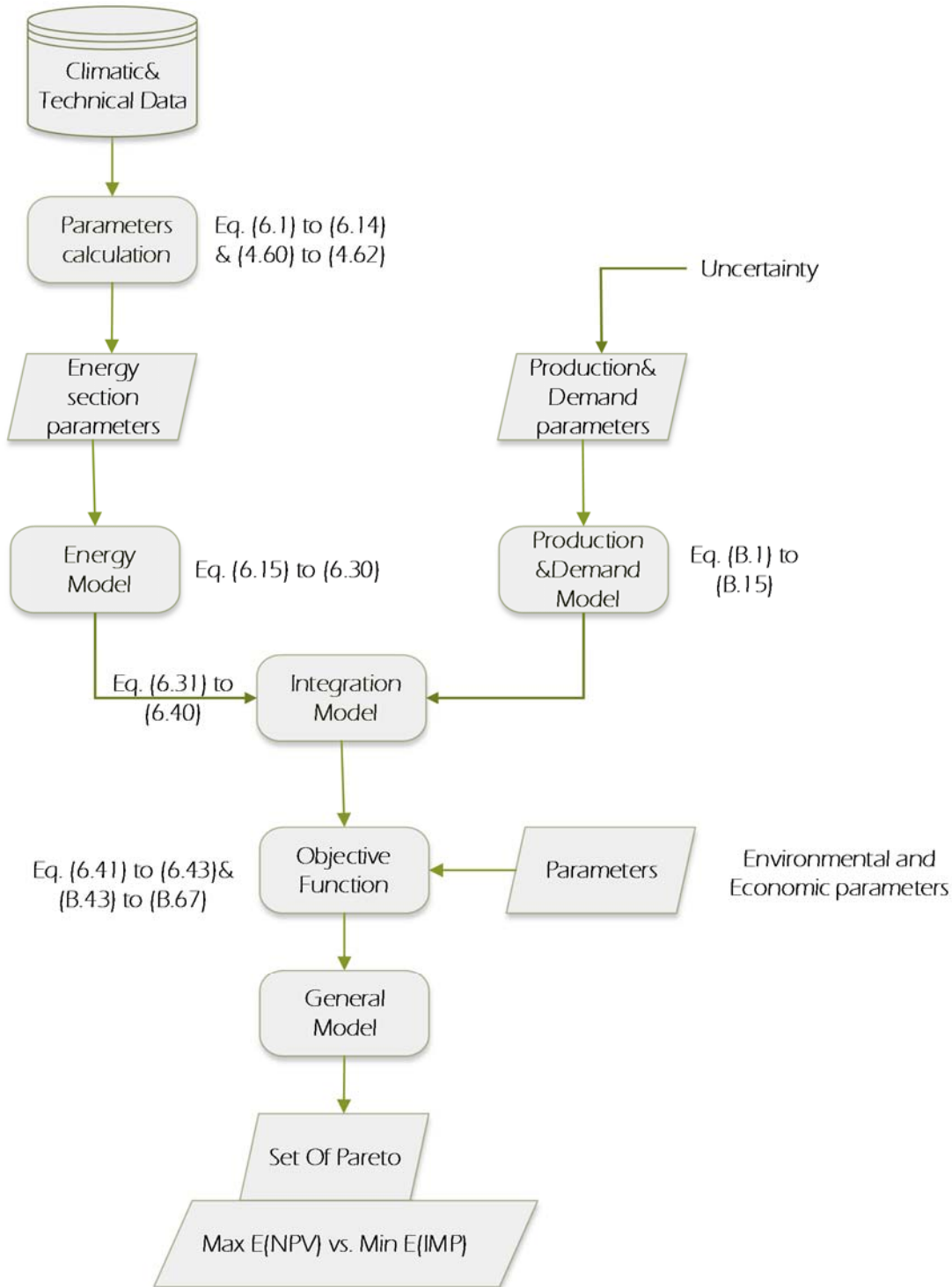


Fig. 6. 2. The general structure of the model.

The model equations are classified into two parts; the adopted model part (Mele et al., 2011) and the extended part. On the other hand, the model includes three main blocks of equations: material production and flows; energy generation and flows; objective functions. The production and demand model (Eq. B.1 to B.15) is the same as Chapter 5 provided in Appendix B.3. The following



section proposes parameter calculations, energy section parameters, energy model, and integration model.

### 6.2.1. Energy generation constraints section

This section details the mathematical formulation of each specific model corresponding to possible technology to be installed to form the energy network. It stands out that it is not a finite number of technologies since the analyst can add more technologies by implementing the corresponding specific models. It is also not necessary that the dimensioned system incorporates them all but, at the user level, it will first define the possible technologies to be installed (regarding the parameter of each power or maximum capacity model) and, then the model will solve what combination of those that are possible is optimum.

The equations corresponding to the installation limits and the energy balance apply to all flows for the total energy generated in each time interval. Here, the model proposed by Alabert et al. (2016) is extended and modified, but before that, it requires introducing pre-optimization equations of the individual system components.

#### 6.2.1.1. Modeling of the individual system components

The developed model is generic, and the formulations presented in section 6.2 can be applied to any small-scale to large-scale problems providing adequate data of resource availability, climate, and demand. Table 6.1 introduces the energy technologies implemented in use in the model.

Table. 6. 1. Enumeration and classification of specific models.

Autonomous Resources	External Resources
Windmill	Electrical grid
Photovoltaic solar	
Cogeneration power plant	

Parameter calculations of the cogeneration power plant were explained in **section 4.4.1.1** through equations (4.60) to (4.62) of **Chapter 4**. Parameter calculations of the windmill and solar photovoltaic panel are described in the following:

#### I. Horizontal axis windmill parameters calculations

The horizontal axis windmill model is presented based on the study conducted by Manyonge et al. (2012). The modification referring to the limiting factor is highlighted. The previous model was based on the maximum number of turbines, while in this case, it has been transformed into the maximally available surface so that the equivalent surface parameter occupied by a turbine is introduced. The model used for power coefficient  $CP$  is given as in Fernando et al. (2015).

In the pre-optimization phase (the parameter calculations), it is necessary to calculate the generated power  $TurbPw_{g,t}$  of a turbine in region  $g$  and period  $t$ . The generated power depends on the power coefficient  $Cp_{g,t}$  and captured power  $TurbPwHW_{g,t}$  (see Eq. (6.1)).

$$TurbPw_{g,t} = TurbPwHW_{g,t} \times Cp_{g,t} \quad \forall g,t \quad (6.1)$$

The captured power depends on the rotor diameter  $RotD$ , wind velocity  $WV_{g,t}$  and density of air  $\rho_{air}$ . Note that the generated power gets value if:

$CutInWV \leq WV_{g,t} \leq CutOutWV$  and  $CP_{g,t} \geq 0$ , else it is zero.

$$TurbPwHW_{g,t} = \frac{1}{2} \rho_{air} \pi \left(\frac{RotD}{2}\right)^2 WV_{g,t}^3 \quad \forall g,t \quad (6.2)$$

The analytical approximation model of the power coefficient is indicated as below:

$$CP_{g,t} = c_1 \left( \frac{c_2}{\Lambda_{g,t}} - \beta c_3 - c_4 \right) e^{-\frac{c_5}{\Lambda_{g,t}}} + \lambda_{g,t} c_6 \quad \forall g,t \quad (6.3)$$

Here,  $c_{1-6}$  are empirical power coefficient parameters,  $\beta$  is the azimuth angle of the pitch,  $\lambda_{g,t}$  tip speed ratio (often known as TSR) and  $\Lambda_{g,t}$  is tip speed ratio at  $i^{th}$  time step and these two design parameters are calculated by Eq. (6.4) and Eq. (6.5):

$$\lambda_{g,t} = \frac{\omega nom \left(\frac{2\pi}{60}\right) \left(\frac{RotD}{2}\right)}{WV_{g,t}} \quad \forall g,t \quad (6.4)$$

$$\frac{1}{\Lambda_{g,t}} = \frac{1}{\lambda_{g,t} + 0.08\beta} - \frac{0.035}{\beta^3 + 1} \quad \forall g,t \quad (6.5)$$

Note that  $\lambda_{g,t}$  depends on the nominal turbine rotation speed ( $\omega nom$ ) and the rotor diameter ( $RotD$ ), and  $\Lambda_{g,t}$  depends on the azimuth angle of the pitch ( $\beta$ ).

In addition to  $TurbPw_{g,t}$ , the design parameter  $PwIMax_{ei}$  should be calculated. This parameter denotes the maximum power to be installed.

$$PwIMax_{ei} = \frac{SurfMaxHW}{SurfPwHW} \quad ei = wind\ energy \quad (6.6)$$

Here, the turbine surface per generated power ( $SurfPwHW$ ) is necessary to calculate through the equivalent surface area of a turbine ( $SurfTEqHW$ ) and nominal turbine power ( $TurbNomPw$ ).

$$SurfPwHW = \frac{SurfTEqHW}{TurbNomPw} \quad (6.7)$$

Note that the parameters  $SurfMaxHW$ ,  $TurbNomPw$ , and  $SurfTEqHW$  vary in different turbine models. Eq. (6.8) defines the unit Price per power.

$$PrPwHW = \frac{TurbPr}{TurbNomPw} \quad (6.8)$$

Table. 6.2 describes the input parameters of the HW model based on the datasheet proposed in Appendix B.3 and Table. 6.3 explains the parameters to be calculated in the pre-optimization phase.

Table. 6. 2. Input parameters of a specific windmill model.

Identifier	Description	Unit
$\omega_{nom}$	Nominal turbine rotation speed	[RPM]
$RotD$	Rotor diameter	[m]
$WV_{g,t}$	Wind velocity in region $g$ and period $t$	[m/s]
$\beta$	The azimuth angle of the pitch	[°]
$c_{1-6}$	Empirical power coefficient parameters	[-]
$SurfTEqHW$	The equivalent surface area of a turbine	[m <sup>2</sup> /turb]
$TurbNomPw$	Nominal turbine power	[kW]
$SurfMaxHW$	Maximum surface available for horizontal windmill axis	[m <sup>2</sup> ]
$TurbPr$	Price of a turbine	[€]
$\rho_{air}$	Density of air	[kg / m <sup>3</sup> ]
$CutInWV$	Cut -in speed	[m/s]
$CutOutWV$	Cut -out speed	[m/s]

Table. 6. 3. Calculated parameters in the pre-optimization phase for a specific windmill model.

Identifier	Description	Unit
$\lambda_{g,t}$	The tip speed ratio (often known as TSR)	[-]
$\Lambda_{g,t}$	The tip speed ratio at $i^{th}$ time step	[-]
$CP_{g,t}$	Power coefficient in region $g$ and period $t$	[-]
$SurfPwHW$	The relation between the surface and power	[m <sup>2</sup> /kW]
$PwIMax_{ei}^*$	Maximum power to install	[kW]
$PrPwHW$	Price per unit of power	[€/kW]
$TurbPwHW_{g,t}$	Captured power by a turbine in region $g$ and period $t$	[kW]
$TurbPw_{g,t}$	Power generated by a turbine in region $g$ and period $t$	[kW]

\*  $ei$  denotes wind energy

## II. Photovoltaic arrays parameter calculations

The photovoltaic energy generation model is based on the study by Darras et al. (2010). It operates by importing the radiation and temperature data from a database to calculate the power per unit

of the installed surface. An incorporated variation considers surface equivalent occupied by each panel, distinguishing between catchment surface and occupied surface.

This section aims to calculate two main parameters of the power per available surface ( $PwSurfPV_{g,t}$ ) and the maximum power to install ( $PwIMax_{ei}$ ) defined by Eq. (6.9) and (6.10).

$$PwSurfPV_{g,t} = \frac{PanPw_{g,t}}{PanSurf} \quad \forall g, t \quad (6.9)$$

$$PwIMax_{ei} = \frac{SurfMaxPV}{SurfPwPV} \quad ei = \text{solar energy} \quad (6.10)$$

Hence, it is necessary to calculate first the power generated by a panel ( $PanPw_{g,t}$ ) and the surface per unit of power ( $SurfPwPV$ ). Note that the panel surface ( $PanSurf$ ), the maximum available surface ( $SurfMaxPV$ ), panel nominal power ( $PanNomPw$ ), and the equivalent surface ( $SurfTEqPV$ ) depend on the solar panel model and vary model to model.

$$PanPw_{g,t} = \frac{GT_{g,t}}{GR} [PanNomPw + \mu_p \times PanNomPw \times (PanT_{g,t} - STA)] \quad \forall g, t \quad (6.11)$$

Here,  $GT_{g,t}$  is the solar irradiance in region  $g$  and period  $t$ . The panel temperature  $PanT_{g,t}$  is calculated as below, and other parameters in the above equation are defined in Table. 6.4. Note that the panel temperature depends on the ambient temperature ( $TA_{g,t}$ ) and the solar irradiance in region  $g$  and period  $t$ .

$$PanT_{g,t} = TA_{g,t} + GT_{g,t} \times \frac{NOCT-20}{800} \quad \forall g, t \quad (6.12)$$

For attaining the maximum power to install ( $PwIMax_{ei}$ ), it is necessary to calculate the surface per unit of power ( $SurfPwPV$ ), defined by Eq. (6.13).

$$SurfPwPV = \frac{SurfTEqPV}{PanNomPw} \quad (6.13)$$

In addition, Eq. (6.14) defines the panel price per unit of power:

$$PrPwPV = \frac{PanPr}{PanNomPw} \quad (6.14)$$

Table. 6.4 describes the input parameters of the photovoltaic model based on the datasheet proposed in Appendix B.3 and Table. 6.5 explains the parameters to be calculated in the pre-optimization phase.

Table. 6. 4. Input parameters of a specific photovoltaic model.

Identifier	Description	Unit
$TA_{g,t}$	Ambient temperature in region $g$ and period $t$	[°C]
$GT_{g,t}$	Solar irradiance in region $g$ and period $t$	[kW/m <sup>2</sup> ]
$NOCT$	Normal Cell Operating Temperature	[°C]
$GR$	Solar irradiance under standard condition	[kW/m <sup>2</sup> ]
$SurfTEqPV$	The equivalent surface occupied by a panel	[m <sup>2</sup> /panel]
$PanNomPw$	Panel nominal power	[kW]
$SurfMaxPV$	Maximum surface available for a photovoltaic	[m <sup>2</sup> ]
$PanPr$	Price of a panel	[€]
$\mu_p$	Coefficient of variation of power per temperature	[% / °C]
$STA$	The ambient temperature under standard condition	[°C]
$PanSurf$	Panel surface	[m <sup>2</sup> ]

Table. 6. 5. Calculated parameters in the pre-optimization phase for a specific photovoltaic model.

Identifier	Description	Unit
$PwSurfPV_{g,t}$	Power per available surface in region $g$ and period $t$	[kW/m <sup>2</sup> ]
$SurfPwPV$	The relation between the surface and power	[m <sup>2</sup> /kW]
$PwIMax_{ei}^*$	Maximum power to install	[kW]
$PrPwPV$	Panel price per unit of power	[€/kW]
$PanPw_{g,t}$	Power generated by a panel in region $g$ and period $t$	[kW]
$PanT_{g,t}$	Temperature of a panel in region $g$ and period $t$	[°C]

\*  $ei$  denotes solar energy

### 6.2.1.2. Individual resources pre-optimization model

The importance of the pre-optimization calculations introduced previously is to calculate the maximum power to be installed and the power generation, which refers to the surface unit. Once this is done, the values are exported to the optimization model.

#### A. Windmill pre-optimization model

$$SurfInsHW_{ei,g} = PwI_{ei,g} \times SurfPwHW \quad (6.15)$$

$$\forall g, \\ ei = \text{wind energy}$$

$$TurbNum_{ei,g} = \frac{PwI_{ei,g}}{TurbNomPw} \quad (6.16)$$

$$PwIG_{ei,g,t,sc} = TurbNum_{ei,g} \times TurbPw_{g,t} \quad (6.17)$$

$$PwIGMax_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \quad (6.18)$$

$$\forall g, t, sc \\ ei = \text{wind energy}$$

$$PwIGMin_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \times MinPwHW \quad (6.20)$$

### B. Solar photovoltaic pre-optimization model

$$SurfPV_{ei,g} = \frac{PwI_{ei,g} \times PanSurf}{PanNomPw} \quad (6.21)$$

$$\forall g, \\ ei = \text{solar energy}$$

$$SurfInsPV_{ei,g} = PwI_{ei,g} \times SurfPwPV \quad (6.22)$$

$$PwIG_{ei,g,t,sc} = SurfPV_{ei,g} \times PwSurfPV_{g,t} \quad (6.23)$$

$$PwIGMax_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \quad (6.24)$$

$$\forall g, t, sc \\ ei = \text{solar energy}$$

$$PwIGMin_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \times MinPwPV \quad (6.25)$$

For both photovoltaic solar panel and windmill, the installation capacity constraints on energy generation are expressed in equations (6.26) and (6.27):

$$PwI_{ei,g} \leq PwIMax_{ei} \quad \forall ei, g \quad (6.26)$$

$$\sum_{ei} PwI_{ei,g} \times SurfPwI_{ei} \leq SurfTMax \quad \forall g \quad (6.27)$$

### C. Cogeneration unit pre-optimization model

The cogeneration power plant is considered a renewable energy generator. Here,  $EnIG_{ei,g,t,sc}$  represents the energy generated in the cogeneration power plant in sub-region  $g$ , in period  $t$  and scenario  $sc$ .

$$EnIG_{ei,g,t} = P_{eg} \times SL \times W_{i,g,t,sc} \quad \forall i, g, t, sc \\ ei = \text{biomass energy} \quad (6.28)$$

$$PwIGMax_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \quad \forall g, t, sc \quad (6.29)$$

$$PwIGMin_{ei,g,t,sc} = PwIG_{ei,g,t,sc} \times MinPgCO \quad ei = \text{biomass energy} \quad (6.30)$$

Here,  $P_{eg}$  is the power generated per ton of raw material,  $SL$  denotes time slot,  $W_{i,g,t,sc}$  is the waste amount produced from material  $i$  in region  $g$  in period  $t$ , and scenario  $sc$  and  $MinPgCO$  is defined as the minimum power generated coefficient.

Regarding integrated energy/material SC model and energy non-storable characteristics, **two different planning periods** (month  $t$  and year  $t''$  for the energy and material, respectively) are considered.

### 6.2.2. Modeling of the integrated system components

While the energy demand depends on the production process rate, the equations noted in this section link energy generation to the production system, and this way, it forms the integrated part of the model. All the equations representing energy generation belong to the general model. Equation (6.31) shows energy balance to meet the demand during a period  $t$ :

$$\sum_e \sum_{ei} [EnIJ_{e,ei,g,t,sc} \times EfIJ_{e,ei}] + \sum_{e \in EX(e,x)} \sum_x [EnXJ_{e,x,g,t,sc} \times EfXJ_{e,x}] = TotalDemand_{g,t,sc} \quad \forall g, t, sc \quad (6.31)$$

The total energy demand ( $TotalDemand_{g,t,sc}$ ) is equal to the energy demand needed per unit of raw material  $Demand_{g,t}$  multiplied by the amount of raw material  $PU_{i,g,t,sc}$  consumed in sub-region  $g$ , each period  $t$ , and scenario  $sc$ .  $EnIJ_{e,ei,g,t,sc}$  represents the energy flow between the energy generation unit  $ei$  and demand region  $g$ , each period  $t$  and scenario  $sc$  and  $EnXJ_{e,x,g,t,sc}$  is energy flow between an external energy resource and a demand point (production plant). The total flows should satisfy the total energy demand in each region.  $EfIJ_{e,ei}$  and  $EfXJ_{e,x}$  are conversion efficiencies between energy resources (internal and external resources) and production plants. The energy generated by each internal renewable resource will be transferred to the process plant to satisfy the energy demand or/and sold to the grid.

$$\sum_e EnIJ_{e,ei,g,t,sc} \times EfIJ_{e,ei} + \sum_{e \in EX(e,x)} EnIX_{e,ei,x,g,t,sc} \times EfIX_{e,x} = EnIG_{ei,g,t,sc} \quad \forall ei, g, t, sc \quad (6.32)$$

Acronym  $IJ$  denotes the flows between internal energy generation resource and demand spot  $IX$  refer to internal and external energy flows and,  $XJ$  is the flow between the external energy resource and demand spot.

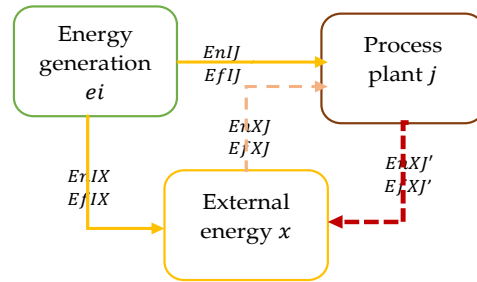


Fig. 6. 3. Flows and efficiencies between system elements.

The Big-M method is applied to define upper and lower generation limits so that equations result linear.  $Gn_{ei,g,t,sc}$  is a binary variable. The parameters  $PwIG_{ei,g,t,sc}$  and  $PwIGMin_{ei,g,t,sc}$  are used to calculate the power to install.

$$PwIG_{ei,g,t,sc} \leq PwIMax_{ei} \times Gn_{ei,g,t,sc} \quad \forall ei, g, t, sc \quad (6.33)$$

$$PwIG_{ei,g,t,sc} \geq -PwIMax_{ei} \times Gn_{ei,g,t,sc} \quad \forall ei, g, t, sc \quad (6.34)$$

$$PwIG_{ei,g,t,sc} \leq PwIGMax_{ei,g,t,sc} + PwIMax_{ei} \times (Gn_{ei,g,t,sc} - 1) \quad \forall ei, g, t, sc \quad (6.35)$$

$$PwIG_{ei,g,t,sc} \geq PwIGMin_{ei,g,t,sc} - PwIMax_{ei} \times (Gn_{ei,g,t,sc} - 1) \quad \forall ei, g, t, sc \quad (6.36)$$

The value of M should be large enough to make the problem feasible and small enough to reduce it. In this case, M corresponds to the maximum power  $PwIMax_{ei}$  to be installed.

