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CONTROL AND OPTIMIZATION OF AN SBR FOR NITROGEN REMOVAL: FROM MODEL CALIBRATION TO PLANT OPERATION

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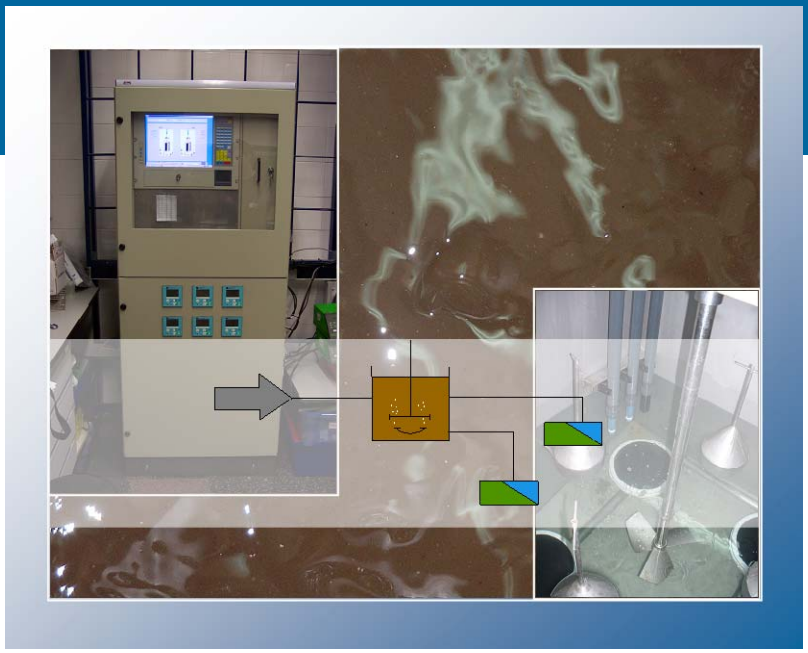

Control and optimization of an SBR for nitrogen removal

From model calibration to plant operation.

Lluís Corominas Tabares

PhD Thesis - 2006

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CERTIFIQUEN

Que el llicenciat Lluís Corominas Tabares ha dut a terme, sota la seva direcció, el treball que, amb el títol *Control and Optimization of an SBR for nitrogen removal: from model calibration to plant operation*, presenta en aquesta memòria, la qual constitueix la seva Tesi per optar al Grau de Doctor per la Universitat de Girona.

I perquè en prengueu coneixement i tingui els efectes que correspongui, presentem davant la Facultat de Ciències de la Universitat de Girona l'esmentada Tesi, signant aquesta certificació a

Girona, 21 de Març del 2006

Maria Dolors Balaguer Condom Jesús Colprim Galceran

Agraïments / Acknowledgements

Després d'escriure tota la tesi em vé molt de gust escriure els agraïments per deixar constància del suport que he rebut durant aquests 5 anys. I ho he fet una mica lluny dels discursos clàssics, de manera agosarada i estalviant paraules:

Una porta que es tanca,
La ment que s'allibera,
Els pensaments damunt la taula,
I la mirada endavant.

Enrera queden els anys,
I les anècdotes viscudes,
Els savis còmplices continuen,
Amb la nova sang impacient.

Les amistats resten en un núvol,
Allí encara s'hi escolten,
Els ritmes marxosos dels inicis,
i l'harmonia dels temps actuals.

Una ombra pintada
m'ha acompanyat de nit i de dia,
la flor que arrela al cor,
i els que han servit l'esperança

No són només paraules sinó pensaments,
No és només paper sinó sentiment,
No són només fets sinó coneixement,
Un petit pas cap a la veritat,
O un reconfort en la ignorància?

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ELS RITMES MARXOSOS
NOVA SANG
HARMONIA

lequia

Resum

Dins el marc de la Nova Cultura de l'Aigua s'està exercint més pressió per assegurar el compliment dels requeriments ambientals. En el camp del tractament de les aigües residuals, es requereix una disminució dels nutrients que s'aboquen en les aigües superficials i per tant es fa necessari millorar la qualitat de l'efluent dels processos de tractament d'aigües residuals. El tractament d'aquestes aigües mitjançant processos biològics ha estat àmpliament utilitzat tant per aigües urbanes com industrials establint condicions aeròbies i anòxiques per eliminar la matèria orgànica i el nitrogen.

El Reactor Seqüencial per Càrregues (SBR per *Sequencing Batch Reactor*) és un sistema de fangs activats utilitzat pel tractament de les aigües residuals. A diferència dels sistemes que funcionen en continu els processos de reacció i sedimentació es realitzen en un sol reactor establint una seqüència temporal de fases d'omplerta, reacció, sedimentació i buidat. El fet de que es requereixi poc espai combinat amb la flexibilitat per tractar cabals i composicions variables han fet de l'SBR un sistema eficaç pel tractament de l'aigua residual de comunitats petites.

Les condicions d'operació més adequades per l'SBR han estat àmpliament estudiades tant per aigua residual sintètica com real. Un pas endavant consisteix en incrementar la productivitat de la planta, disminuir les necessitats de personal, reduir el consum d'energia i incrementar la fiabilitat del procés, fets que es poden aconseguir utilitzant estratègies de control. Així doncs, l'objectiu general d'aquesta tesis és dissenyar un sistema de control i optimització per la tecnologia SBR assegurant l'eliminació de matèria orgànica i nitrogen, utilitzant models calibrats com a eina de suport.