### 6.2.2.1. External resource equations

The constraints corresponding to the installation limits and the energy balance according to the flows define the external energy resources section.

$$EnXP_{e,x,g,t,sc} = EnXJ_{e,x,g,t,sc} \times EfXJ_{e,x} \quad \forall g, t, EX(e, x), sc \quad (6.37)$$

$$EnXS_{e,x,g,t,sc} = \sum_{ei} EnIX_{e,ei,x,g,t,sc} \times EfIX_{e,x} \quad \forall g, t, EX(e, x), sc \quad (6.38)$$

$$PwXP_{e,x,g,t,sc} = EnXP_{e,x,g,t,sc} / SL \quad \forall g, t, EX(e, x), sc \quad (6.39)$$

$$PwXS_{x,g,t,sc} = EnXS_{e,x,g,t,sc} / SL \quad \forall g, t, EX(e, x), sc \quad (6.40)$$

$EnXP_{e,x,g,t,sc}$  and  $EnXS_{e,x,g,t,sc}$  are the energy quantities to buy and sell at each period on each external resource, which defines the corresponding  $PwXP_{e,x,g,t,sc}$  and  $PwXS_{x,g,t,sc}$  powers.

### 6.2.3. Objective function

The model explores the optimum economic and environmental performance of the network. The economic objective is represented by the net present value (NPV), whereas the environmental impact is quantified according to Life Cycle Assessment (LCA) principles explained in the previous chapter.

#### 6.2.3.1. Expected Net Present Value

The expected NPV is maximized as an objective function. Hence, the calculated NPV for each scenario  $sc$  is multiplied by the associated probability  $Prob_{sc}$  of each scenario  $sc$  as expressed in Eq. (6.41). The  $NPV_{sc}$  can be determined from the discounted cash flows  $CF_{t'',sc}$  generated in each of the time intervals  $t''$  in which the entire time horizon:

$$E[NPV] = \sum_{sc} Prob_{sc} \times NPV_{sc} \quad (6.41)$$

$$NPV_{sc} = \sum_{t''} \frac{CF_{t'',sc}}{(1+ir)^{t''-1}} \quad \forall sc \quad (6.42)$$

The equations related to cash flow calculations are provided in Appendix B.3.

#### 6.2.3.2. Expected environmental impacts

The environmental impact as an objective function is defined through the  $DAM_{sc}$  variable and to be minimized. The equations related to the life cycle inventory calculations are provided in Appendix B.3.

$$DAM_{sc} = GWPCul_{sc} + GWPPr_{sc} + GWPQ_{sc} \quad (6.43)$$



#### 6.2.4. Multi-objective equations

The overall bi-MILP formulation can be expressed in compact form as follows:

$$(M) \quad \min_{x, X, N} \{-E[NPV(x, X, N)]; E[DAM(x, X, N)]\}$$

s.t. constraints (6.1)-(6.43) and the equation provided in Appendix B

$$x \in \mathbb{R}, \quad X \in \{0,1\}, \quad N \in \mathbb{Z}^+$$

Note that the solution method is the same as in previous chapters, and it is provided in Appendix B. Here, the proposed multi-renewable energy resource integrated model shows more flexibility in managing energy demand. According to the integrated energy/material SC model and referring to the non-storable characteristic of energy, it is considered two different planning periods as mentioned previously.

### 6.3. Case study

The capabilities of the proposed model are tested through a case study based on the sugar-bioethanol industry of Argentina. The country is divided into 24 regions with associated ethanol, raw and white sugar demands. The employed data is from Mele et al. (2011), plus other additional information provided in Appendix section B.3.

#### 6.3.1. Windmill model

As a horizontal axis system, the 850 kW model of GAMESA G58 (Gamesa, 2008) is chosen. The design data set is depicted in Appendix section B.3.

Regional wind velocity  $WV_{g,t}$  was extracted from The world Meteorological Service Data Base ("Home | World Weather Information Service"). Fig. 6.4 shows the calculated regional power coefficient  $C_p$  and how it varies during a year. The graph indicates the availability of wind power during a year in each region of Argentina.

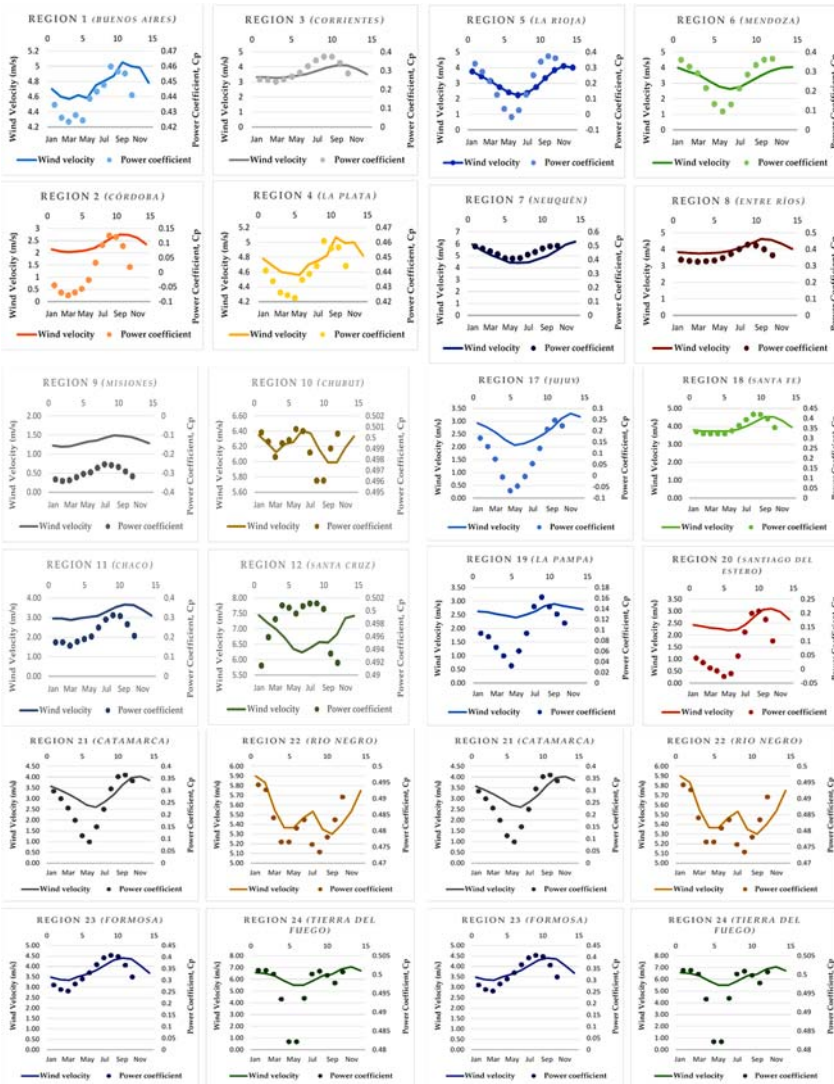


Fig. 6. 4. Regional wind velocity and associated power coefficient  $C_p$  calculated for each month of a year.

The obtained results prove that the regions with more stability in wind velocity and fewer variations in  $C_p$  (i.e.,  $g_3, g_7, g_8, g_{11}, g_{15}, g_{18},$  and  $g_{23}$ ) are potentially assumed to install wind turbines. Furthermore, to obtain  $TurbPw_{g,t}$  (the power generated by a turbine in region  $g$  and during month  $t$  (Eq. (6.8)), it is necessary to calculate the power coefficient  $C_p$  and the captured power by each turbine ( $TurbPw_{HW_{g,t}}$ ) corresponding to each region based on the design parameters of GAMESA G58 and metrological data (see Appendix B.3). The power generated in region  $g$  and month  $t$  has been calculated and proposed in Table 6.2. Note that the maximum number of the windmill is assumed to be 60. The pre-optimization parameters are depicted in the following:

Table. 6. 6. Pre-optimization parameters.

<b>SurfPwHW</b>	<b>3.48</b>	<b>[m<sup>2</sup>/kW]</b>
<b>PwIMax<sub>ei</sub>*</b>	<b>43000</b>	<b>[kW]</b>
<b>PrPwHW</b>	<b>882.35</b>	<b>[€/kW]</b>

\* *ei* denotes wind energy

Table. 6. 7. Generated power calculated for each region in each month.

		Month											
		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
Region		<i>TurbPw<sub>g,t,sc</sub></i> (kW)											
(Buenos Aires)	g1	58.70	53.95	52.57	54.88	53.03	61.15	64.17	67.26	77.01	74.23	73.14	62.65
(Córdoba)	g2	0	0	0	0	0	0	0	0	0	0	0	0
(Corrientes)	g3	12.15	11.95	10.98	12.15	13.82	16.55	22.01	28.68	33.82	33.82	25.52	16.07
(La Plata)	g4	62.65	58.21	53.95	53.03	52.11	58.70	61.15	64.68	78.13	73.68	74.23	64.68
(La Rioja)	g5	22.29	14.47	8.49	0	0	0	0	3.40	11.95	24.92	33.46	30.01
(Mendoza)	g6	30.01	22.29	16.79	8.66	0	0	0	8.49	15.84	24.02	30.01	31.36
(Neuquén)	g7	134.97	101.10	77.01	61.15	45.95	45.53	46.80	59.18	72.59	100.46	134.97	153.19
(Entre Ríos)	g8	24.62	23.15	22.29	22.86	23.73	26.76	33.10	42.62	55.20	52.61	42.47	30.79
(Misiones)	g9	0	0	0	0	0	0	0	0	0	0	0	0
(Chubut)	g10	166.51	158.17	148.87	157.00	159.35	171.36	168.33	151.17	138.69	138.69	153.49	165.31
(Chaco)	g11	0	0	0	0	6.85	7.76	11.71	16.58	19.97	19.19	13.55	7.99
(Santa Cruz)	g12	263.59	240.48	221.41	196.42	166.51	157.59	170.14	184.98	183.72	205.50	254.41	261.46
(Salta)	g13	8.72	6.63	0	0	0	0	0	0	8.23	16.23	19.97	14.52
(San Juan)	g14	31.30	24.60	16.94	9.76	0	0	7.76	13.87	22.01	30.29	36.37	36.09
(San Luis)	g15	46.83	43.07	40.08	34.99	33.12	37.20	48.77	63.56	78.77	84.80	77.09	59.85
(Tucumán)	g16	13.07	10.91	8.82	0	0	0	0	7.61	16.63	25.98	25.73	20.22
(Jujuy)	g17	0	0	0	0	0	0	0	0	0	8.00	11.55	9.25
(Santa Fe)	g18	23.73	21.82	21.82	21.82	21.82	24.72	30.85	40.02	50.91	50.53	41.01	28.36
(La Pampa)	g19	0	0	0	0	0	0	0	0	0	0	0	0
(Santiago del Estero)	g20	0	0	0	0	0	0	0	0	7.48	8.00	0	0
(Catamarca)	g21	17.64	13.60	9.69	0	0	0	0	9.25	19.12	29.18	30.85	25.22
(Rio Negro)	g22	132.03	127.21	107.63	95.81	95.81	102.17	106.53	94.77	91.68	97.91	106.53	121.29
(Formosa)	g23	15.26	12.90	12.22	15.84	18.91	23.73	31.71	41.01	45.11	43.03	31.13	20.32
(Tierra del Fuego)	g24	185.29	179.00	162.67	129.61	104.34	104.34	130.21	162.67	173.49	211.26	228.49	198.83

Based on Alabert et al. (2016 a), the minimum energy generation coefficient *MinPwHW* is assumed to be equal to 1, and the operational price per unit of wind energy *PrEnHW* is considered to be 0 €/kWh.

### 6.3.2. Photovoltaic Arrays model

The **Kyocera KD225GH-4YB2** model is selected as a photovoltaic solar generator because of the case study discussed in this work. Related data is shown in Appendix B.3. Solar irradiance  $GT_{g,t}$  is calculated using the Solar Electricity Handbook (Boxwell, 2010) for each month  $t$  in each region  $g$  (Fig. 6.5).

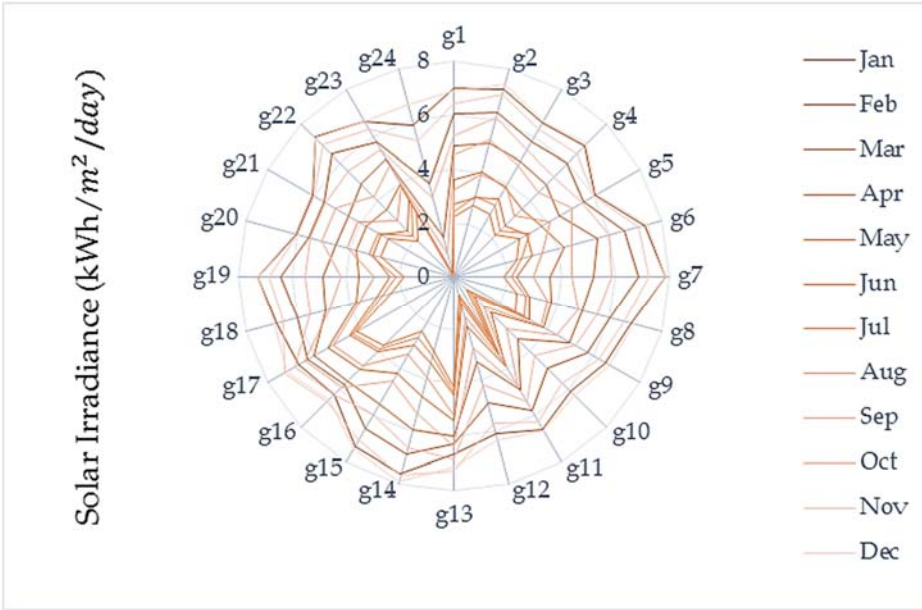


Fig. 6. 5. Solar Irradiance GT, associated with regions in each period.

Ambient temperature  $TA_{g,t}$  is extracted from the world weather information service (“Argentina | World Weather Information Service”) and depicted in Fig. 6.6.

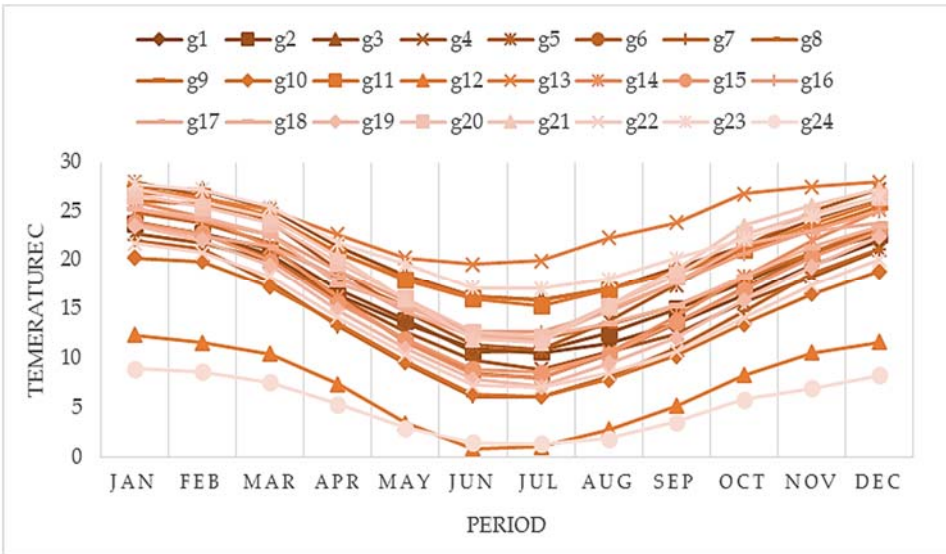


Fig. 6. 6. Temperature profile TA, associated with regions in each period.

The obtained results prove that the regions with more stability the solar irradiance (i.e.,  $g_2$ ,  $g_3$ ,  $g_5$ ,  $g_{13}$ , and  $g_{17}$ ) are potentially assumed to install solar photovoltaic arrays. Furthermore, to attain the amount of regional power generated per unit available area in each period  $t$  ( $PwSurfPV_{g,t}$ ) (Eq. (6.14)), it is necessary to calculate the generated power by each panel  $PanPw_{g,t}$  corresponding to each region based on the design parameters of Kyocera model KD225GH-4YB2 and solar irradiance data (see Table. 6.8). Thus,  $PwSurfPV_{g,t}$  in each region, and month  $t$  has been calculated and proposed in Table. 6.9.

Table. 6. 8. Solar power generated by the panel.

Region	Month												
	Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec	
	<i>PanPw<sub>g,t</sub>(kW)</i>												
(Buenos Aires)	1.98	1.72	4.6	4.57	4.62	4.58	4.75	4.81	4.87	5.05	5	4.98	4.78
(Córdoba)	2.03	1.79	2.06	2.03	2.06	2.1	2.2	2.4	2.62	2.75	2.73	2.61	2.35
(Corrientes)	1.84	1.61	3.32	3.27	3.33	3.41	3.53	3.74	3.96	4.11	4.11	3.86	3.51
(La Plata)	1.95	1.70	4.69	4.6	4.58	4.56	4.7	4.75	4.82	5.07	4.99	5	4.82
(La Rioja)	1.69	1.55	3.44	3.13	2.75	2.41	2.23	2.38	2.75	3.32	3.84	4.1	4
(Mendoza)	2.08	1.86	3.75	3.54	3.14	2.78	2.63	2.77	3.13	3.5	3.81	4	4.04
(Neuquén)	2.25	1.97	5.45	5.05	4.75	4.42	4.41	4.44	4.71	4.97	5.44	5.94	6.18
(Entre Ríos)	1.92	1.71	3.78	3.75	3.77	3.8	3.9	4.09	4.34	4.63	4.57	4.34	4.02
(Misiones)	1.81	1.60	1.19	1.21	1.27	1.33	1.36	1.43	1.49	1.48	1.45	1.37	1.28
(Chubut)	1.76	1.41	6.24	6.12	6.23	6.26	6.41	6.37	6.15	5.99	5.99	6.18	6.33
(Chaco)	1.84	1.61	2.95	2.88	2.97	3.02	3.08	3.31	3.53	3.67	3.64	3.40	3.10
(Santa Cruz)	1.82	1.47	7.20	6.99	6.71	6.35	6.24	6.39	6.57	6.56	6.81	7.35	7.42
(Salta)	1.85	1.75	3.01	2.85	2.56	2.31	2.21	2.38	2.67	3.11	3.52	3.67	3.44
(San Juan)	2.14	1.95	3.83	3.55	3.20	2.98	2.92	3.08	3.41	3.74	4.01	4.18	4.17
(San Luis)	2.08	1.86	4.35	4.28	4.14	4.09	4.20	4.49	4.80	5.08	5.19	5.05	4.72
(Tucumán)	1.76	1.63	3.27	3.15	2.93	2.65	2.47	2.68	3.08	3.53	3.88	3.87	3.68
(Jujuy)	1.88	1.78	2.77	2.55	2.27	2.07	2.13	2.28	2.48	2.73	3.10	3.30	3.18
(Santa Fe)	1.92	1.70	3.73	3.73	3.73	3.73	3.83	4.03	4.28	4.53	4.53	4.30	3.95
(La Pampa)	2.07	1.84	2.60	2.53	2.47	2.40	2.50	2.63	2.83	2.90	2.83	2.77	2.70
(Santiago del Estero)	1.70	1.56	2.37	2.30	2.27	2.20	2.23	2.45	2.78	3.07	3.10	2.97	2.65
(Catamarca)	1.69	1.56	3.40	3.20	2.97	2.70	2.60	2.85	3.18	3.63	3.98	4.03	3.85
(Rio Negro)	2.09	1.85	5.83	5.55	5.37	5.37	5.47	5.53	5.35	5.30	5.40	5.53	5.75
(Formosa)	1.85	1.60	3.37	3.33	3.50	3.63	3.80	4.05	4.30	4.40	4.35	4.03	3.68
(Tierra del Fuego)	1.76	1.08	6.50	6.30	5.87	5.50	5.50	5.88	6.30	6.43	6.88	7.07	6.73

Table. 6. 9. Power per available surface of a panel in each month and region.

Region	Month												
	Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec	
	<i>PwSurfPV<sub>g,t</sub> (kW/m<sup>2</sup>)</i>												
(Buenos Aires)	1.21	1.05	0.85	0.64	0.49	0.40	0.44	0.58	0.81	0.93	1.12	1.20	1.21
(Córdoba)	1.23	1.09	0.89	0.72	0.55	0.50	0.56	0.71	0.94	1.07	1.21	1.27	1.23
(Corrientes)	1.12	0.98	0.84	0.67	0.59	0.48	0.55	0.69	0.83	0.94	1.08	1.13	1.12
(La Plata)	1.19	1.04	0.84	0.64	0.49	0.40	0.45	0.58	0.80	0.94	1.14	1.21	1.19
(La Rioja)	1.03	0.94	0.78	0.66	0.56	0.51	0.59	0.74	0.90	0.96	1.03	1.04	1.03
(Mendoza)	1.26	1.13	0.96	0.75	0.54	0.44	0.49	0.62	0.82	1.06	1.24	1.29	1.26
(Neuquén)	1.37	1.20	0.91	0.64	0.42	0.34	0.40	0.54	0.80	1.05	1.28	1.37	1.37
(Entre Ríos)	1.17	1.04	0.86	0.66	0.52	0.44	0.50	0.65	0.86	0.97	1.14	1.19	1.17
(Misiones)	1.10	0.97	0.85	0.67	0.57	0.47	0.54	0.67	0.77	0.91	1.07	1.14	1.10
(Chubut)	1.07	0.86	0.59	0.35	0.20	0.13	0.16	0.29	0.51	0.76	1.01	1.11	1.07
(Chaco)	1.12	0.98	0.84	0.67	0.59	0.48	0.55	0.69	0.83	0.94	1.09	1.14	1.12
(Santa Cruz)	1.11	0.89	0.61	0.36	0.20	0.13	0.17	0.30	0.52	0.78	1.04	1.15	1.11
(Salta)	1.12	1.06	1.02	0.93	0.78	0.73	0.76	0.90	1.10	1.16	1.23	1.21	1.12
(San Juan)	1.30	1.18	1.03	0.83	0.62	0.53	0.57	0.71	0.95	1.17	1.33	1.36	1.30
(San Luis)	1.26	1.13	0.97	0.75	0.54	0.44	0.49	0.62	0.82	1.06	1.24	1.29	1.26
(Tucumán)	1.07	0.99	0.96	0.87	0.71	0.66	0.70	0.85	1.04	1.09	1.15	1.12	1.07
(Jujuy)	1.14	1.08	1.04	0.95	0.80	0.75	0.79	0.93	1.13	1.19	1.25	1.23	1.14
(Santa Fe)	1.17	1.03	0.86	0.66	0.53	0.44	0.50	0.65	0.86	0.97	1.14	1.19	1.17
(La Pampa)	1.26	1.12	0.86	0.63	0.44	0.35	0.40	0.54	0.76	0.99	1.21	1.26	1.26
(Santiago del Estero)	1.03	0.95	0.78	0.66	0.56	0.51	0.59	0.73	0.89	0.95	1.03	1.04	1.03
(Catamarca)	1.03	0.95	0.78	0.66	0.56	0.51	0.59	0.73	0.89	0.95	1.02	1.04	1.03
(Rio Negro)	1.27	1.12	0.86	0.63	0.44	0.35	0.40	0.55	0.77	1.00	1.22	1.27	1.27
(Formosa)	1.12	0.97	0.86	0.69	0.59	0.48	0.55	0.69	0.84	0.94	1.08	1.13	1.12
(Tierra del Fuego)	1.07	0.66	0.28	0.03	0.00	0.00	0.00	0.00	0.17	0.57	0.97	1.22	1.07

Based on Alabert et al. (2016 a), the minimum energy generation coefficient  $MinPwPV$  is assumed to be equal to 1, and the operational price per unit of photovoltaic energy  $PrEnPV$  is considered to be 0 €/kWh. Maximum available surface for photovoltaic  $SurfMaxPV$  is 300000 m<sup>2</sup>. The pre-optimization parameters are depicted in the following:

Table. 6. 10. Pre-optimization parameters.

<b><i>SurfPwPV</i></b>	<b>6.67</b>	<b>[m<sup>2</sup>/kW]</b>
<b><i>PwIMax<sub>ei</sub>*</i></b>	<b>45000</b>	<b>[kW]</b>
<b><i>PrPwHW</i></b>	<b>3000</b>	<b>[€/kW]</b>

\*  $ei$  denotes solar energy

### 6.3.3. Cogeneration power plant

The cogeneration power plant has been explained in detail in Chapter 4 (section 4.4.1). It is assumed that the energy output per ton of sugarcane is 66 kWh/t, and the minimum energy generation coefficient  $MinPgCO$  is equal to 1. It is also assumed that the power plant capacity is 50 MW, and power generation is available continuously for 7800 hours annually. Based on IEA (2010), the estimated installation costs of the cogeneration plant is 800€/KW.

## 6.4. Results

Regarding the aim of proposing a quantitative tool, it targets at determining the optimal integration of renewable technologies to meet the energy (in this particular case electricity)

demand to produce the main products (sugar and ethanol) and cover the market demand over 12 months and during four years of the planning horizon. The bi-criteria model was written in GAMS and solved with the MILP solver CPLEX 12.9 on an Intel® Core™ i7-3770 Octa-core Processor 3.40 GHz and 7.88 GB of RAM. It is focused on minimizing the cost but also included results on the environmental sustainability of the network.

**Pareto set of solutions**

The optimality of the multi-objective problem is validated by obtained environmental impact (represented by  $kg\ CO_2$  emissions) and NPV that resulted in minimal GWP100  $-3.43 \times 10^9\ kg\ CO_2$  and maximal NPV  $\text{€}4.50 \times 10^9$ , respectively. In the following, in Fig. 6.7, the Pareto set of solutions is presented, in which each point implies an optimum network configuration. In the optimal area, there is minimum risk in making decisions. Between two points of A (Utopia) and B (Particular solution), NPV and GWP100 variations are negligible. Out of this bond, it faces dramatic changes and variations in both zones of Nadir and Utopia.

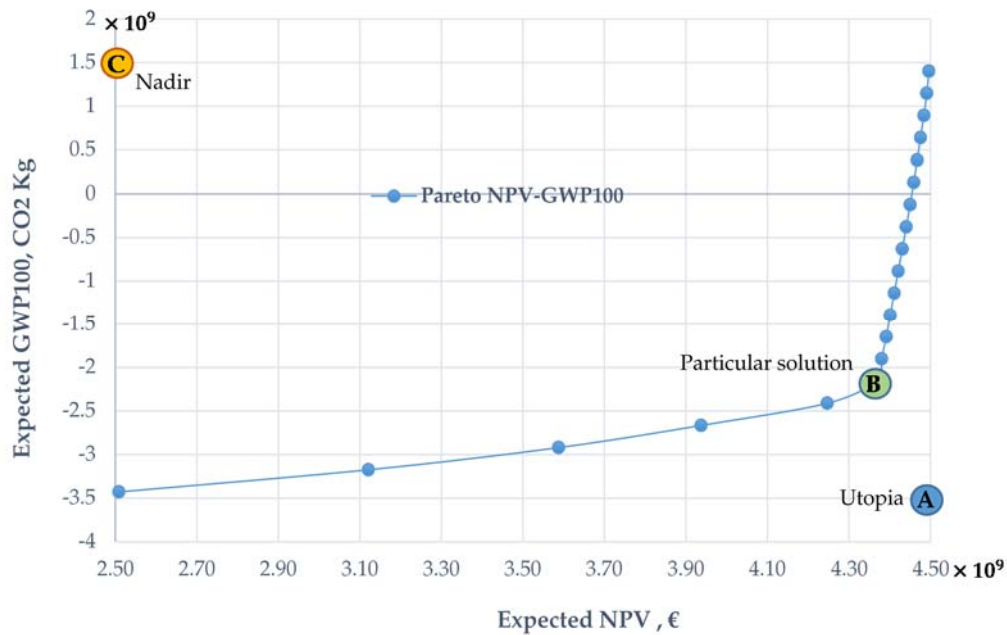


Fig. 6. 7. Pareto set of solutions.

**Design configuration for the particular solution**

The decision on the optimum configuration of the system mainly depends on its local resource (energy/raw material) availability and the installation and operational costs. Fig. 6.8 shows the SC configuration for a specific solution. In this, the SC consists of five sugar mills and ten ethanol distilleries. All these production plants are located in 10 regions, 5 of them having sugarcane plantations. These regions are the optimum locations because of raw material availability and stability in climatic conditions during a year. For instance, cogeneration power plants are installed in the zones having sugarcane plantations because of the availability of bagasse. Storage facilities are installed in four intermediate regions to facilitate product transportation.



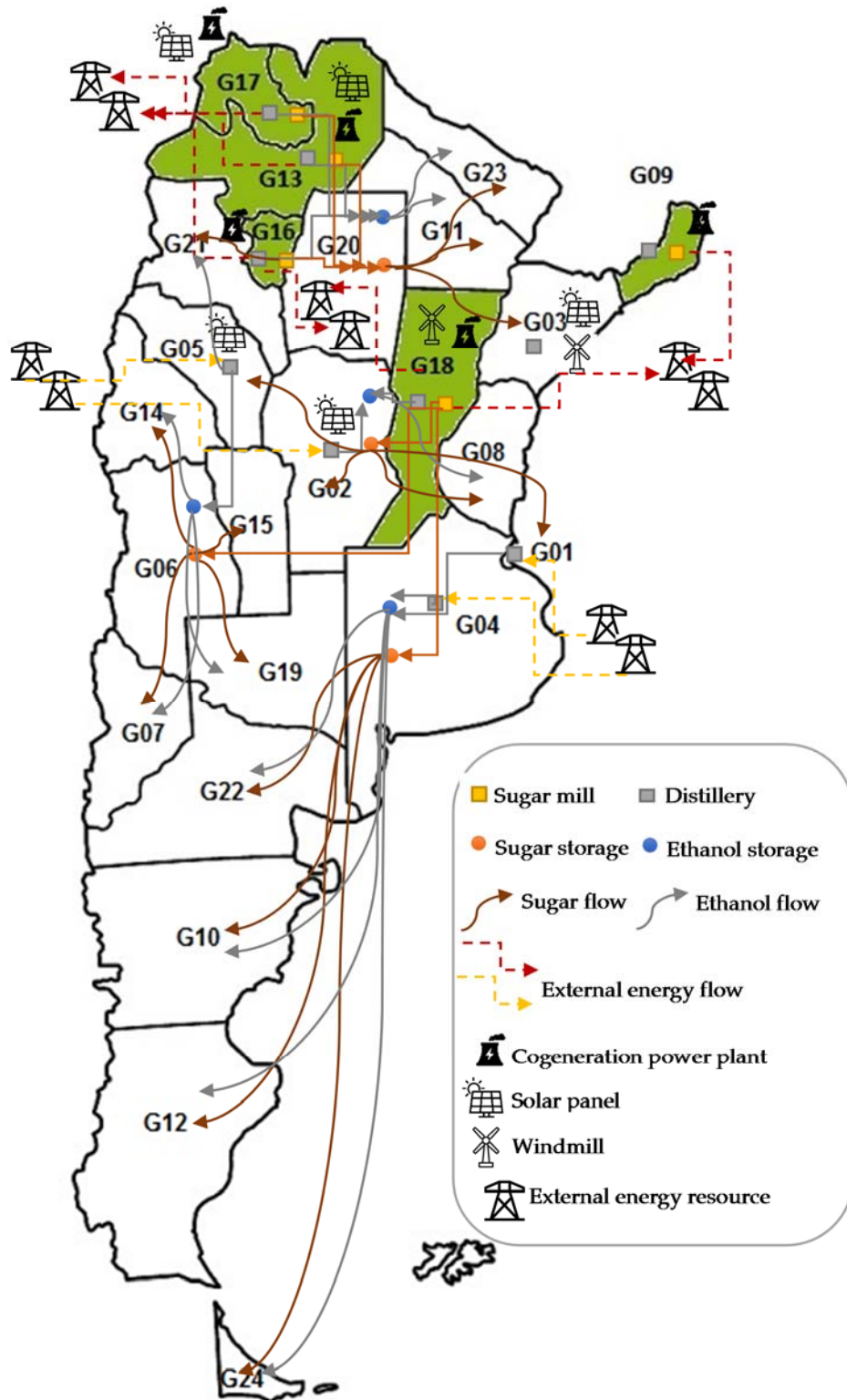


Fig. 6. 8. SC configuration for Particular solution (point B in Fig. 6.7).

There are solar arrays and windmills in regions where the most constant solar irradiation and higher  $C_p$  coefficient during a period with the installed capacity, as depicted in Table. 6.11.



Table. 6. 11. Regional Installed power capacity (MW) of each technology.

Particular solution	NPV (€)	GWP100 (kgCO <sub>2</sub> )	
	$4.37 \times 10^9$	$-2.16 \times 10^9$	
<b>Renewable energy generation technology</b>	Windmill	Solar panel	Cogeneration power plant
<b>Region</b>			
Córdoba ( $g_2$ )	-	√ 45MW	-
Corrientes ( $g_3$ )	√ 43MW	√ 22MW	-
La Rioja ( $g_5$ )	-	√ 45MW	-
Misiones ( $g_9$ )	-	-	√ 65MW
Salta ( $g_{13}$ )	-	√ 16MW	√ 65MW
Tucumán ( $g_{16}$ )	-	-	√ 65MW
Jujuy ( $g_{17}$ )	-	√ 16MW	√ 65MW
Santa Fe ( $g_{18}$ )	√ 22MW	-	√ 65MW

Hence, regions Misiones ( $g_9$ ), Salta( $g_{13}$ ), Tucumán( $g_{16}$ ), Jujuy( $g_{17}$ ), and Santa Fe( $g_{18}$ ) are autonomously able to provide their energy demand and sell their exceeded energy to the grid.

Regarding two extreme solutions of the Pareto curve, in the minimal GWP100 solution, the SC includes seven sugar mills utilizing sugar production technologies  $T_1$  and  $T_2$  five distilleries  $T_5$  that convert sugarcane into ethanol and produce bagasse as the waste. Most of these production facilities are located in five provinces that have sugar cane plantations. The consumption of sugar cane in this solution is 100% (i.e., all the available sugar cane is consumed). It results in significant reductions in  $CO_2$  emissions mainly because sugar cane cultivation is carbon negative, so that it has a negative contribution to global warming. Hence, the choice of the cogeneration in the minimum impact solution is motivated by their lower values of GWP100 and excess available bagasse as the cogeneration feedstock compared to other renewable energy generators.

Despite cogeneration power plants fed by residues of the process plant, those resources such as solar and wind generate energy independently. Hence, in regions with high Power Coefficients  $C_p$  and constant climatic condition such  $g_1$  (Autonomous City of Buenos Aires, CABA) and  $g_4$  (Buenos Aires), it is feasible to implement wind turbines, which results in a high contribution of wind power in the energy/material SC. It has the most effective share of 60% in the integrated energy/material SC, and the NPV improves to 43% than the minimum environmental impact solution. In the following, the share of each renewable resource for maximum NPV and minimum GWP100 solutions is depicted in Fig. 6.9.

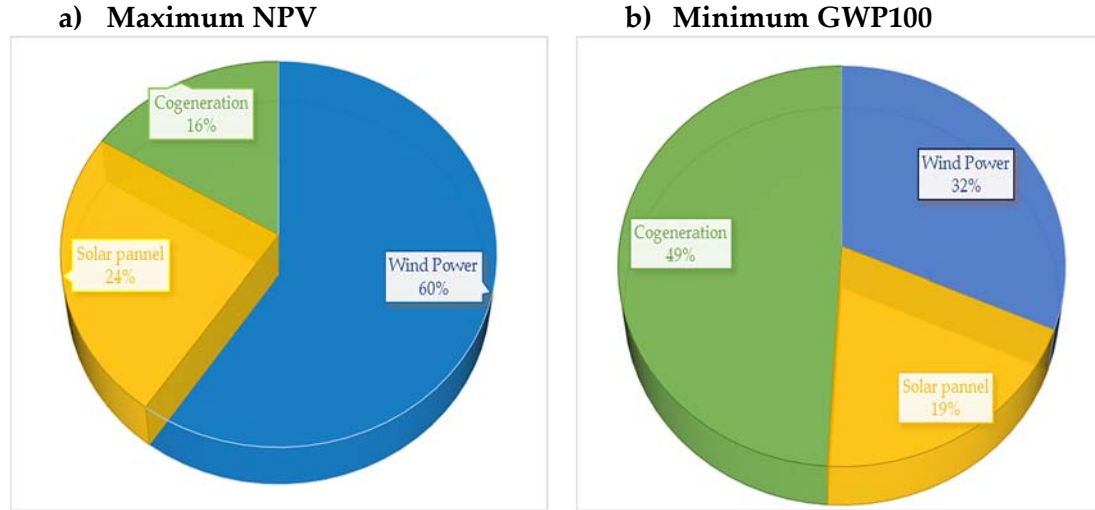


Fig. 6. 9. Renewable resource share in a) Maximum NPV b) Minimum GWP100 solutions.

In Table. 6.12, the benefits of the integrated material/energy SC are compared in short.

Table. 6. 12. Energy/Material SC comparison.

	Individual Material (Chapter 4)	Single integrated energy resource (Chapter 5)	Multi integrated energy resource (Chapter 6)
NPV(€)	$3.03 \times 10^9$	$3.18 \times 10^9$	$4.50 \times 10^9$
GWP100 (kg CO <sub>2</sub> )	$-1.72 \times 10^9$	$-1.8 \times 10^9$	$-3.43 \times 10^9$

**Uncertainty management and sensitivity analysis**

The problem is solved under product demand is uncertainty. Therefore, the number of scenarios is reduced to three (Max, Mean, Min) with an associated occurrence probability of 25%, 50%, and 25%, respectively (Case 5 Chapter 5). Fig. 6.9 illustrates the expected overall generated energy and energy demand during ten years (2018 to 2028). The network responds to the energy demand in all scenarios. Thus, the results assure that an energy surplus of 10 to 40% for all demand levels, especially in low demand scenarios, creates possibilities to market it.

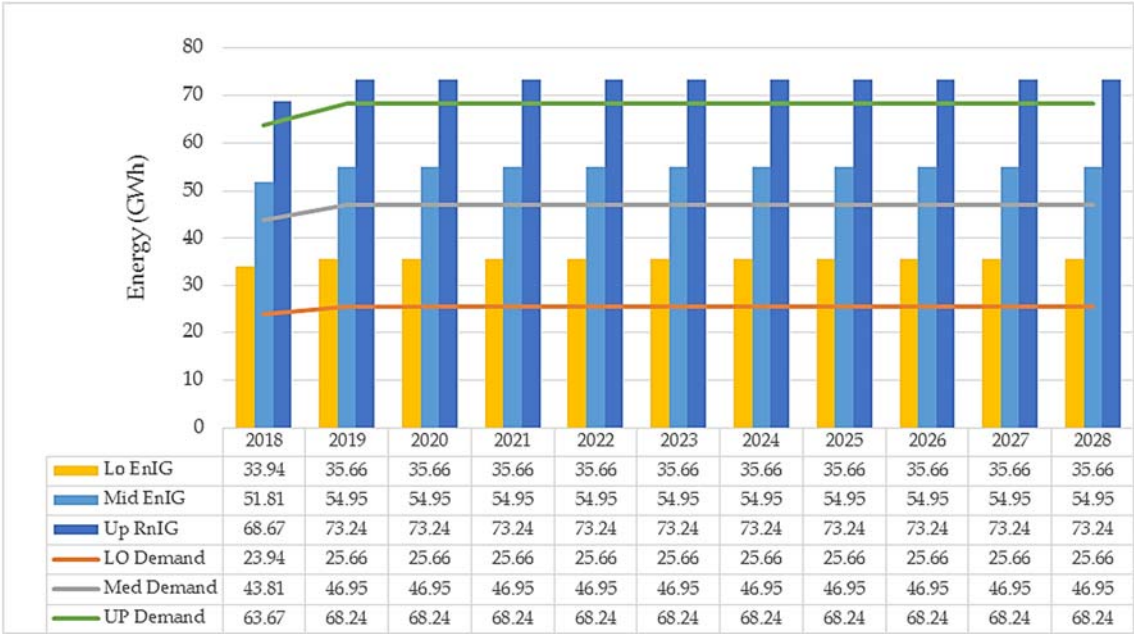


Fig. 6. 10. Expected energy generated/delivered for satisfying demand.

The sensitivity analysis is to determine which decision variables have more weight in the system's profitability. The associated ENPVs are obtained by changing  $\pm 20\%$  of unit investment and operation costs and, the results are depicted in Fig. 10. It is deduced that there is more sensitivity to the Capital Expenditure (CAPEX) than the Operating Expenses (OPEX). Hence, by 15% increase in CAPEX, NPV decreases 15% while, if OPEX increases the same, NPV drops only 7%.

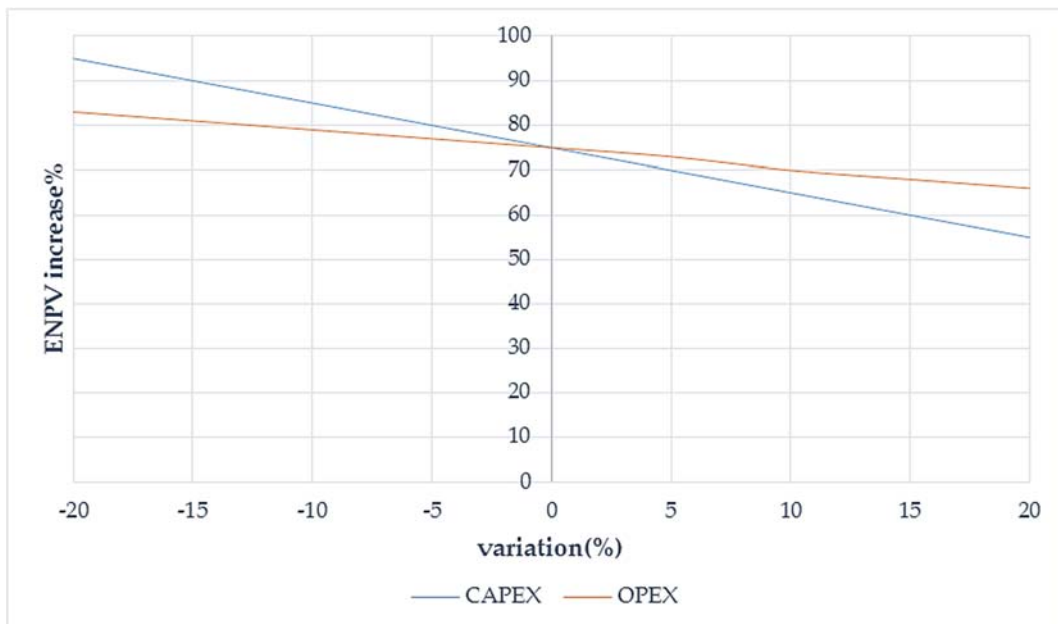


Fig. 6. 11. Sensitivity analysis for CAPEX and OPEX.

Following this notion, different scenarios are considered regarding the CAPEX values obtained by renewable investment unit cost variations.

Table. 6. 13. NPV associated with renewables unit cost variations.

Renewable investment cost variation (%)	$\infty$	-10	-20	-30	-40	-50	-60	-70	-80	-90	-100
NPV( $10^{10}$ €)	0.3	0.565	0.6	0.665	0.7	0.785	0.8	0.889	0.9	1.0	1.17

It is assumed two extreme situations: Ideal case as the unit installation cost of renewables is equal to 0, and the worst case of the unit installation cost of renewables is infinite. Figure 6.12 illustrates the results.

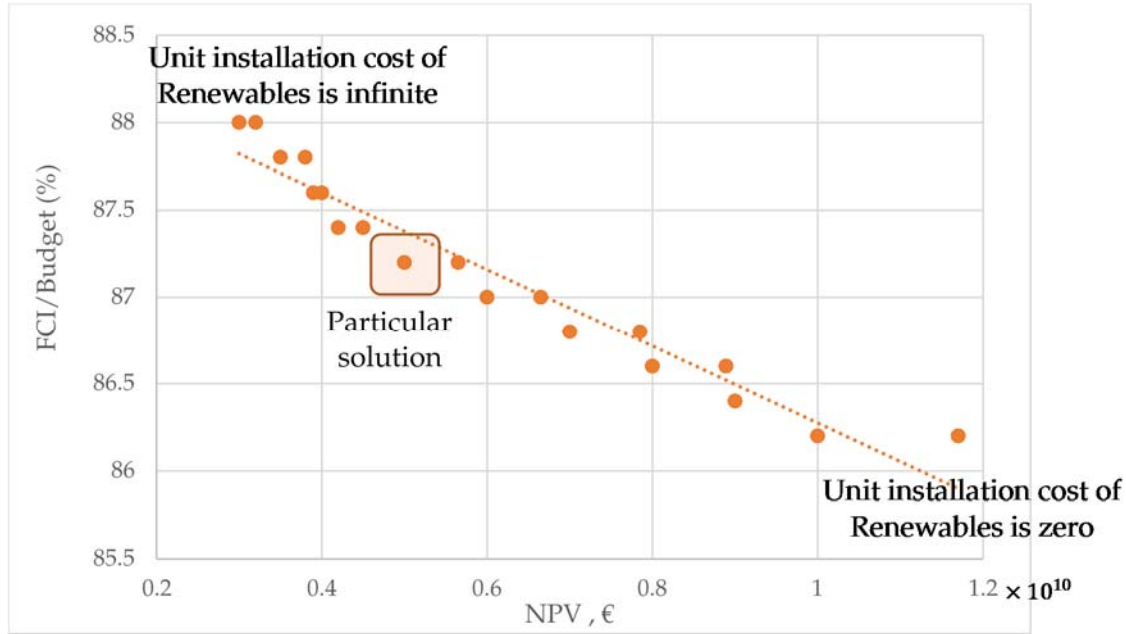


Fig. 6. 12. Fixed installation cost portion for each scenario versus NPV.

In the ideal scenario, the unit installation cost of renewables is assumed to be zero, so 87% of the total budget allocates for installing production plants with a maximum NPV amount of  $\text{€}1.17 \times 10^{10}$ . On the other side, as the unit installation cost of renewable is infinite, it reaches the base model (Melé et al., 2011) with 300 billion euros of NPV and more installation cost assigned. The area limited between two extremes represents the integrated system configurations that say with different installation unit costs of renewables, fixed cost investment share varies between 87 to 88 percent of the total budget, and we have different configurations with proper NPVs.

The share of installation costs of the ideal, particular, and worst cases in the budget are represented in Fig. 6.13. Here, FCI and CIns denote the fixed cost installation of the process plants and renewable energy generators.

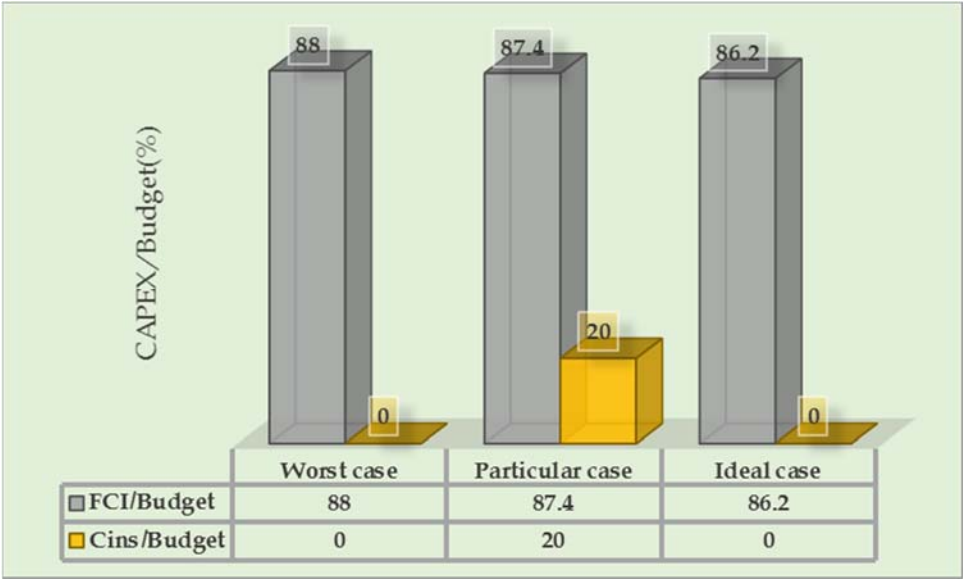


Fig. 6. 13. The cost of renewables and process plant installation for Ideal cases, Particular and Worst cases.

Note that in the worst case, the production plants need to provide energy from external resources, whereas in the ideal case, the internal energy demand is satisfied, and excess energy of 87.60 GWh is to sell annually (see Fig. 6.14).

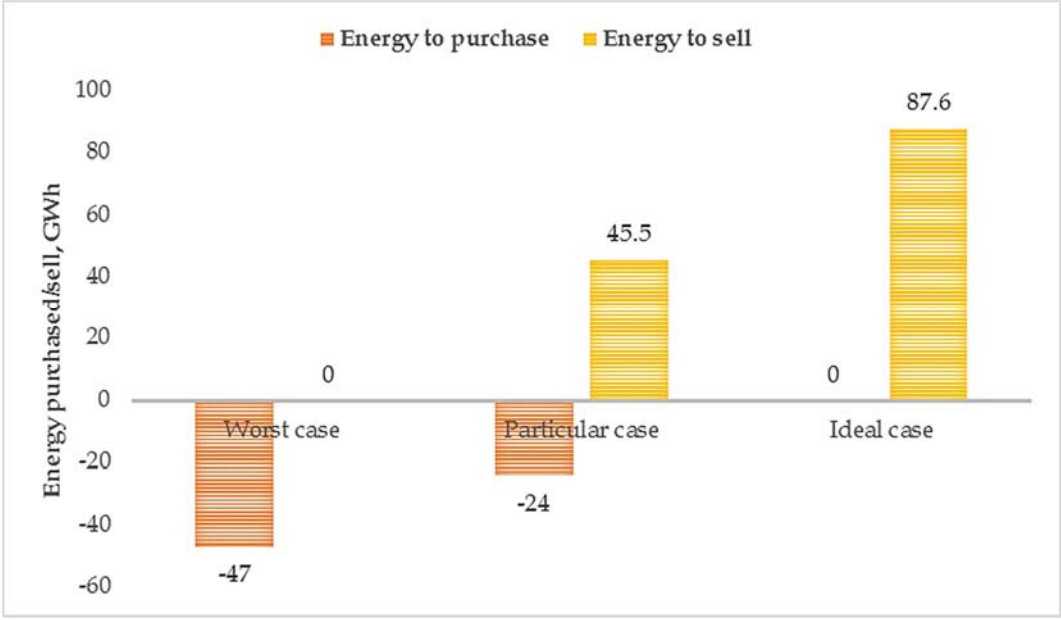


Fig. 6. 14. Purchase/Sell Energy amount in Ideal case, Particular and Worst cases.

In the worst case, and regarding the high operational cost (energy to buy), although it is invested more in production plant capacity installation, it is produced more petite than the ideal case (Fig. 6.14).

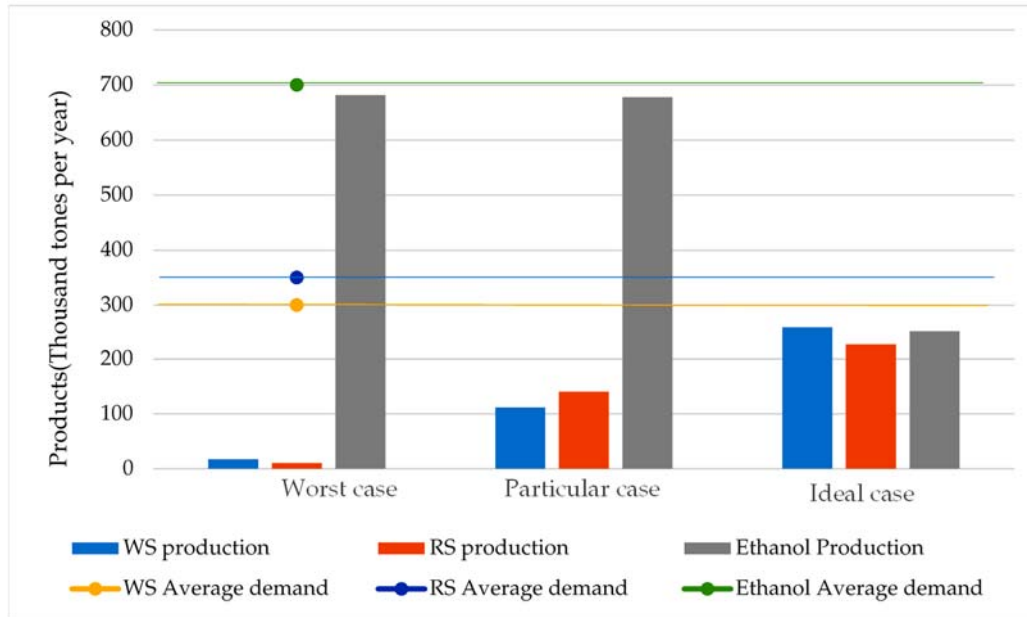


Fig. 6. 15. Production vs. Demand amount in Ideal case, Particular and Worst cases.

Since the operating costs in the energy section are almost zero, it motivates the production section to operate in a higher capacity. Thus, in the ideal case, the production capacity is maximum.

### 6.5. Conclusions

This chapter introduced a general model to optimize an integrated multi-energy/material SC with economic and environmental concerns. The model includes four segments of equations: material production, energy generation, integrated energy/material equations, and objective function, and it aimed to show the quantitative profitability of integration for both economic and environmental issues under uncertain conditions.

The model was applied to the same case study of previous chapters, i.e., the Argentinean sugar cane industry considered 24 regions of Argentina as potential sites and associated climatic features and availability of renewable energy resources. In the first part, the Pareto solutions were proposed and discussed the economic profitability of renewable resources integration. Focused on a particular optimum configuration by the Pareto set of solutions, the exploitation benefits of renewable energies integration in a production process system were analyzed.

Compared to the initial model proposed in chapter 4, the economic criteria represented by NPV increased significantly along with environmental impacts decrease. It deduced that the energy integration motivates the processing system to exploit the maximum production capacity. Thus, it leads to improving the economic and environmental criteria simultaneously. This deduction illustrates in the ideal, particular, and worst cases. For instance, in the worst case, it is obliged to

purchase energy from external resources and, the demand satisfaction level is too low for raw and white sugar.

On the other hand, in the ideal case, the system tends to generate as much energy as possible. So there are more sites involve in renewable energy installation, and the system tends to generate more energy than material.

In this particular case, although the integrated system should deal with different tactical and strategic limitations, an integrated network is compromising with all these restrictions and propose a flexible and robust solution. As a result, it satisfies the internal energy demand in the regions with sugarcane plantations and also generates exceeded energy to sell.

## 6.6. Nomenclature

### *Abbreviations*

LCA	Life Cycle Assessment
CAPEX	Capital Expenditure
MILP	Mixed Integer Linear Programming
NPV	Net Present Value
OPEX	Operating Expense
SC	Supply Chain

### *Index*

$e$	Set for Energy types ( $e e = 1, \dots, E$ )
$ei$	Set for Energy resources ( $ei ei = 1, \dots, EI$ )
$g$	Set for Regions ( $g g = 1, \dots, G$ )
$sc$	Set of scenarios ( $sc sc = 1, \dots, SC$ )
$t$	Set for Planning periods ( $t t = 1, \dots, T$ )
$x$	Set for External energy suppliers ( $x x = 1, \dots, X$ )

### *Sets*

EX( $e, x$ )	Subset of ordered pairs that link energy types $e$ to external resource $x$
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### *Parameters*

$\beta$	The azimuth angle of the pitch
$\varepsilon$	Auxiliary boundary for the $\varepsilon$ -constraint method
$\lambda_{g,t}$	The tip speed ratio in region $g$ in period $t$
$\Lambda_{g,t}$	The tip speed ratio at $t^{th}$ time step in region $g$ in period $t$
$\mu_p$	Coefficient of variation of power per temperature
$\rho_{air}$	Density of air
$\omega_{nom}$	Nominal turbine rotation speed
$Cp_{g,t}$	power coefficient in region $g$ in period $t$
$CutInWV$	Cut-in speed
$CutOutWV$	Cut-out speed
$Demand_{g,t,sc}$	energy demand needed per unit of raw material $i$ in period $t$ , for scenario $sc$

$EfIJ_{e,ei}$	Conversion efficiency between internal energy resource $ei$ type $e$ and the process plant $i$
$EfIX_{e,x}$	Conversion efficiency of the excess energy type $e$ sent to the external energy generation resource $x$
$EfXJ_{e,x}$	Conversion efficiency between external resource $x$ energy type $e$ and the process plant $i$
$GR$	Solar irradiance under standard condition
$GT_{g,t}$	Solar irradiance in region $g$ and period $t$
$ir$	Interest rate
$MinPgCO$	Minimum power generation coefficient
$MinPwHW$	Minimum power generation by windmill
$MinPwPV$	Minimum power generation by photovoltaic
$NOCT$	Normal Cell Operating Temperature
$P_{eg}$	Power generated by the cogeneration per ton of biomass
$PanNomPw$	Panel nominal power
$PanPr$	Price of a panel
$PanPw_{g,t}$	Power generated by a panel in region $g$ and period $t$
$PanSurf$	Panel surface
$PanT_{g,t}$	Temperature a panel in region $g$ and period $t$
$prob_{sc}$	the probability of scenario $sc$
$PrPwHW$	Price per unit of wind power
$PrPwPV$	Panel price per unit of power
$PwIMax_{ei}$	the maximum power to install energy resource $ei$
$PwSurfPV_{g,t}$	Power per available surface in region $g$ and period $t$
$RotD$	Rotor diameter
$SL$	Slot length
$STA$	The ambient temperature under standard condition
$SurfMaxHW$	Maximum surface available for horizontal windmill axis
$SurfMaxPV$	Maximum surface available for a photovoltaic
$SurfPwHW$	The relation between the surface and power
$SurfPwPV$	The relation between the surface and power
$SurfTEqHW$	The equivalent surface area of a turbine
$SurfTEqPV$	The equivalent surface occupied by a panel
$SurfTMax$	Maximum total surface
$SurfPwI_{ei}$	Area occupation per unit power of each $ei$
$TA_{g,t}$	Ambient temperature in region $g$ and period $t$
$TurbNomPw$	Nominal turbine power
$TurbPr$	Price of a turbine
$TurbPw_{g,t}$	Power generated by a turbine in region $g$ and period $t$
$TurbPwHW_{g,t}$	Captured power by a turbine in region $g$ and period $t$
$WV_{g,t}$	Wind velocity in region $g$ and period $t$

**Variables**

$CF_{t'',sc}$	Cash flow in period $t''$ in scenario $sc$
$DAM_{sc}$	Environmental metric to be optimized in scenario $sc$



$E[NPV]$	Expected net present value
$EnIG_{ei,g,t,sc}$	Energy type $e$ generated in region $g$ and period $t$ in scenario $sc$
$EnIJ_{e,ei,g,t,sc}$	Energy flux type $e$ between renewable source $ei$ and demand of region $g$ in period $t$ in scenario $sc$
$EnIX_{e,ei,x,g,t}$	Energy flux type $e$ between renewable source $ei$ and external source $x$ region $g$ in period $t$
$EnXJ_{e,x,g,t,sc}$	Energy flux type $e$ between external source $x$ and demand of region $g$ in period $t$ in scenario $sc$
$EnXP_{e,x,g,t,sc}$	Energy type $e$ purchased from external source $x$ in period $t$ in scenario $sc$
$EnXS_{e,x,g,t,sc}$	Energy type $e$ sales to external source $x$ in period $t$ in scenario $sc$
$GWPCul_{sc}$	GWP100 amount in cultivation process in scenario $sc$
$GWPPr_{sc}$	GWP100 amount in the production process in scenario $sc$
$GWPQ_{sc}$	GWP100 amount in transportation process in scenario $sc$
$NPV_{sc}$	Net Present Value in scenario $sc$
$PwI_{ei,g}$	Power to install a renewable source $ei$ , in each region $g$
$PwIG_{ei,g,t,sc}$	Power to generate by a renewable source $ei$ , in each region $g$ , each period $t$ in scenario $sc$
$PwIGMax_{ei,g,t,sc}$	Maximum power to generate by renewable source $ei$ in each region $g$ and period $t$ in scenario $sc$
$PwIGMin_{ei,g,t,sc}$	Minimum power to generate by renewable source $ei$ in each region $g$ and period $t$ in scenario $sc$
$PwXP_{e,x,g,t,sc}$	Power purchased from external source $x$ in period $t$ in scenario $sc$
$PwXS_{x,g,t,sc}$	Power selling to external source $x$ in period $t$ in scenario $sc$
$SurfInsHW_{ei,g}$	Equivalent windmill surface to occupy in region $g$
$SurfInsPV_{ei,g}$	Equivalent photovoltaic surface to occupy in region $g$
$SurfPV_{ei,g}$	Photovoltaic surface to install in region $g$
$TotalDemand_{g,t,sc}$	Energy demand of region $g$ and period $t$ in scenario $sc$
$TurbNum_{ei,g}$	Number of the turbine to install in region $g$
$W_{i,g,t,sc}$	Amount of wastes of $i$ generated in region $g$ and period $t$ in scenario $sc$

#### **Binary Variables**

$Gn_{ei,g,t,sc}$	By the Big-M method, the local binary variable is used to define lower and higher generation limits
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*Part III*

*Conclusions and Future works*



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## CONCLUSIONS AND FUTURE WORKS

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This thesis has addressed Sustainable Supply Chains in the process industries, focused on Energy Management of large-scale systems. Hence, this thesis has developed a general model to facilitate the management and assure robust and viable solutions.

Since retrofitting the actual process industries towards sustainability is a goal, applying this novel model allows the decision-makers to tackle several issues simultaneously to accomplish the several conflicting objectives. Precisely, this contribution has employed multi-objective strategies and promoted the model both at the strategic and tactical management levels (Chapter 4). Moreover, the systematic combination of the multi-objective approach with uncertainty management has extended the borders of the solution space (Chapter 5 and 6), and the numerical results have proved the significant effects of this combination on the solution's flexibility and robustness compared with the ones obtained through conventional PSE approaches. Notably, the work has resulted in contributions to the following areas.

- ☞ To exploit the mathematical programming effectively to combine material/energy networks and optimize its performance.
  - Applying multi-objective optimization to drive robustly sustainable process and solutions;
  - Using MILP to deal with the complexity due to the nature of material/energy networks;
  - Using the  $\varepsilon$ -constraint method to obtain the Pareto sets of solutions to obtain compromise solutions quickly;
- ☞ Applying economic and environmental metrics simultaneously and analyzing the economic and environmental risks to manage the effects of uncertainty through the network;
- ☞ Using the scenario-based model to deal with large numbers of uncertain parameters and investigate the adequate numbers of scenarios to be as representative as possible;
- ☞ Exploiting scenario reduction strategies and simplified scenario approach to analyze and compare;

It is worthy to note that the proposed model is general enough to apply to any size of the process industries, small-scale to large-scale and country-size problems. Applying the model to a case study has validated the model's efficiency and effectiveness, and numerical results illustrated the viability and capability of the model applied to integrated material/energy networks.

The integrated discussion of the conclusions obtained from each issue is next exposed, organized according to chapters 4 to 6:

- ☛ Multi-Objective issues (notably to deal with conflicting objectives),
- ☛ Uncertainty issues (to enhance flexibility and robustness in solutions)
- ☛ Sustainability issues (to obtain compromised solutions)
- ☛ Integration issues (to manage the complexity in large-scale networks)

### 7.1. Multi-Objective issues

Multi-objective optimization is a systematic and simultaneous process of optimizing several objective functions. Hence, the optimal solutions happen in the presence of trade-offs between two or more conflicting objectives. As explained in chapter 3, three MOO classes are a priori, interactive, and a posteriori (generation) methods. Despite a priori and interactive, generation methods are not very common due to the extensive computational efforts and less available software. However, they are efficient methods to manage the conflicting objectives since the generation methods involve the DM only in the second phase of the solution process (having all the alternatives in the form of the Pareto set or other proper representation). Consequently, applying these methods reduces the DM bias effects. The most commonly used generation method is the  $\varepsilon$ -constraint, described profoundly in chapter 3, and it is the primary solution strategy of this thesis.

Besides, regarding the literature review, the multi-objective approach is the best to deal with complex, and this thesis has advanced uniquely to apply to large-scale complex networks. This contribution has validated the MOO capabilities through the design and planning of integrated material/energy networks. In particular, the case study accounts for renewable energy resources as alternative energy sources for satisfying energy demands in industrial sectors in Argentina.

To demonstrate the benefits of applying MOO, numerical results (as the particular sub-results), associated with economic and environmental objectives, indicate that in both cases of single and multi-energy resources networks (**Chapter 4 and 6**), the compromised solutions are more viable comparing with the solutions obtained by SOO. The obtained results through this thesis reinforce the idea that the MOO is the proper approach to apply to complex, large-scale problems, and in this particular case, applying it to energy-material management is a promising option to deal with several conflicting objectives efficiently.

### 7.2. Uncertainty issues

Due to the uncertain nature of PSE problems, inevitably, uncertainty issues should be considered in the problem-solving processes. Mainly, stochastic programming has been applied to large numbers of PSE problems as a preventive approach. Stochastic programming aims to efficiently control the effect of uncertain/unpredictable conditions over the resulting solutions for a large-scale network.

This thesis has exploited the scenario-based approach to deal with large numbers of uncertain parameters. The Monte Carlo sampling method generated random scenarios with the normal distribution that represent the uncertainty space. By using a scenario reduction algorithm, different reduced sets of scenarios were generated in different sizes. The problem was solved for each reduced set. The design decision variables got fixed, and the problem was solved again with different fixed variables for the same set of scenarios. The results revealed that notably that the representativeness of a reduced set depends on the numbers of uncertain parameters. The objective variations are perfectly centered by the adequate reduced set of scenarios and result in robust solutions.

Besides, a simplified scenario-based approach was used to reduce computational complexity. The idea behind this strategy is to use a set containing three scenarios: (Mean value  $+\gamma$ , Mean value, Mean value  $-\gamma$ ). Despite less computational efforts, the simplified scenarios method provides the results with poor quality, compared to the results obtained by the optimum reduced set, and similar to the results obtained by the smaller size of scenarios.

This contribution utilized risk metrics to measure the uncertainty effects. Commonly, Values at risk (VaR) is the most used metric. The stochastic approach is appealing for the risk-averse decision-makers, while the opportunity value (OV) in the deterministic case is much higher than the stochastic one corresponding to a certain level of risk. Chapter 5 was profoundly dedicated to uncertainty issues and presented a clear image of VaR and OV for the risk-averse and risk-taker decision-makers.

Although this contribution grants an optimal solution, the accuracy in the description of the system behavior is maintained. Hence, future works should address the quality of the obtained design.

### **7.3. Sustainability issues**

Regarding sustainability criteria, here, it is mainly aimed to maintain or develop the sustainability level in a large-scale industrial network. This contribution has focused on carbon emissions reduction strategies to answer sustainability issues. A combined approach that consists of integrating LCA and optimization was applied, as former studies have done. Therefore, a bi-criterion MILP seeks to maximize the network's NPV and life cycle environmental performance simultaneously. Besides, the carbon emissions in the design and operation phases were translated to the costs aimed to minimize.

The combined model (mentioned above) was applied to the case studies. It is deduced from the results that multi-renewable energy resource networks demonstrate better environmental performance than a single resource one. Besides, uncertainty does not directly affect environmental impact but controls the variations by using adequate scenario numbers.

As a sub conclusion, the results indicate the CO<sub>2</sub> emissions reduction through the supply chain using renewable resources and the dependency on fossil-based energies has been reduced significantly through biofuel production and exploiting renewable resources. Also, it leads to

paying less landfill tax to be seen as an improvement in the economic objective. Note that the uncertain quality of renewable resources should be considered in future works. However, the uncertain quality of renewable resources should be considered in future works.

#### 7.4. Integration issues

The synergies associated with integrating material and energy supply chains compared to the stand-alone systems have been studied through this thesis. The management of many decision variables simultaneously with various uncertain parameters becomes then a significant challenge. The novel model is capable of managing all these variables and uncertain parameters. It is proved using a multi-scenario multi-objective design and planning supply chain model as a test-bed. It facilitates reaching out to more possible solutions and searching for solution alternatives behaving in different manners within the uncertain parameter space (see **Chapter 6**). Besides, the approach allows narrowing down the number of alternatives to be analyzed, ensuring that the final solution performs well for a wide range of criterion targets. The integration can be used in different engineering problems, ensuring the quality of the final solution even for those in which process uncertainties have to be explicitly considered over the solution performance.

#### 7.5. Future works

The main future research direction would be classified in:

- Social sustainability issues:

While sustainability in social issues is the neglected component in sustainable development, there is a need for a novel integrated method that allows considering and evaluating the social acceptance/risk of the selected decision criteria. Besides, social sustainability mainly focuses on the context of many current initiatives in sustainability and responsibility, including supply chain management. Notably, it is needed to utilize metrics, indicators, and frameworks of social impacts and initiatives related to their abilities to evaluate the social sustainability of supply chains. Integrated approaches such as applying a set of composite indicators and looking beyond traditional system boundaries are required in the future to develop social sustainability performance.

- Robustness measuring within a solution identification framework:

Structural robustness measures are needed to evaluate alternative solutions based on a trade-off between different objectives. The procedure can be integrated into the optimization process. The above is particularly interesting for its further application on large and complex problems, such as large-scale process industries.

- Decentralized management and game theory

This framework can apply to decentralized supply chain problems to explore its capabilities to produce a solution that simultaneously improves the performances of each of the SC entities.







## *Appendices*



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**PUBLICATIONS**


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Here is a list of the publications carried out so far within the scope of this thesis.

### A.1. Conference proceeding articles

#### Published

- Morakabatchiankar, S., Hjaila, K., Graells, M., & Espuña, A. (2017). Developing a Multi-Objective Strategic-Tactical Optimization Model for Sustainable Production Supply Chains Considering Electricity Cogeneration: Sugar Cane Bioenergy Industry. In *Computer Aided Chemical Engineering* (Vol. 40, pp. 2179–2184). Elsevier. <https://doi.org/10.1016/B978-0-444-63965-3.50365-2>
- Morakabatchiankar, S., Hjaila, K., Mele, F. D., Graells, M., & Espuña, A. (2018). Economic and environmental benefits of waste-based energy closed-loop integration in process industries under uncertainty. In *Computer Aided Chemical Engineering* (Vol. 43, pp. 501–506). Elsevier. <https://doi.org/10.1016/B978-0-444-64235-6.50089-9>
- Morakabatchiankar, S., Mele, F. D., Graells, M., & Espuña, A. (2019). Optimal design and planning multi resource-based energy integration in process industries. In *Computer Aided Chemical Engineering* (Vol. 46, pp. 1075–1080). Elsevier B.V. <https://doi.org/10.1016/B978-0-12-818634-3.50180-6>
- Morakabatchiankar, S., Mele, F. D., Graells, M., & Espuña, A. (2020). Optimal Design and planning supply chains of multi-renewable resource-based energy/material applied in process industries. In *14th Mediterranean Congress of Chemical Engineering, virtual event, 16-20 November*. Grupo Pacifico. <https://doi.org/10.48158/mecce-14.dg.06.06>

#### Submitted

- Morakabatchiankar, S., Mele, F. D., & Graells, Moisés, Espuña, A. (2021). Simplified targeting models for Sustainable Supply Chains retrofitting in process industries. (Accepted to published in *Computer-Aided Chemical Engineering*).

### A.2. Other congresses and workshops

- Medina-González, S.; Morakabatchiankar, S.; Graells, M.; Guillén-Gosálbez, G.; Espuña, A.; Puigjaner, L. Sustainable Design of a Bio-Based Energy Network Under Multiple Objectives and Availability/quality Uncertainty. 11th Conference on sustainable development of energy, water, and environment systems, (04-09 September 2016).

*Appendix A. Publications*

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**CASE STUDY DATA AND COMPLEMENTARY INFORMATION**


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**B.1 Complementary information of Chapter 4**
 **Cogeneration datasheet**

Table. B. 1. Design data of the cogeneration power plant (Bocci et al., 2009).

Identifier	Value	Unit
Atmospheric pressure	1	bar
Process pressure	2.1	bar
Thermal power needed	62	MW
Gasifier steam to biomass ratio	0.5	
Gasifier temperature	800	°C
Combustor temperature	940	°C
MCFC temperature	610	°C
MCFC stack efficiency	55	%
MCFC voltage	0.77	V
Combustor air excess	25	%
Gasifier efficiency	90	%
Internal steam turbine efficiency	85	%
Mechanical efficiency( $\eta_{mT}$ )	98	%
Auxiliary devices efficiency( $\eta_{aux}$ )	95	%
Alternator efficiency	98	%
Air and fuel gas specific heat ( $C_p$ )	1006	kJ / kgK
Lower Heat Value bagasse ( <b>LHV</b> )	7.40	MJ / kg
Recovery heat inlet water temperature	15	°C
Turbine minimum gas mass flow fraction	30	%
Recovery heat inlet drop temperature	29	K
Minimum recovery heat inlet drop temperature	10	K
Electrical referential efficiency	27	%
Thermal referential efficiency	70	%

Appendix B. Case study Data

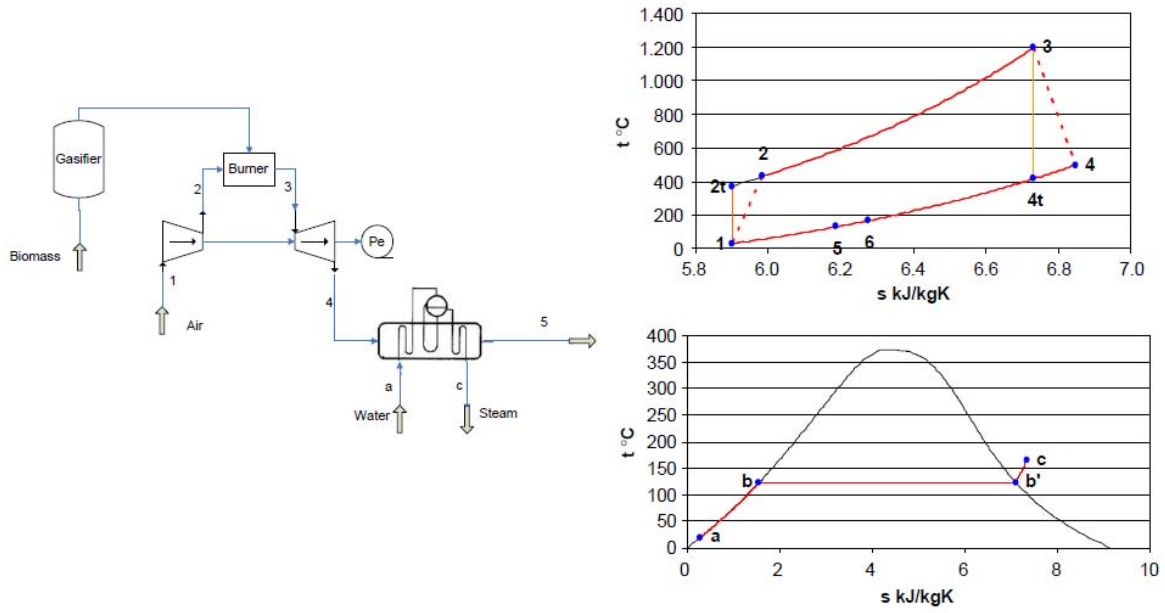


Fig. B. 1. Thermodynamic diagram of the gas turbine cogeneration power plant (Bocci et al., 2009).



## B.2 Complementary information of Chapter 5

### a. Equations associated with the production section

#### Mass balances equations

$$\begin{aligned} & \sum_{s \in IS(i,s)} ST_{i,s,g,t-1,sc} + PT_{i,g,t,sc} + PU_{i,g,t,sc} + \\ & \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{i,l,g',g,t,sc} = \sum_{s \in IS(i,s)} ST_{i,s,g,t,sc} + DTS_{i,g,t,sc} + \quad \forall i, g, t, sc \quad (B.1) \\ & \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{i,l,g,g',t,sc} + W_{i,g,t,sc} \end{aligned}$$

#### Total production rate

$$PT_{i,g,t,sc} = -\sum_p \text{sign} \rho_{p,i} \times PE_{i,p,g,t,sc} \quad \forall i, g, t, sc \quad (B.2)$$

$$PE_{i,p,g,t,sc} = |\rho_{p,i}| \sum_{i' \in IM(i',p)} PE_{i',p,g,t,sc} \quad \forall i, p, g, t, sc \quad (B.3)$$

#### Mass flow and inventory constraints

$$PU_{i,g,t,sc} \leq \text{CapCrop}_{g,t} \quad i = \text{Raw material}, \quad \forall g, t, sc \quad (B.4)$$

$$\sum_{i \in IS(i,s)} ST_{i,s,g,t,sc} \leq \text{SCap}_{s,g,t} \quad \forall s, g, t, sc \quad (B.5)$$

$$ALL_{i,g,t,sc} = \sigma DTS_{i,g,t,sc} \quad \forall i, g, t, sc \quad (B.6)$$

$$2ALL_{i,g,t,sc} \leq \sum_{s \in IS(i,s)} \text{SCap}_{s,g,t} \quad \forall i, g, t, sc \quad (B.7)$$

$$DTS_{i,g,t,sc} \leq SD_{i,g,t,sc} \quad \forall i, g, t, sc \quad (B.8)$$

$$X_{l,g,g',t} + X_{l,g',g,t} = 1 \quad \forall l, g, g', t (g \neq g') \quad (B.9)$$

$$\underline{Q}_l X_{l,g,g',t} \leq \sum_{i \in IL(i,l)} Q_{i,l,g,g',t,sc} \leq \overline{Q}_l X_{l,g,g',t} \quad \forall l, g, g' (g \neq g'), t, sc \quad (B.10)$$

#### Production and storage capacity constraints

$$\tau |\rho_{p,i}| PCap_{p,g,t} \leq PE_{i,p,g,t,sc} \leq |\rho_{p,i}| PCap_{p,g,t} \quad \forall g, t, IM(i,p), sc \quad (B.11)$$

While the production and storage capacity variables are considered design variables, the following equations are the same as equations (4.12) to (4.15) in Chapter 4.

$$PCap_{p,g,t} = PCap_{p,g,t-1} + PCapE_{p,g,t} \quad \forall p, g, t \quad (B.12)$$

$$\underline{PCap}_p NP_{p,g,t} \leq PCapE_{p,g,t} \leq \overline{PCap}_p NP_{p,g,t} \quad \forall p, g, t \quad (B.13)$$

$$\text{SCap}_{s,g,t} = \text{SCap}_{s,g,t-1} + \text{SCap}E_{s,g,t} \quad \forall s, g, t \quad (B.14)$$

$$\underline{\text{SCap}}_s NS_{s,g,t} \leq \text{SCap}E_{s,g,t} \leq \overline{\text{SCap}}_s NS_{s,g,t} \quad \forall s, g, t \quad (B.15)$$

### b. Energy generation and constraints

#### Energy balances and flows equations

$$\begin{aligned} & \sum_e [\text{EnI}J_{e,g,t,sc} \times \text{EfI}J_e] + \sum_{e \in EX(e,x)} \sum_x [\text{EnX}J_{e,x,g,t,sc} \times \text{EfX}J_{e,x}] = \\ & \text{TotalDemand}_{g,t,sc} \quad \forall g, t, sc \quad (B.16) \end{aligned}$$

In a scenario, the energy type  $e$  generating by the internal resource aimed to send to the process plant or market to the external energy demanders as the equation (B.17) defines and indicates the energy balance between internal and external resources in period  $t$ .

$$\text{EnI}J_{e,g,t,sc} \times \text{EfI}J_e + \text{EnI}X_{e,x,g,t,sc} \times \text{EfI}X_{e,x} = \text{EnI}G_{e,g,t,sc} \quad \forall g, t, EX(e,x), sc \quad (B.17)$$

#### Installation and generation capacity constraints

The installation capacity and constraint are design variables so that they are the same as Eq. (4.18) and (4.19) of Chapter 4.

$$PwI_g \leq PwIMax \quad \forall g \quad (B.18)$$

$$PwI_g \times SurfPwl \leq SurfTMax \quad \forall g \quad (B.19)$$

The following equations (B.20) to (B.23) correspond to the Big-M method, introducing the binary variable  $Gn_{g,t,sc}$  as the generation decision, aims to avoid nonlinearity.

$$PwIG_{g,t,sc} \leq PwIMax \times Gn_{g,t,sc} \quad \forall g, t, sc \quad (B.20)$$

$$PwIG_{g,t,sc} \geq -PwIMax \times Gn_{g,t,sc} \quad \forall g, t, sc \quad (B.21)$$

$$PwIG_{g,t,sc} \leq PwIGMax_{g,t,sc} + PwIMax \times (Gn_{g,t,sc} - 1) \quad \forall g, t, sc \quad (B.22)$$

$$PwIG_{g,t,sc} \geq PwIGMin_{g,t,sc} - PwIMax \times (Gn_{g,t,sc} - 1) \quad \forall g, t, sc \quad (B.23)$$

As noted previously, it is necessary to choose a value of M sufficiently large to make the problem feasible for each scenario  $sc$  and small enough to limit it. In this case, M corresponds to the maximum power  $PwIMax$  to be installed. Here,  $PwIGMax_{g,t,sc}$  and  $PwIGMin_{g,t,sc}$  are parameters calculated based on specific energy resource models (see Eq. (B.24) and (B.26)).

$$PwIGMax_{g,t} = PwIG_{g,t,sc} \quad \forall g, t, sc \quad (B.24)$$

$$PwIGMin_{g,t,sc} = PwIG_{g,t,sc} \times MinPgcO \quad \forall g, t, sc \quad (B.25)$$

$$PwIG_{g,t,sc} = EnIG_{g,t,sc} / SL \quad \forall g, t, sc \quad (B.26)$$

### External resource equations

$$EnXP_{e,x,g,t,sc} = enXJ_{e,x,g,t,sc} \times EfXJ_{e,x} \quad \forall g, t, EX(e, x), sc \quad (B.27)$$

$$EnXS_{e,x,g,t,sc} = enIX_{e,x,g,t,sc} \times EfIX_{e,x} \quad \forall g, t, EX(e, x), sc \quad (B.28)$$

$$PwXP_{x,g,t,sc} = \sum_e EnXP_{e,x,g,t,sc} / SL \quad \forall g, t, EX(e, x), sc \quad (B.29)$$

$$PwXS_{x,g,t,sc} = \sum_e EnXS_{e,x,g,t,sc} / SL \quad \forall g, t, EX(e, x), sc \quad (B.30)$$

## c. Objective functions

### Economic objective

The economic objective is the net present value (NPV) from the discounted cash flows  $CF_{t,sc}$  that is generated in each period  $t$  in scenario  $sc$  for the entire time horizon.

$$NPV_{sc} = \sum_t \frac{CF_{t,sc}}{(1+ir)^{t-1}} \quad \forall sc \quad (B.31)$$

The fraction of the total depreciable capital  $TOTAL_t$  has been defined in **Chapter 4 (Eq. (4.33))**.

$$TOTAL_t = \frac{FCI}{T} + \frac{CIns}{T} + \frac{GHGIns}{T} \quad \forall t \quad (B.32)$$

$$CF_{t,sc} = NE_{t,sc} - TOTAL_t \quad t = 1, \dots, T - 1, \forall sc \quad (B.33)$$

The salvage value  $sv$  has been defined in **section 4.3.3.1**.

$$CF_{t,sc} = NE_{t,sc} - TOTAL_t + sv(FCI + CIns + GHGIns) \quad t = T \quad (B.34)$$

### Total fixed cost investment

#### i. The fixed costs of the production plant

Total fixed cost investment includes  $FCI$  and  $CIns$  determined in **section 4.3.3.1. (Eq. (4.35))** of **Chapter 4**.

$$FCI = \sum_p \sum_g \sum_t [\alpha_{p,g,t}^{Pr} \times NP_{p,g,t} + \beta_{p,g,t}^{Pr} \times PCapE_{p,g,t}] + \sum_s \sum_g \sum_t [\alpha_{s,g,t}^{St} \times NS_{s,g,t} + \beta_{s,g,t}^{St} \times SCapE_{s,g,t} \times PCapE_{p,g,t}] + \sum_l \sum_t TMC_{l,t} \times NT_{l,t} \quad (B.35)$$

#### ii. The fixed costs of the renewable energy installation

$CIns$  is determined in **section 4.3.3.1. (Eq. (4.35))** of **Chapter 4**.  $GHGIns$  is the fixed costs variables, corresponding to the installation of the renewable energy resource and consequent  $CO_2$  emissions.

$$CIns = PrPwI \sum_g PwI_g \quad (B.36)$$

$$GHGIns = GHGPr \left[ \sum_g GHGPwI \times PwI_g + \sum_{e \in EX(e,x)} \sum_x \sum_g \sum_t \sum_{sc} [(PwXP_{e,x,g,t,sc} + PwXS_{x,g,t,sc}) \times GHGPw_x] \right] \quad (B.37)$$

iii. **Total fixed costs constraint**

$$FCI + CIns + GHGIns \leq \overline{FIC} \quad (B.38)$$

**Net earnings**

$$NE_{t,sc} = (1 - \varphi)(Rev_{t,sc} - FOC_{t,sc} - TOC_{t,sc} - COP_{t,sc} - GHGCOP_{t,sc}) + \varphi DEP_t \quad \forall t, sc \quad (B.39)$$

$$Rev_{t,sc} = \sum_{i \in SEP(i)} \sum_g DTS_{i,g,t,sc} \times PR_{i,g,t} \quad \forall t, sc \quad (B.40)$$

The depreciation term is calculated with the straight-line method, similar to (Kostin et al., 2012) formulated in their work.

$$DEP_t = (1 - sv) \times TOTAL_t \quad \forall t \quad (B.41)$$

**The production operating costs**

$$FOC_{t,sc} = \sum_i \sum_{p \in IM(i,p)} \sum_g UPC_{i,p,g,t} \times PE_{i,p,g,t,sc} + \sum_i \sum_{s \in IS(i,s)} USC_{i,s,g,t} \times ALL_{i,g,t,sc} + DC_{t,sc} \quad \forall t, sc \quad (B.42)$$

$$DC_{t,sc} = \sum_i \sum_g W_{i,g,t,sc} \times LT_{i,g} \quad \forall t, sc \quad (B.43)$$

**The transportation costs**

$$TOC_{t,sc} = FC_{t,sc} + LC_{t,sc} + MC_{t,sc} + GC_{t,sc} \quad \forall t, sc \quad (B.44)$$

$$Fuel\ Usage_{i,l,g,g',t,sc} = \frac{2EL_{g,g'}}{FE_l} \times \frac{Q_{i,l,g,g',t,sc}}{TCap_l} \quad \forall i, l, g, g', t, sc \quad (B.45)$$

Thereupon, the total fuel cost in each period is as the following:

$$FC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l Fuel\ Usage_{i,l,g,g',t,sc} \times FPl_t \quad \forall t, sc \quad (B.46)$$

The labor transportation cost is a function of the driver wage  $DW_{l,t}$ . Moreover, the total delivery time is as below:

$$Total\ Delivery\ time_{i,l,g,g',t,sc} = \frac{Q_{i,l,g,g',t,sc}}{TCap_l} \left( \frac{2EL_{g,g'}}{SP_l} + LUT_l \right) \quad \forall i, l, g, g', t, sc \quad (B.47)$$

Here,  $SP_l$  and  $LUT_l$  represent the average speed and loading/unloading time of transportation mode  $l$ , respectively. Therefore, the labor cost  $LC_{t,sc}$  is defined as the following:

$$LC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l Total\ Delivery\ Time_{i,l,g,g',t,sc} \times DW_{l,t} \quad \forall t, sc \quad (B.48)$$

The general maintenance cost of the transportation systems depends on the total distance driven and the unit cost of the traveled distance  $ME_l$ .

$$MC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l \frac{Q_{i,l,g,g',t,sc}}{TCap_l} \times 2EL_{g,g'} \times ME_l \quad \forall t, sc \quad (B.49)$$

Finally in this part, the general costs  $GC_t$  and average number of transportation modes  $NT_{l,t}$  are obtained by **Eq. (4.50) and (4.51)**.

$$GC_t = \sum_l \sum_{t' \leq t} GE_{l,t'} \times NT_{l,t'} \quad \forall t \quad (B.50)$$

$$\sum_{t \leq T} NT_{l,t} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \frac{\text{Total Delivery time}_{i,l,g,g',t}}{avl_l} \sum_{t' \leq T} NT_{l,t'} = \quad \forall l \quad (B.51)$$

$$\sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \frac{\text{Total Delivery time}_{i,l,g,g',t}}{avl_l}$$

**The operation costs of renewable energy resource**

$$COP_{t,sc} = \sum_e \sum_g PrEnI_e \times EnIG_{e,g,t} + \sum_{e \in EX(e,x)} \sum_x \sum_g [PrEnP_{e,x} \times EnXP_{e,x,g,t,sc} - PrEnS_{e,x} \times EnXS_{e,x,t,sc}] \quad \forall t, sc \quad (B.52)$$

Here, the costs of  $CO_2$  emissions caused by operating the energy generation unit are calculated and added to the operational costs.

$$GHGCOP_{t,sc} = GHGPr [\sum_e \sum_g GHGENI_e \times EnIG_{e,g,t,sc} + \sum_{e \in EX(e,x)} \sum_x GHGENX_{e,x} \times EnXP_{e,x,g,t,sc}] \quad \forall t, sc \quad (B.42)$$

Note that the allowable emissions amount has a limitation for the entire horizon.

$$GHGPwl \sum_g Pwl_g + \sum_e \sum_g GHGENI_e \times EnIG_{e,g,t,sc} \leq GHGMax \quad \forall t, sc \quad (B.43)$$

**Environmental objective**

$$GWPCul_{sc} = \omega_i^{PU} \sum_i \sum_g \sum_t PU_{i,g,t,sc} \quad \forall sc \quad (B.44)$$

$$GWPPr_{sc} = \sum_i \sum_p \sum_g \sum_t \omega_p^{Pr} \times PE_{i,p,g,t,sc} \quad \forall sc \quad (B.45)$$

$$GWPQ_{sc} = \sum_i \sum_l \sum_g \sum_{g'} \sum_t \omega_l^{Tr} \times EL_{g,g'} \times Q_{i,l,g,g',t,sc} \quad \forall sc \quad (B.46)$$

The environmental impact, as an objective function, is defined through the expected  $DAM_{sc}$  as an environmental metric to be minimized.

$$DAM_{sc} = GWPCul_{sc} + GWPPr_{sc} + GWPQ_{sc} \quad (B.47)$$

### B.3 Complementary information of Chapter 6

#### ✂ Wind turbine datasheet

Table. B. 2. Windmill data from the technical data sheet of GAMESA G58.

<b>Identifier</b>	<b>Value</b>	<b>Unit</b>
$\rho_{air}^*$	1.225	$kg/m^3$
<i>TurbNomPw</i>	850	<i>KW</i>
<i><math>\omega_{nom}</math></i>	30.8	<i>RPM</i>
<i>RotD</i>	52	<i>m</i>
$\beta$	0	$^\circ$
<i>CutInWV</i>	3	<i>m/s</i>
<i>CutOutWV</i>	21	<i>m/s</i>
<i>TurbPr</i>	750,000	€
<i>SurfTEqHW</i>	2,950	<i>m<sup>2</sup> / Turb</i>
<i>SurfMaxHW</i>	2,642	<i>m<sup>2</sup> / Turb</i>

\* The ISA or International Standard Atmosphere states the density of air is 1.225 kg/m<sup>3</sup> at sea level and 15 degrees C

Table. B. 3. Coefficients of the Wind Turbine.

$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$c_6$
0.5176	46	0.4	0	21	0.0068

Table. B. 4. Monthly data of regional Wind velocity.

Month													
Region		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
		Wind velocity $WV_{g,t}(m/s)$											
(Buenos Aires)	g1	4.7	4.6	4.57	4.62	4.58	4.75	4.81	4.87	5.05	5	4.98	4.78
(Córdoba)	g2	2.14	2.06	2.03	2.06	2.1	2.2	2.4	2.62	2.75	2.73	2.61	2.35
(Corrientes)	g3	3.33	3.32	3.27	3.33	3.41	3.53	3.74	3.96	4.11	4.11	3.86	3.51
(La Plata)	g4	4.78	4.69	4.6	4.58	4.56	4.7	4.75	4.82	5.07	4.99	5	4.82
(La Rioja)	g5	3.75	3.44	3.13	2.75	2.41	2.23	2.38	2.75	3.32	3.84	4.1	4
(Mendoza)	g6	4	3.75	3.54	3.14	2.78	2.63	2.77	3.13	3.5	3.81	4	4.04
(Neuquén)	g7	5.94	5.45	5.05	4.75	4.42	4.41	4.44	4.71	4.97	5.44	5.94	6.18
(Entre Ríos)	g8	3.83	3.78	3.75	3.77	3.8	3.9	4.09	4.34	4.63	4.57	4.34	4.02
(Misiones)	g9	1.22	1.19	1.21	1.27	1.33	1.36	1.43	1.49	1.48	1.45	1.37	1.28
(Chubut)	g10	6.35	6.24	6.12	6.23	6.26	6.41	6.37	6.15	5.99	5.99	6.18	6.33
(Chaco)	g11	2.95	2.95	2.88	2.97	3.02	3.08	3.31	3.53	3.67	3.64	3.40	3.10
(Santa Cruz)	g12	7.44	7.20	6.99	6.71	6.35	6.24	6.39	6.57	6.56	6.81	7.35	7.42
(Salta)	g13	3.14	3.01	2.85	2.56	2.31	2.21	2.38	2.67	3.11	3.52	3.67	3.44
(San Juan)	g14	4.04	3.83	3.55	3.20	2.98	2.92	3.08	3.41	3.74	4.01	4.18	4.17
(San Luis)	g15	4.44	4.35	4.28	4.14	4.09	4.20	4.49	4.80	5.08	5.19	5.05	4.72
(Tucumán)	g16	3.38	3.27	3.15	2.93	2.65	2.47	2.68	3.08	3.53	3.88	3.87	3.68
(Jujuy)	g17	2.93	2.77	2.55	2.27	2.07	2.13	2.28	2.48	2.73	3.10	3.30	3.18
(Santa Fe)	g18	3.80	3.73	3.73	3.73	3.73	3.83	4.03	4.28	4.53	4.53	4.30	3.95
(La Pampa)	g19	2.63	2.60	2.53	2.47	2.40	2.50	2.63	2.83	2.90	2.83	2.77	2.70
(Santiago del Estero)	g20	2.43	2.37	2.30	2.27	2.20	2.23	2.45	2.78	3.07	3.10	2.97	2.65
(Catamarca)	g21	3.58	3.40	3.20	2.97	2.70	2.60	2.85	3.18	3.63	3.98	4.03	3.85
(Rio Negro)	g22	5.90	5.83	5.55	5.37	5.37	5.47	5.53	5.35	5.30	5.40	5.53	5.75
(Formosa)	g23	3.48	3.37	3.33	3.50	3.63	3.80	4.05	4.30	4.40	4.35	4.03	3.68
(Tierra del Fuego)	g24	6.58	6.50	6.30	5.87	5.50	5.50	5.88	6.30	6.43	6.88	7.07	6.73

<https://weatherspark.com/y/28981/Average-Weather-in-Buenos-Aires-Argentina-Year-Round>

Table. B. 5. Windmill captured power calculated for each region in each month.

		Month											
Region		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
		<i>TurbPwHW<sub>g,t</sub>(kW)</i>											
<b>(Buenos Aires)</b>	<b>g1</b>	135.05	126.61	124.15	128.27	124.97	139.41	144.76	150.24	167.52	162.60	160.65	142.06
<b>(Córdoba)</b>	<b>g2</b>	12.75	11.37	10.88	11.37	12.05	13.85	17.98	23.39	27.05	26.47	23.13	16.88
<b>(Corrientes)</b>	<b>g3</b>	48.03	47.60	45.48	48.03	51.58	57.22	68.05	80.78	90.31	90.31	74.81	56.25
<b>(La Plata)</b>	<b>g4</b>	142.06	134.19	126.61	124.97	123.34	135.05	139.41	145.66	169.52	161.62	162.60	145.66
<b>(La Rioja)</b>	<b>g5</b>	68.60	52.95	39.89	27.05	18.21	14.43	17.54	27.05	47.60	73.65	89.65	83.25
<b>(Mendoza)</b>	<b>g6</b>	83.25	68.60	57.70	40.27	27.95	23.66	27.65	39.89	55.77	71.94	83.25	85.77
<b>(Neuquén)</b>	<b>g7</b>	272.62	210.57	167.52	139.41	112.32	111.56	113.85	135.91	159.69	209.41	272.62	307.02
<b>(Entre Ríos)</b>	<b>g8</b>	73.08	70.26	68.60	69.70	71.38	77.16	89.00	106.33	128.83	124.22	106.05	84.71
<b>(Misiones)</b>	<b>g9</b>	2.37	2.20	2.29	2.64	3.03	3.24	3.81	4.30	4.18	3.93	3.35	2.74
<b>(Chubut)</b>	<b>g10</b>	332.71	316.58	298.79	314.32	318.85	342.17	336.24	303.17	279.59	279.59	307.60	330.38
<b>(Chaco)</b>	<b>g11</b>	33.41	33.41	30.94	33.92	36.00	38.17	47.09	57.29	64.07	62.52	51.01	38.73
<b>(Santa Cruz)</b>	<b>g12</b>	536.35	484.93	443.98	392.17	332.71	315.45	339.79	369.11	366.61	410.76	515.68	531.53
<b>(Salta)</b>	<b>g13</b>	40.43	35.47	29.99	21.90	16.03	14.09	17.63	24.68	39.29	56.57	64.07	53.05
<b>(San Juan)</b>	<b>g14</b>	85.65	73.05	58.02	42.77	34.43	32.40	38.17	51.68	68.06	83.77	94.98	94.47
<b>(San Luis)</b>	<b>g15</b>	113.89	107.15	101.74	92.46	89.02	96.51	117.37	143.68	170.65	181.38	167.66	137.09
<b>(Tucumán)</b>	<b>g16</b>	50.01	45.34	40.66	32.83	24.21	19.52	24.90	37.82	57.38	75.69	75.20	64.56
<b>(Jujuy)</b>	<b>g17</b>	32.55	27.55	21.57	15.15	11.48	12.63	15.32	19.72	26.56	38.75	46.75	41.63
<b>(Santa Fe)</b>	<b>g18</b>	71.38	67.69	67.69	67.69	67.69	73.27	84.82	101.63	121.19	120.52	103.42	80.17
<b>(La Pampa)</b>	<b>g19</b>	23.53	22.86	20.94	19.52	17.98	20.32	23.53	29.33	31.72	29.33	27.55	25.60
<b>(Santiago del Estero)</b>	<b>g20</b>	18.55	17.24	15.83	15.15	13.85	14.49	19.13	27.80	37.51	38.75	33.96	24.21
<b>(Catamarca)</b>	<b>g21</b>	59.43	51.13	42.62	33.96	25.60	22.86	30.11	41.63	62.39	81.70	84.82	74.23
<b>(Rio Negro)</b>	<b>g22</b>	267.15	258.20	222.37	201.06	201.06	212.51	220.38	199.19	193.66	204.83	220.38	247.29
<b>(Formosa)</b>	<b>g23</b>	54.58	49.64	48.18	55.77	61.96	71.38	86.41	103.42	110.81	107.07	85.35	64.76
<b>(Tierra del Fuego)</b>	<b>g24</b>	369.73	357.23	325.26	262.65	216.42	216.42	263.77	325.26	346.35	422.69	459.04	397.09

Table. B. 6. Monthly Tip speed ratio calculated for each region.

		Month											
		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Region		Tip speed ratio $\lambda_{g,t}$											
(Buenos Aires)	$g_1$	17.84	18.23	18.35	18.15	18.31	17.65	17.43	17.22	16.61	16.77	16.84	17.54
(Córdoba)	$g_2$	39.19	40.71	41.31	40.71	39.93	38.12	34.94	32.01	30.49	30.72	32.13	35.68
(Corrientes)	$g_3$	25.18	25.26	25.65	25.18	24.59	23.76	22.42	21.18	20.40	20.40	21.73	23.89
(La Plata)	$g_4$	17.54	17.88	18.23	18.31	18.39	17.84	17.65	17.40	16.54	16.81	16.77	17.40
(La Rioja)	$g_5$	22.36	24.38	26.79	30.49	34.80	37.61	35.24	30.49	25.26	21.84	20.45	20.96
(Mendoza)	$g_6$	20.96	22.36	23.69	26.71	30.17	31.89	30.27	26.79	23.96	22.01	20.96	20.76
(Neuquén)	$g_7$	14.12	15.39	16.61	17.65	18.97	19.02	18.89	17.80	16.87	15.42	14.12	13.57
(Entre Ríos)	$g_8$	21.90	22.19	22.36	22.24	22.07	21.50	20.50	19.32	18.13	18.35	19.34	20.84
(Misiones)	$g_9$	68.63	70.35	69.48	66.21	63.23	61.84	58.62	56.28	56.85	58.02	61.17	65.44
(Chubut)	$g_{10}$	13.21	13.43	13.69	13.46	13.40	13.09	13.16	13.63	14.00	14.00	13.56	13.24
(Chaco)	$g_{11}$	28.42	28.42	29.16	28.28	27.72	27.19	25.35	23.75	22.88	23.06	24.68	27.06
(Santa Cruz)	$g_{12}$	11.27	11.65	12.00	12.51	13.21	13.45	13.12	12.76	12.79	12.31	11.42	11.30
(Salta)	$g_{13}$	26.67	27.86	29.47	32.72	36.31	37.90	35.17	31.44	26.93	23.85	22.88	24.36
(San Juan)	$g_{14}$	20.77	21.90	23.65	26.18	28.14	28.71	27.19	24.58	22.42	20.92	20.06	20.10
(San Luis)	$g_{15}$	18.89	19.27	19.61	20.24	20.50	19.96	18.70	17.48	16.50	16.17	16.60	17.75
(Tucumán)	$g_{16}$	24.85	25.67	26.62	28.59	31.65	34.00	31.35	27.27	23.73	21.64	21.69	22.82
(Jujuy)	$g_{17}$	28.67	30.31	32.89	37.00	40.58	39.31	36.86	33.88	30.68	27.05	25.41	26.41
(Santa Fe)	$g_{18}$	22.07	22.46	22.46	22.46	22.46	21.88	20.83	19.62	18.50	18.53	19.50	21.23
(La Pampa)	$g_{19}$	31.95	32.25	33.21	34.00	34.94	33.54	31.95	29.68	28.92	29.68	30.31	31.06
(Santiago del Estero)	$g_{20}$	34.58	35.43	36.46	37.00	38.12	37.55	34.23	30.22	27.35	27.05	28.27	31.65
(Catamarca)	$g_{21}$	23.46	24.66	26.21	28.27	31.06	32.25	29.42	26.41	23.08	21.10	20.83	21.78
(Rio Negro)	$g_{22}$	14.21	14.38	15.11	15.63	15.63	15.34	15.16	15.67	15.82	15.53	15.16	14.58
(Formosa)	$g_{23}$	24.13	24.91	25.16	23.96	23.13	22.07	20.71	19.50	19.06	19.28	20.79	22.80
(Tierra del Fuego)	$g_{24}$	12.75	12.90	13.31	14.29	15.25	15.25	14.27	13.31	13.04	12.20	11.87	12.45



Table. B. 7. Monthly Tip speed ratio in  $i^{th}$  time step calculated for each region.

		Month											
		Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
<b>Region</b>		<b>Tip speed ratio at <math>i^{th}</math> time step</b>											
		$\frac{1}{\Lambda_{g,t}}$											
<i>(Buenos Aires)</i>	$g1$	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
<i>(Córdoba)</i>	$g2$	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00	-0.01
<i>(Corrientes)</i>	$g3$	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01
<i>(La Plata)</i>	$g4$	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
<i>(La Rioja)</i>	$g5$	0.01	0.01	0.00	0.00	-0.01	-0.01	-0.01	0.00	0.00	0.01	0.01	0.01
<i>(Mendoza)</i>	$g6$	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01
<i>(Neuquén)</i>	$g7$	0.03	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03	0.04
<i>(Entre Ríos)</i>	$g8$	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.01
<i>(Misiones)</i>	$g9$	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02	-0.02
<i>(Chubut)</i>	$g10$	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
<i>(Chaco)</i>	$g11$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00
<i>(Santa Cruz)</i>	$g12$	0.05	0.05	0.05	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.05	0.05
<i>(Salta)</i>	$g13$	0.00	0.00	0.00	-0.01	-0.01	-0.01	-0.01	0.00	0.00	0.01	0.01	0.01
<i>(San Juan)</i>	$g14$	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01
<i>(San Luis)</i>	$g15$	0.02	0.02	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.03	0.02	0.02
<i>(Tucumán)</i>	$g16$	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.01	0.01	0.01	0.01
<i>(Jujuy)</i>	$g17$	0.00	0.00	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00
<i>(Santa Fe)</i>	$g18$	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.01
<i>(La Pampa)</i>	$g19$	0.00	0.00	-0.01	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00
<i>(Santiago del Estero)</i>	$g20$	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	0.00	0.00	0.00	0.00	0.00
<i>(Catamarca)</i>	$g21$	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01
<i>(Rio Negro)</i>	$g22$	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03
<i>(Formosa)</i>	$g23$	0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.01	0.01
<i>(Tierra del Fuego)</i>	$g24$	0.04	0.04	0.04	0.03	0.03	0.03	0.03	0.04	0.04	0.05	0.05	0.04

Table. B. 8. Power coefficient  $C_p$  calculated for each region in each month.

		Month											
Region		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
		$C_{p_{g,t}}$											
(Buenos Aires)	g1	0.43	0.43	0.42	0.43	0.42	0.44	0.44	0.45	0.46	0.46	0.46	0.44
(Córdoba)	g2	-0.04	-0.07	-0.08	-0.07	-0.06	-0.03	0.03	0.09	0.13	0.12	0.09	0.02
(Corrientes)	g3	0.25	0.25	0.24	0.25	0.27	0.29	0.32	0.36	0.37	0.37	0.34	0.29
(La Plata)	g4	0.44	0.43	0.43	0.42	0.42	0.43	0.44	0.44	0.46	0.46	0.46	0.44
(La Rioja)	g5	0.32	0.27	0.21	0.13	0.04	-0.02	0.03	0.13	0.25	0.34	0.37	0.36
(Mendoza)	g6	0.36	0.32	0.29	0.21	0.13	0.10	0.13	0.21	0.28	0.33	0.36	0.37
(Neuquén)	g7	0.50	0.48	0.46	0.44	0.41	0.41	0.41	0.44	0.45	0.48	0.50	0.50
(Entre Ríos)	g8	0.34	0.33	0.32	0.33	0.33	0.35	0.37	0.40	0.43	0.42	0.40	0.36
(Misiones)	g9	-0.33	-0.34	-0.34	-0.32	-0.30	-0.30	-0.27	-0.25	-0.26	-0.27	-0.29	-0.32
(Chubut)	g10	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50
(Chaco)	g11	0.17	0.17	0.16	0.18	0.19	0.20	0.25	0.29	0.31	0.31	0.27	0.21
(Santa Cruz)	g12	0.49	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.49	0.49
(Salta)	g13	0.22	0.19	0.15	0.08	0.01	-0.02	0.03	0.10	0.21	0.29	0.31	0.27
(San Juan)	g14	0.37	0.34	0.29	0.23	0.18	0.17	0.20	0.27	0.32	0.36	0.38	0.38
(San Luis)	g15	0.41	0.40	0.39	0.38	0.37	0.39	0.42	0.44	0.46	0.47	0.46	0.44
(Tucumán)	g16	0.26	0.24	0.22	0.17	0.10	0.05	0.11	0.20	0.29	0.34	0.34	0.31
(Jujuy)	g17	0.17	0.13	0.07	-0.01	-0.07	-0.05	0.00	0.05	0.12	0.21	0.25	0.22
(Santa Fe)	g18	0.33	0.32	0.32	0.32	0.32	0.34	0.36	0.39	0.42	0.42	0.40	0.35
(La Pampa)	g19	0.09	0.09	0.07	0.05	0.03	0.06	0.09	0.14	0.16	0.14	0.13	0.11
(Santiago del Estero)	g20	0.04	0.02	0.00	-0.01	-0.03	-0.02	0.05	0.13	0.20	0.21	0.18	0.10
(Catamarca)	g21	0.30	0.27	0.23	0.18	0.11	0.09	0.15	0.22	0.31	0.36	0.36	0.34
(Río Negro)	g22	0.49	0.49	0.48	0.48	0.48	0.48	0.48	0.48	0.47	0.48	0.48	0.49
(Formosa)	g23	0.28	0.26	0.25	0.28	0.31	0.33	0.37	0.40	0.41	0.40	0.36	0.31
(Tierra del Fuego)	g24	0.50	0.50	0.50	0.49	0.48	0.48	0.49	0.50	0.50	0.50	0.50	0.50



## Solar panel

Table. B. 9. Photovoltaic data from the technical data sheet of Kyocera KD225GH-4YB2.

Identifier	Value	Unit
<b>GR</b>	1	$KW/m^2$
<b>STA</b>	25	$^{\circ}C$
<b>PanNomPw</b>	225	$W$
$\mu_p$	-0.0046	$\%/^{\circ}C$
<b>NOCT</b>	45	$^{\circ}C$
<b>PanSurf</b>	1.645	$m^2$
<b>SurfTEqPV</b>	1.5	$m^2$
<b>PanPr</b>	675	$\text{€}$

Table. B. 10. Monthly data of regional temperature.

Region		Month											
		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
		$TA_{g,t} (^{\circ}C)$											
(Buenos Aires)	g1	23.6	22.8	20.6	16.4	13.5	11	10.6	11.5	13.5	16.4	19.5	22
(Córdoba)	g2	23.8	22.8	21.2	17	13.9	10.7	10.8	12.6	15	17.7	20.8	22.7
(Corrientes)	g3	27.5	27.2	25.3	21.5	18.5	16.3	16	17	19.3	21.4	24.2	26.3
(La Plata)	g4	22.8	21.8	20	16.2	12.7	9.9	8.9	10.7	12.5	15.7	18.4	21.1
(La Rioja)	g5	28	26.6	24	19	14.8	11.4	10.9	13.8	17.5	21.3	25	27.3
(Mendoza)	g6	24	22.8	20.2	15.9	11.9	8.5	8.1	10.4	13.5	17.2	20.7	23.2
(Neuquén)	g7	22.1	21.2	17.8	13.3	9.5	6.2	6.1	8.2	11	14.8	18.7	21.2
(Entre Ríos)	g8	24.9	23.8	21.8	18.2	15.4	12.5	12	13.4	15.3	18.2	20.9	23.5
(Misiones)	g9	26.1	25.8	24.3	20.7	18.2	16.3	15.9	17.2	18.7	21.1	23.3	25.5
(Chubut)	g10	20.3	19.9	17.3	13.5	9.7	6.4	6.2	7.9	10.3	13.5	16.6	18.9
(Chaco)	g11	27	26.5	24.6	20.8	18	16.1	15.4	17	18.9	21.2	23.7	26
(Santa Cruz)	g12	12.4	11.6	10.5	7.4	3.5	0.9	1.1	2.8	5.2	8.3	10.6	11.7
(Salta)	g13	27.4	26.4	25.2	22.7	20.3	19.6	20	22.3	23.9	26.8	27.5	28
(San Juan)	g14	26	24.5	21.4	16.2	11.7	8.4	8	10.6	14.3	18.4	22.1	25.2
(San Luis)	g15	23.9	22.8	20	15.6	12	8.9	8.6	10.4	13.7	17	20.4	23
(Tucumán)	g16	25.3	24.1	22.6	18.9	15.8	12.7	12.7	14.7	17.7	20.7	23.1	25
(Jujuy)	g17	23.6	22.5	21.4	18.3	14.8	12.2	11.9	15	17.8	21.7	23	23.8
(Santa Fe)	g18	25.3	24.4	22.6	17.6	15.3	12.4	12.2	13.6	15.4	18.4	21.4	23.5
(La Pampa)	g19	23.6	22.1	19.5	14.9	11	7.9	7.2	9.5	12.1	15.9	19.4	22.5
(Santiago del Estero)	g20	26.7	25.5	23.8	19.8	16.1	12.7	12.2	15.3	18.5	22.7	24.8	26.5
(Catamarca)	g21	27.3	26	24.4	20.4	16	12	11.6	15.4	19.1	23.6	25.6	27.3
(Rio Negro)	g22	21.8	20.8	18.4	14.2	10.4	7.3	7.1	8.5	10.7	14.1	17.5	20.1
(Formosa)	g23	27.8	27.2	25.5	21.8	19.6	17.2	17.1	18.1	20.2	22.2	24.5	26.5
(Tierra del Fuego)	g24	9	8.7	7.6	5.4	3	1.5	1.4	1.9	3.6	5.9	7	8.3

<https://en.climate-data.org/south-america/argentina-11/>

Table. B. 11. Solar irradiance.

		Month											
		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
Region	$g_{t}$	$GT_{g,t}(\text{kWh/m}^2/\text{day})$											
(Buenos Aires)	$g_1$	7.01	6.06	4.86	3.61	2.7	2.2	2.43	3.22	4.49	5.22	6.41	6.92
(Córdoba)	$g_2$	7.17	6.31	5.13	4.04	3.06	2.77	3.09	3.93	5.25	6.08	6.97	7.37
(Corrientes)	$g_3$	6.61	5.78	4.93	3.86	3.36	2.68	3.08	3.87	4.75	5.43	6.32	6.67
(La Plata)	$g_4$	6.88	5.97	4.83	3.57	2.69	2.17	2.43	3.2	4.45	5.25	6.47	6.96
(La Rioja)	$g_5$	6.08	5.56	4.54	3.77	3.12	2.81	3.24	4.11	5.08	5.52	6.01	6.13
(Mendoza)	$g_6$	7.36	6.56	5.52	4.23	2.99	2.41	2.64	3.41	4.55	5.98	7.09	7.48
(Neuquén)	$g_7$	7.88	6.89	5.18	3.56	2.32	1.85	2.16	2.95	4.37	5.86	7.27	7.89
(Entre Ríos)	$g_8$	6.83	6.03	4.96	3.75	2.94	2.43	2.77	3.59	4.8	5.51	6.57	6.91
(Misiones)	$g_9$	6.48	5.72	4.98	3.84	3.24	2.67	3.03	3.77	4.4	5.23	6.22	6.69
(Chubut)	$g_{10}$	6.11	4.91	3.35	1.94	1.07	0.71	0.87	1.58	2.79	4.23	5.7	6.33
(Chaco)	$g_{11}$	6.61	5.78	4.93	3.86	3.36	2.68	3.08	3.87	4.75	5.43	6.32	6.67
(Santa Cruz)	$g_{12}$	6.11	4.91	3.35	1.94	1.07	0.71	0.87	1.58	2.79	4.23	5.7	6.33
(Salta)	$g_{13}$	6.64	6.26	6	5.39	4.45	4.16	4.34	5.2	6.38	6.83	7.27	7.15
(San Juan)	$g_{14}$	7.65	6.9	5.94	4.66	3.39	2.87	3.07	3.92	5.3	6.65	7.67	7.94
(San Luis)	$g_{15}$	7.36	6.56	5.52	4.23	2.99	2.41	2.64	3.41	4.55	5.98	7.09	7.48
(Tucumán)	$g_{16}$	6.27	5.76	5.58	4.95	4	3.68	3.88	4.76	5.87	6.28	6.67	6.57
(Jujuy)	$g_{17}$	6.64	6.26	6	5.39	4.45	4.16	4.34	5.2	6.37	6.83	7.27	7.15
(Santa Fe)	$g_{18}$	6.83	6.03	4.96	3.75	2.94	2.43	2.77	3.59	4.8	5.51	6.57	6.91
(La Pampa)	$g_{19}$	7.31	6.44	4.88	3.52	2.4	1.88	2.16	2.97	4.21	5.55	6.89	7.28
(Santiago del Estero)	$g_{20}$	6.08	5.56	4.54	3.77	3.12	2.81	3.24	4.11	5.08	5.52	6.01	6.13
(Catamarca)	$g_{21}$	6.08	5.56	4.54	3.77	3.12	2.81	3.24	4.11	5.08	5.52	6.01	6.13
(Río Negro)	$g_{22}$	7.31	6.44	4.88	3.52	2.4	1.88	2.16	2.97	4.21	5.55	6.89	7.28
(Formosa)	$g_{23}$	6.65	5.76	5.03	3.96	3.34	2.72	3.1	3.92	4.79	5.45	6.3	6.65
(Tierra del Fuego)	$g_{24}$	5.83	3.58	1.49	0.15	0	0	0	0	0.89	3.04	5.23	6.6

<http://www.solarelectricityhandbook.com/solar-irradiance.html>

Table. B. 12. The temperature of a panel in each month and region.

		Month											
		Jan	Feb	Mar	Apr	May	June	Jul	Aug	Sep	Oct	Nov	Dec
Region	$PanT_{g,t}$	$(^{\circ}\text{C})$											
(Buenos Aires)	23.61	22.81	20.61	16.40	13.50	11.00	10.60	11.50	13.51	16.41	19.51	22.01	23.61
(Córdoba)	23.81	22.81	21.21	17.01	13.90	10.70	10.80	12.61	15.01	17.71	20.81	22.71	23.81
(Corrientes)	27.51	27.21	25.31	21.51	18.50	16.30	16.00	17.01	19.31	21.41	24.21	26.31	27.51
(La Plata)	22.81	21.81	20.01	16.20	12.70	9.90	8.90	10.70	12.51	15.71	18.41	21.11	22.81
(La Rioja)	28.01	26.61	24.01	19.00	14.80	11.40	10.90	13.81	17.51	21.31	25.01	27.31	28.01
(Mendoza)	24.01	22.81	20.21	15.91	11.90	8.50	8.10	10.40	13.51	17.21	20.71	23.21	24.01
(Neuquén)	22.11	21.21	17.81	13.30	9.50	6.20	6.10	8.20	11.01	14.81	18.71	21.21	22.11
(Entre Ríos)	24.91	23.81	21.81	18.20	15.40	12.50	12.00	13.40	15.31	18.21	20.91	23.51	24.91
(Misiones)	26.11	25.81	24.31	20.71	18.20	16.30	15.90	17.20	18.71	21.11	23.31	25.51	26.11
(Chubut)	20.31	19.91	17.30	13.50	9.70	6.40	6.20	7.90	10.30	13.51	16.61	18.91	20.31
(Chaco)	27.01	26.51	24.61	20.81	18.00	16.10	15.40	17.01	18.91	21.21	23.71	26.01	27.01
(Santa Cruz)	12.41	11.61	10.50	7.40	3.50	0.90	1.10	2.80	5.20	8.31	10.61	11.71	12.41
(Salta)	27.41	26.41	25.21	22.71	20.31	19.61	20.01	22.31	23.91	26.81	27.51	28.01	27.41
(San Juan)	26.01	24.51	21.41	16.21	11.70	8.40	8.00	10.61	14.31	18.41	22.11	25.21	26.01
(San Luis)	23.91	22.81	20.01	15.61	12.00	8.90	8.60	10.40	13.71	17.01	20.41	23.01	23.91
(Tucumán)	25.31	24.11	22.61	18.91	15.81	12.70	12.71	14.71	17.71	20.71	23.11	25.01	25.31
(Jujuy)	23.61	22.51	21.41	18.31	14.81	12.21	11.91	15.01	17.81	21.71	23.01	23.81	23.61
(Santa Fe)	25.31	24.41	22.61	17.60	15.30	12.40	12.20	13.60	15.41	18.41	21.41	23.51	25.31
(La Pampa)	23.61	22.11	19.51	14.90	11.00	7.90	7.20	9.50	12.11	15.91	19.41	22.51	23.61
(Santiago del Estero)	26.71	25.51	23.81	19.80	16.10	12.70	12.20	15.31	18.51	22.71	24.81	26.51	26.71
(Catamarca)	27.31	26.01	24.41	20.40	16.00	12.00	11.60	15.41	19.11	23.61	25.61	27.31	27.31
(Río Negro)	21.81	20.81	18.41	14.20	10.40	7.30	7.10	8.50	10.71	14.11	17.51	20.11	21.81
(Formosa)	27.81	27.21	25.51	21.81	19.60	17.20	17.10	18.11	20.21	22.21	24.51	26.51	27.81
(Tierra del Fuego)	9.01	8.70	7.60	5.40	3.00	1.50	1.40	1.90	3.60	5.90	7.01	8.31	9.01

a. Equations associated with the Chapter 6 mathematical model

$$CF_{t'',sc} = NE_{t'',sc} - TOTAL_{t''} \quad t'' = 1, \dots, T - 1, \forall sc \quad (B.48)$$

$$TOTAL_{t''} = \frac{FCI}{T} + \frac{CIns}{T} + \frac{GHGIns}{T} \quad \forall t'' \quad (B.49)$$

The economic criteria consider costs corresponding to system elements installation and pondered operation costs for each renewable resource.

$$CIns = \sum_{ei} \sum_g PrPwl_{ei} \times Pwl_{ei,g} \quad (B.50)$$

$$\begin{aligned} COP_{t,sc} = & \sum_{ei} \sum_g PrEnI_{ei} \times EnIG_{ei,g,t,sc} + \\ & \sum_{e \in EX(e,x)} \sum_x \sum_g [PrEnP_{e,x} \times EnXP_{e,x,g,t,sc} - PrEnS_{e,x} \times \\ & EnXS_{e,x,t,sc}] \quad \forall t, sc \quad (B.51) \end{aligned}$$

Both the environmental and the economic criteria calculate separately the contribution of the installation corresponding to power and capacity of the system's operation that encompasses generation and energy transfers.

$$\begin{aligned} GHGIns = & GHGPr [\sum_{ei} \sum_g GHGPwl_{ei} \times Pwl_{ei,g} + \\ & \sum_{e \in EX(e,x)} \sum_x \sum_g \sum_t \sum_{sc} [(PwXP_{e,x,g,t,sc} + PwXS_{x,g,t,sc}) \times GHGPw_x] \quad (B.52) \end{aligned}$$

$$\begin{aligned} GHGCOP_{t,sc} = & GHGPr [\sum_e \sum_{ei} \sum_g GHGEnI_{e,ei} \times EnIG_{ei,g,t,sc} + \\ & \sum_{e \in EX(e,x)} \sum_x GHGEnX_{e,x} \times EnXP_{e,x,g,t,sc}] \quad \forall t, sc \quad (B.53) \end{aligned}$$

A restriction of the maximum value of emissions from the total installation is also considered for the sizing horizon.

$$GHGPwl \sum_g Pwl_g + \sum_e \sum_{ei} \sum_g GHGEnI_{e,ei} \times EnIG_{ei,g,t,sc} \leq GHGMax \quad \forall t, sc \quad (B.54)$$

An upper limit on the total capital investment is defined by Eq. (B.55):

$$FCI + CIns + GHGIns \leq \overline{FIC} \quad (B.55)$$

In the calculation of the cash flow corresponding to the last period  $t'' = T$ . It is assumed that part of the total fixed capital investment ( $FCI$ ,  $CIns$ , and  $GHGIns$ ) may be recovered at the end of the planning horizon.

$$CF_{t'',sc} = NE_{t'',sc} - TOTAL_{t''} + sv(FCI + CIns + GHGIns) \quad \forall sc, t = T \quad (B.56)$$

$FCI$  denotes the total fixed cost investment of production plants:

$$\begin{aligned} FCI = & \sum_p \sum_g \sum_{t''} [\alpha_{p,g,t''}^{Pr} \times NP_{p,g,t''} + \beta_{p,g,t''}^{Pr} \times PCapE_{p,g,t''}] + \sum_s \sum_g \sum_{t''} [\alpha_{s,g,t''}^{St} \times \\ & NS_{s,g,t''} + \beta_{s,g,t''}^{St} \times SCapE_{s,g,t''} \times PCapE_{p,g,t''}] + \sum_l \sum_{t''} TMC_{l,t''} \times NT_{l,t''} \quad (B.52) \end{aligned}$$

The net earnings are given by the difference between the incomes  $Rev_{t,sc}$  and the facility operation cost  $FOC_{t,sc}$ , transportation cost  $TOC_{t,sc}$ , operation cost  $COP_{t,sc}$  and operational emission costs  $GHGCOP_{t,sc}$  of renewables as stated in equation (B.53):

$$\begin{aligned} NE_{t,sc} = & (1 - \varphi)(Rev_{t,sc} - FOC_{t,sc} - TOC_{t,sc} - COP_{t,sc} \\ & - GHGCOP_{t,sc}) + \varphi DEP_t \quad \forall t, sc \quad (B.53) \end{aligned}$$

$$NE_{t'',sc} = \sum_t NE_{t,sc} \quad (B.54)$$

In equation (B.55),  $SEP(i)$  represents the set of products  $i$  that can be sent to the market.

Appendix B. Case study Data

$$Rev_{t,sc} = \sum_{i \in SEP(i)} \sum_g DTS_{i,g,t,sc} \times PR_{i,g,t} \quad \forall t, sc \quad (B.55)$$

The operating costs are obtained by multiplying the unit production and storage costs ( $UPC_{i,p,g,t}$  and  $USC_{i,s,g,t}$ , respectively) with the corresponding production rates and average inventory levels, respectively. This term also includes the disposal cost  $DC_{t,sc}$ .

$$FOC_{t,sc} = \sum_i \sum_{p \in IM(i,p)} \sum_g UPC_{i,p,g,t} \times PE_{i,p,g,t,sc} + \sum_i \sum_{s \in IS(i,s)} USC_{i,s,g,t} \times AIL_{i,g,t,sc} + DC_{t,sc} \quad \forall t, sc \quad (B.56)$$

The disposal cost is a function of the amount of waste generated and landfill tax  $LT_{i,g}$ :

$$DC_{t,sc} = \sum_i \sum_g W_{i,g,t,sc} \times LT_{i,g} \quad \forall t, sc \quad (B.57)$$

The transportation cost includes the fuel  $FC_{t,sc}$ , labor  $LC_{t,sc}$ , maintenance  $MC_{t,sc}$ , and general  $GC_{t,sc}$  costs:

$$TOC_{t,sc} = FC_{t,sc} + LC_{t,sc} + MC_{t,sc} + GC_{t,sc} \quad \forall t, sc \quad (B.58)$$

The fuel cost is a function of the fuel price  $FP_{l,t}$  and fuel usage:

$$FC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l \left[ \frac{2EL_{g,g'} \times Q_{i,l,g,g',t,sc}}{FE_l \times Cap_l} \right] \times FP_{l,t} \quad \forall t, sc \quad (B.59)$$

Furthermore, as shown in equation (B.60), the labor transportation cost is a function of the driver wage ( $DW_{l,t}$ ) and total delivery time (term inside the brackets):

$$LC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l Total\ Delivery\ Time_{i,l,g,g',t,sc} \times DW_{l,t} \quad \forall t, sc \quad (B.60)$$

The general maintenance cost of the transportation systems depends on the total distance driven and the unit cost of the traveled distance  $ME_l$ .

$$MC_{t,sc} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l \frac{Q_{i,l,g,g',t,sc}}{TCap_l} \times 2EL_{g,g'} \times ME_l \quad \forall t, sc \quad (B.61)$$

Finally, the general cost includes transportation insurance, license and registration, and outstanding finances. It can be determined from the general expenses  $GE_{l,t}$  and number of transportation units  $NT_{l,t}$  as follows (Mele et al., 2011):

$$GC_t = \sum_l \sum_{t' \leq t} GE_{l,t'} \times NT_{l,t'} \quad \forall t \quad (B.62)$$

The depreciation term is calculated with the straight-line method, similarly as (Mele et al., 2011) did in their work:

$$DEP_{t''} = (1 - sv) \times TOTAL_{t''} \quad \forall t'' \quad (B.63)$$

The average number of trucks required by the SC is calculated from the flow rates of materials between regions, the transportation mode availability  $avl_l$ , the capacity of a transport container, the average distance traveled between regions, the average speed, and the loading/unloading time, as stated in equation (B.64):

$$\sum_{t' \leq T} NT_{l,t'} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \frac{Q_{i,l,g,g',t,sc}}{avl_l \times TCap_l} \left( \frac{2EL_{g,g'}}{SP_l} + LUT_l \right) \quad \forall l, sc \quad (B.64)$$

Mathematically, the inventory of emissions due to the operation of the network can be expressed as a function of some continuous variables of the model. Precisely, the entries of the life cycle inventory can be calculated from the production rates at the plants  $PE_{i,p,g,t,sc}$  and transportation flows  $Q_{i,l,g,g',t,sc}$  as stated in equations (B.65) to (B.67):

$$GWP_{cul_{sc}} = \omega_i^{PU} \sum_i \sum_g \sum_t PU_{i,g,t,sc} \quad \forall sc \quad (B.65)$$

$$GWPPr_{sc} = \sum_i \sum_p \sum_g \sum_t \omega_p^{Pr} \times PE_{i,p,g,t,sc} \quad \forall sc \quad (B.66)$$

$$GWPQ_{sc} = \sum_i \sum_l \sum_g \sum_{g'} \sum_t \omega_l^{Tr} \times EL_{g,g'} \times Q_{i,l,g',t,sc} \quad \forall sc \quad (B.67)$$

## B.4 Nomenclature

### Abbreviations

BFPP	Biomass-Fired Power Plant
BIGCC	Biomass-Fueled Integrated Gasification Combined Cycle
BIGFC	Biomass Integrated Gasification with Fuel Cells
BPT	Back Pressure Turbine
CAPEX	Capital Expenditure
GHG	Greenhouse Gas
LCA	Life Cycle Assessment
MCFC	Molten Carbonate Fuel Cells
MILP	Mixed Integer Linear Programming
MOO	Multi-Objective Optimization
NPV	Net Present Value
OPEX	Operating Expense
OV	Opportunity Value
PSE	Process System Engineering
SC	Supply Chain
SSC	Sustainable Supply Chain
SSCM	Sustainable Supply Chain Management
VaR	Value at Risk

### Index

$e$	Set for Energy types ( $e e = 1, \dots, E$ )
$ei$	Set for Energy resources ( $ei ei = 1, \dots, EI$ )
$g$	Set for Regions ( $g g = 1, \dots, G$ )
$i$	Set for Material types ( $i i = 1, \dots, I$ )
$k$	Target value( $k k = 1, \dots, K$ )
$l$	Set for Transportation modes ( $l l = 1, \dots, L$ )
$p$	Set for Production technologies ( $p p = 1, \dots, P$ )
$s$	Set for Storage technologies ( $s s = 1, \dots, S$ )
$sc$	Set of scenarios ( $sc sc = 1, \dots, SC$ )
$t$	Set for Planning periods ( $t t = 1, \dots, T$ )
$x$	Set for External energy suppliers ( $x x = 1, \dots, X$ )

### Sets

EX( $e, x$ )	Subset of ordered pairs that link energy types $e$ to external resource $x$
IL( $i, l$ )	Subset of ordered pairs that link materials $i$ to transport modes $l$
IM( $i, p$ )	Subset of ordered pairs that link main products $i$ to technologies $p$

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$IS(i, s)$	Subset of ordered pairs that link materials $i$ to storage technologies $s$
$SEP(i)$	Subset of final products $i$

*Parameters*

$\alpha_{p,g,t}^{Pr}$	Fixed investment coefficient for technology $p$
$\alpha_{s,g,t}^{St}$	Fixed investment coefficient for storage technology $s$
$\beta_{p,g,t}^{Pr}$	Variable investment coefficient for production technology $p$
$\beta_{s,g,t}^{St}$	Variable investment coefficient for storage technology $s$
$\beta$	The azimuth angle of the pitch
$\varepsilon$	Auxiliary boundary for the $\varepsilon$ -constraint method
$\eta$	Net cogeneration efficiency
$\eta_{alt}$	Alternator efficiency
$\eta_{aux}$	Auxiliary devices (pumps, cooling towers, and other components) efficiency
$\eta_{mT}$	Mechanical turbine efficiency
$\eta_t$	Turbine thermodynamic efficiency
$\theta_{sc}^d$	a realization of uncertain parameters in scenario $sc$
$\lambda_{g,t}$	The tip speed ratio in region $g$ in period $t$
$\Lambda_{g,t}$	The tip speed ratio at $t^{th}$ time step in region $g$ in period $t$
$\mu_p$	Coefficient of variation of power per temperature
$\rho_{air}$	Density of air
$\rho_{p,i}$	Material balance coefficient associated with material $i$ and technology $p$
$\sigma$	Storage period
$\tau$	Minimum desired percentage of the available installed capacity
$\varphi$	Tax rate
$\omega_{nom}$	Nominal turbine rotation speed
$\omega_p^{Pr}$	Life cycle environmental burden associated with production technology $p$
$\omega_i^{PU}$	Life cycle environmental burden associated with purchasing material $i$
$\omega_l^{Tr}$	Life cycle environmental burden associated with transportation mode $l$
$\Omega_k$	Target level $k$
$\Omega'_k$	Environmental performance target
$avl_l$	Availability of transportation mode $l$
$C_{sc,sc'}$	the distance between two scenarios
$CapCrop_{g,t}$	Total capacity of raw material production (sugar cane plantations) in region $g$ in period $t$
$c_p$	specific heat
$Cp_{g,t}$	power coefficient in region $g$ in period $t$
$CutInWV$	Cut-in speed
$CutOutWV$	Cut-out speed



$Demand_{g,t}$	energy demand needed per unit of raw material $i$ in period $t$ , for scenario $sc$
$Demand_{g,t,sc}$	energy demand needed per unit of raw material $i$ in period $t$ , for scenario $sc$
$DW_{l,t}$	Driver wage of transportation mode $l$ in period $t$
$EfIJ_e$	Conversion efficiency between internal energy resource type $e$ and the process plant $i$
$EfIJ_{e,ei}$	Conversion efficiency between internal energy resource $ei$ type $e$ and the process plant $i$
$EfIX_{e,x}$	Conversion efficiency of the excess energy type $e$ sent to the external energy generation resource $x$
$EfXJ_{e,x}$	Conversion efficiency between external resource $x$ energy type $e$ and the process plant $i$
$EL_{g,g'}$	Distance between $g$ and $g'$
$f_{sc}^*$	Optimal objective value under scenario $sc$
$\overline{FIC}$	Upper limit on the capital investment
$FE_l$	Fuel consumption of transportation mode $l$
$FP_{l,t}$	Fuel Price of transportation mode $l$ in period $t$
$GE_{l,t}$	General expenses of transportation mode $l$ in period $t$
$GHGEnI_e$	Emissions per unit of energy generated for each type $e$
$GHGMax$	Maximum allowable emissions amount
$GHGPr$	Price of GHG emissions $kg CO_2$ equivalent
$GHGPwl$	Emissions per unit of power
$GR$	Solar irradiance under standard condition
$GT_{g,t}$	Solar irradiance in region $g$ and period $t$
$h$	Enthalpy
$ir$	Interest rate
$LHV$	Lower heating value
$LT_{i,g,t}$	Landfill tax in period $t$
$LUT_l$	Loading/unloading time of transportation mode $l$
$M$	Big positive number
$m_{bio}$	Biomass flow rate
$m_g$	Mass flow rate of the gas
$ME_l$	Maintenance expenses of transportation mode $l$
$MinPgCO$	Minimum power generation coefficient
$MinPwHW$	Minimum power generation by windmill
$MinPwPV$	Minimum power generation by photovoltaic
$N$	Number of scenarios to be removed
$NOCT$	Normal Cell Operating Temperature
$P_{ec}$	power consumed inside the production process
$P_{eg}$	Power generated by the cogeneration per ton of biomass
$PanNomPw$	Panel nominal power
$PanPr$	Price of a panel
$PanPw_{g,t}$	Power generated by a panel in region $g$ and period $t$
$PanSurf$	Panel surface

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$PanT_{g,t}$	Temperature of a panel in region $g$ and period $t$
$\overline{PCap}_p$	Maximum capacity of technology $p$
$\underline{PCap}_p$	Minimum capacity of technology $p$
$PR_{i,g,t}$	Prices of final products $i$
$PrEnI_e$	Price of energy type $e$
$PrEnP_{e,x}$	Purchase price of external energy type $e$ source $x$
$PrEnS_{e,x}$	Selling price of energy type $e$ to external source $x$
$prob_{sc}$	the probability of scenario $sc$
$prob_{sc}^{orig}$	the probability of scenario $sc$ in an original discrete distribution
$PrPwI$	Installation power cost
$PrPwHW$	Price per unit of wind power
$PrPwPV$	Panel price per unit of power
$PwIMax$	the maximum power to be installed
$PwIMax_{ei}$	the maximum power to install energy resource $ei$
$PwSurfPV_{g,t}$	Power per available surface in region $g$ and period $t$
$\overline{Q}_l$	Maximum capacity of transportation mode $l$
$\underline{Q}_l$	Minimum capacity of transportation mode $l$
$RotD$	Rotor diameter
$\overline{SCap}_s$	Maximum capacity of storage technology $s$
$\underline{SCap}_s$	Minimum capacity of storage technology $s$
$SD_{i,g,t}$	Demand of product $i$ in region $g$ in period $t$
$SD_{i,g,t,sc}$	Demand of product $i$ in region $g$ in period $t$ in scenario $sc$
$SL$	Slot length
$SP_l$	Average speed of transportation mode $l$
$STA$	The ambient temperature under standard condition
$sv$	Salvage value
$SurfMaxHW$	Maximum surface available for horizontal windmill axis
$SurfMaxPV$	Maximum surface available for a photovoltaic
$SurfPwHW$	The relation between the surface and power
$SurfPwPV$	The relation between the surface and power
$SurfTEqHW$	The equivalent surface area of a turbine
$SurfTEqPV$	The equivalent surface occupied by a panel
$SurfTMax$	Maximum total surface
$SurfPwI_{ei}$	Area occupation per unit power of each $ei$
$T$	Number of time intervals
$TA_{g,t}$	Ambient temperature in region $g$ and period $t$
$TCap_l$	Capacity of transportation mode $l$
$TMC_{l,t}$	Cost of establishing transportation mode $l$ in period $t$
$TurbNomPw$	Nominal turbine power
$TurbPr$	Price of a turbine
$TurbPw_{g,t}$	Power generated by a turbine in region $g$ and period $t$
$TurbPwHW_{g,t}$	Captured power by a turbine in region $g$ and period $t$

$UPC_{i,p,g,t}$	the unit production cost of product $i$ in region $g$ in period $t$
$USC_{i,s,g,t}$	unit storage cost of product $i$ in region $g$ in period $t$
$WV_{g,t}$	Wind velocity in region $g$ and period $t$

### *Variables*

$v_{sc,sc'}$	a dual variable which means whether scenario $sc$ is removed and assigned to scenario $sc'$
$AIL_{i,g,t}$	Average inventory level of product $i$ in region $g$ in period $t$
$AIL_{i,g,t,sc}$	Average inventory level of product $i$ in region $g$ in period $t$ in scenario $sc$
$CF_t$	Cash flow in period $t$
$CF_{t,sc}$	Cash flow in period $t$ in scenario $sc$
$CIns$	Total cost of installation of all renewable power plants
$COP_t$	Operation cost of all renewable power plants in period $t$
$COP_{t,sc}$	Operational cost of all renewable power plants in period $t$ in scenario $sc$
$DAM$	Environmental metric to be optimized
$DAM_{sc}$	Environmental metric to be optimized in scenario $sc$
$DC_{t,sc}$	Disposal cost in period $t$ in scenario $sc$
$DEP_t$	Depreciation in period $t$
$DTS_{i,g,t}$	Amount of material $i$ delivered in region $g$ and period $t$
$DTS_{i,g,t,sc}$	Amount of material $i$ delivered in region $g$ and period $t$ in scenario $sc$
$E[DAM]$	Expected environmental damage
$EnIG_{e,g,t}$	Energy type $e$ generated in region $g$ and period $t$
$EnIG_{e,g,t,sc}$	Energy type $e$ generated in region $g$ and period $t$ in scenario $sc$
$EnIG_{ei,g,t,sc}$	Energy type $e$ generated in region $g$ and period $t$ in scenario $sc$
$EnIJ_{e,g,t}$	Energy flux type $e$ between renewable source and demand of region $g$ in period $t$
$EnIJ_{e,g,t,sc}$	Energy flux type $e$ between renewable source and demand of region $g$ in period $t$ in scenario $sc$
$EnIJ_{e,ei,g,t,sc}$	Energy flux type $e$ between renewable source $ei$ and demand of region $g$ in period $t$ in scenario $sc$
$EnIX_{e,x,g,t}$	Energy flux type $e$ between renewable source and external source $x$ region $g$ in period $t$
$EnIX_{e,x,g,t,sc}$	Energy flux type $e$ between renewable source $ei$ and external source $x$ region $g$ in period $t$ in scenario $sc$
$EnIX_{e,ei,x,g,t,sc}$	Energy flux type $e$ between renewable source $ei$ and external source $x$ region $g$ in period $t$
$E[NPV]$	Expected net present value
$EnXJ_{e,x,g,t}$	Energy flux type $e$ between external source $x$ and demand of region $g$ in period $t$
$EnXJ_{e,x,g,t,sc}$	Energy flux type $e$ between external source $x$ and demand of region $g$ in period $t$ in scenario $sc$
$EnXP_{e,x,g,t}$	Energy type $e$ purchased from external source $x$ in period $t$

## Appendix B. Case study Data

$EnXP_{e,x,g,t,sc}$	Energy type $e$ purchased from external source $x$ in period $t$ in scenario $sc$
$EnXS_{e,x,g,t}$	Energy type $e$ sales to external source $x$ in period $t$
$EnXS_{e,x,g,t,sc}$	Energy type $e$ sales to external source $x$ in period $t$ in scenario $sc$
$f_{exp}^{err}$	absolute error between the expected performance of original and reduced distribution
$f_{exp}^{orig}$	Expected objective function obtained using the original set of scenarios
$f_{exp}^{new}$	Expected objective function obtained using the reduced set of scenarios
$FC_t$	Fuel cost in period $t$
$FC_{t,sc}$	Fuel cost in period $t$ in scenario $sc$
$FCI$	Fixed capital investment
$FOC_t$	Facility operating cost in period $t$
$FOC_{t,sc}$	Facility operating cost in period $t$ in scenario $sc$
$Fuel\ Usage_{i,l,g,g',t}$	Fuel consumption for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$
$Fuel\ Usage_{i,l,g,g',t,sc}$	Fuel consumption for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$ in scenario $sc$
$GC_t$	General cost in period $t$
$GC_{t,sc}$	General cost in period $t$ in scenario $sc$
$GHGCOPI_t$	Total GHG operational emissions $kg\ CO_2$ equivalent in period $t$
$GHGCOPI_{t,sc}$	Total GHG operational emissions $kg\ CO_2$ equivalent in period $t$ in scenario $sc$
$GHGIns$	Total GHG Installation emissions $kg\ CO_2$ equivalent for all renewable power plants
$GWPCul$	GWP100 amount in the cultivation process
$GWPCul_{sc}$	GWP100 amount in cultivation process in scenario $sc$
$GWPPr$	GWP100 amount in the production process
$GWPPr_{sc}$	GWP100 amount in the production process in scenario $sc$
$GWPQ$	GWP100 amount in the transportation process
$GWPQ_{sc}$	GWP100 amount in transportation process in scenario $sc$
$LC_t$	Labor cost in period $t$
$LC_{t,sc}$	Labor cost in period $t$ in scenario $sc$
$MC_t$	Maintenance cost in period $t$
$MC_{t,sc}$	Maintenance cost in period $t$ in scenario $sc$
$n_{sc,sc'}$	Probability displacement between scenarios
$NE_t$	Net earnings in period $t$
$NE_{t,sc}$	Net earnings in period $t$ in scenario $sc$
$NP_{p,g,t}$	Number of plants with technology $p$ established in region $g$ and period $t$
$NPV$	Net Present Value
$NPV_{sc}$	Net Present Value in scenario $sc$

$NS_{s,g,t}$	Number of storages with storage technology $s$ established in region $g$ and period $t$
$PE_{i,p,g,t}$	Production rate of material $i$ associated with technology $p$ established in region $g$ and period $t$
$PE_{i,p,g,t,sc}$	Production rate of material $i$ associated with technology $p$ established in region $g$ and period $t$ in scenario $sc$
$PCap_{p,g,t}$	Existing capacity of technology $p$ in region $g$ and period $t$
$prob_{sc}^{new}$	new probability of scenario $sc$ in the reduced distribution
$PT_{i,g,t}$	Total production rate of material $i$ in region $g$ and period $t$
$PT_{i,g,t,sc}$	Total production rate of material $i$ in region $g$ and period $t$ in scenario $sc$
$PU_{i,g,t}$	Purchases of material $i$ in region $g$ and period $t$
$PU_{i,g,t,sc}$	Purchases of material $i$ in region $g$ and period $t$ in scenario $sc$
$PwI_g$	Power to install at own source in region $g$
$PwI_{ei,g}$	Power to install a renewable source $ei$ , in each region $g$
$PwIG_{g,t}$	Power to generate by a renewable source, in each region $g$ , each period $t$
$PwIG_{g,t,sc}$	Power to generate by a renewable source, in each region $g$ , each period $t$ in scenario $sc$
$PwIG_{ei,g,t,sc}$	Power to generate by a renewable source $ei$ , in each region $g$ , each period $t$ in scenario $sc$
$PwIGMax_{g,t}$	Maximum power to generate by renewable source in each region $g$ and period $t$
$PwIGMax_{g,t,sc}$	Maximum power to generate by renewable source in each region $g$ and period $t$ in scenario $sc$
$PwIGMax_{ei,g,t,sc}$	Maximum power to generate by renewable source $ei$ in each region $g$ and period $t$ in scenario $sc$
$PwIGMin_{g,t}$	Minimum power to generate by renewable source in each region $g$ and period $t$
$PwIGMin_{g,t,sc}$	Minimum power to generate by renewable source in each region $g$ and period $t$ in scenario $sc$
$PwIGMin_{ei,g,t,sc}$	Minimum power to generate by renewable source $ei$ in each region $g$ and period $t$ in scenario $sc$
$PwXP_{e,x,g,t}$	Power purchased from external source $x$ in period $t$
$PwXP_{e,x,g,t,sc}$	Power purchased from external source $x$ in period $t$ in scenario $sc$
$PwXS_{x,g,t}$	Power selling to external source $x$ in period $t$
$PwXS_{x,g,t,sc}$	Power selling to external source $x$ in period $t$ in scenario $sc$
$Q_{i,l,g,g',t}$	Flow rate of material $i$ transported by mode $l$ from region $g$ to region $g'$ in period $t$
$Q_{i,l,g,g',t,sc}$	Flow rate of material $i$ transported by mode $l$ from region $g$ to region $g'$ in period $t$ in scenario $sc$
$Rev_{t,sc}$	Revenue in period $t$ in scenario $sc$
$SCap_{s,g,t}$	Existing capacity of storage $s$ in region $g$ and period $t$
$SCapE_{s,g,t}$	Capacity expansion of storage $s$ in region $g$ and period $t$
$ST_{i,s,g,t}$	Total inventory of material $i$ in region $g$ stored by technology $s$ in period $t$

Appendix B. Case study Data

$ST_{i,s,g,t,sc}$	Total inventory of material $i$ in region $g$ stored by technology $s$ in period $t$ in scenario $sc$
$SurfInsHW_{ei,g}$	Equivalent windmill surface to occupy in region $g$
$SurfInsPV_{ei,g}$	Equivalent photovoltaic surface to occupy in region $g$
$SurfPV_{ei,g}$	Photovoltaic surface to install in region $g$
$TOC_t$	Transport operating cost in period $t$
$TOC_{t,sc}$	Transport operating cost in period $t$ in scenario $sc$
$TOTAL_t$	total depreciable capital during period $t$
$Total\ Delivery\ time_{i,l,g,g',t}$	Delivery time for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$
$Total\ Delivery\ time_{i,l,g,g',t,sc}$	Delivery time for transporting material $i$ by transportation mode $l$ , between region $g$ and $g'$ in period $t$ in scenario $sc$
$TotalDemand_{g,t}$	Energy demand of region $g$ and period $t$
$TotalDemand_{g,t,sc}$	Energy demand of region $g$ and period $t$ in scenario $sc$
$TurbNum_{ei,g}$	Number of the turbine to install in region $g$
$W_{i,g,t}$	Amount of wastes of $i$ generated in region $g$ and period $t$
$W_{i,g,t,sc}$	Amount of wastes of $i$ generated in region $g$ and period $t$ in scenario $sc$

**Binary Variables**

$Gn_{g,t,sc}$	By the Big-M method, the local binary variable is used to define lower and higher generation limits
$X_{l,g,g',t}$	1 if a transportation link is established between regions $g$ and $g'$ , otherwise 0
$y_{sc}$	whether scenario $sc$ is removed ( $y_{sc} = 1$ ) or not ( $y_{sc} = 0$ )
$Z_{sc}$	1 if NPV attained in scenario $sc$ is below the target level $\Omega$ , otherwise 0
$Z'_{sc}$	Binary variable (1 if the impact in scenario $c$ is above the target limit, 0 otherwise)

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