El disseny i implementació de les estratègies de control es pot realitzar directament mitjançant l'experimentació. Tot i això, la utilització de models representa un avantatge per a definir i avaluar estratègies de control, estalviant temps i diners. Per tant, és necessari obtenir un model calibrat de la planta SBR, basat en el model existent ASM1, que descrigui els processos d'eliminació de matèria orgànica i nitrogen. Per tal de superar les dificultats del procés de calibració i per assegurar que els estudis són de suficient qualitat han aparegut diferents protocols sistematics de treball que poden ser aplicats. Els aspectes més rellevants que es consideren en aquests protocols s'han analitzat de manera separada per cadascun d'ells, abans de començar amb la calibració del model de l'SBR. Posteriorment s'han realitzat dos estudis de calibració: el primer es realitza per tal d'obtenir un model calibrat que s'utilitzarà per avaluar estratègies de control. En aquest cas s'utilitzen només dades històriques per calibrar el model i els punts forts i febles detectats s'identifiquen per millorar posteriors experiències de calibració; en el segon estudi de calibració s'obté un model de fangs activats que serà utilitzat en el desenvolupament d'un sistema de control i supervisió de l'SBR.

Normalment, la tecnologia SBR és operada amb un cicle prefixat i el cap de planta supervisa el procés i adapta manualment aquest cicle. La flexibilitat i l'alt nivell d'automatització dels SBR afavoreix la implementació d'estratègies de control que permeten ajustar a temps real el cicle prefixat. Diferents nivells de control es poden definir depenent de la informació necessària i de les instruccions d'operació aplicades. En aquesta tesis, s'han definit tres nivells de control: el nivell baix, el nivell mitjà i el nivell alt.

El nivell baix està format pel sistema d'adquisició de dades i pel sistema de monitorització que permeten executar un cicle definit i fer l'adquisició de les dades que s'obtenen de l'SBR. A més, es pot contribuir a la millora del funcionament de l'SBR amb l'establiment de llaços interns de control per tal de mantenir certs paràmetres ambientals a un valor desitjat. La monitorització del procés també permet identificar pautes de comportament en les variables en línia (pH, oxigen dissolt i potencial RedOx) que es poden relacionar directament amb les reaccions del procés. Així doncs, s'han analitzat diferents casos històrics d'estudi per tal d'identificar les pautes de comportament i més en concret detectar els punts finals de les reaccions de nitrificació i desnitrificació utilitzant aquestes variables en línia. Es fa èmfasis en el control de l'oxigen dissolt durant les fases aeròbies ja que aquest té influencia en la resta de variables, i per tant pot tenir efectes sobre nivells de control superiors.

En el nivell mitjà de control la durada de les fases aeròbies i anòxiques és ajustada per tal de minimitzar el consum d'energia i d'incrementar la capacitat de la planta. L'objectiu és finalitzar les fases aeròbies quan la nitrificació hagi acabat i les anòxiques quan la desnitrificació sigui completa. La finalització d'aquestes etapes és possible amb el coneixement adquirit anteriorment de les pautes de comportament de les variables en línia. Així doncs, s'ha dissenyat una estratègia de control basada en les dades de velocitat de consum d'oxigen (OUR) i RedOx que s'ha avaluat primer utilitzant un dels models calibrats i posteriorment s'ha implementat en una planta pilot semi-industrial.

El nivell alt de control realitza la supervisió del procés. L'objectiu és assegurar que l'SBR sigui capaç d'adaptar les condicions d'operació a la variabilitat de l'aigua residual sense la necessitat d'una contínua supervisió del cap de planta. Per aquest motiu es proposa un mòdul supervisor que és capaç d'identificar l'estat del procés i adaptar el cicle mitjançant la utilització d'eines de la intel·ligència artificial.

Els nivells de control baix i mitjà s'han implementat en la planta pilot. El nivell alt s'ha dissenat i els diferents mòduls s'estan desenvolupant. El treball futur se centra en la finalització i validació d'aquest sistema de control supervisor.

Resumen

Bajo el concepto de la Nueva Cultura del Agua se está ejerciendo más presión para cumplir con los requerimientos ambientales. En el campo del tratamiento de aguas residuales se requiere una disminución de los nutrientes que se vierten en las aguas superficiales y por lo tanto es necesario mejorar la calidad del efluente de los procesos de tratamiento de las aguas residuales. El tratamiento del agua residual mediante procesos biológicos ha sido ampliamente utilizado para las aguas urbanas e industriales estableciendo condiciones aeróbicas y anóxicas para eliminar simultáneamente la materia orgánica y el nitrógeno.

El Reactor Secuencial por Cargas (SBR de *Sequencing Batch Reactor*) es un sistema de lodos activos utilizado para el tratamiento de aguas residuales. A diferencia de los sistemas que funcionan en continuo los procesos de reacción y sedimentación se llevan a cabo en un solo reactor mediante la secuencia temporal de fases de llenado, reacción, sedimentación y vaciado. El hecho de que se requiera poco espacio combinado con la flexibilidad para tratar caudales y composiciones variables ha favorecido que el SBR sea un sistema eficaz para el tratamiento del agua residual de comunidades pequeñas.

Las condiciones de operación de la tecnología SBR más adecuadas han sido ampliamente estudiadas utilizando tanto agua sintética como real. Un paso más allá consiste en incrementar la productividad de la planta, disminuir las necesidades de personal, reducir el consumo de energía e incrementar la fiabilidad del proceso. Esto se puede conseguir utilizando estrategias de control. Por lo tanto, el objetivo general de esta tesis es diseñar un sistema de control y optimización para la tecnología SBR asegurando la eliminación de materia orgánica y nitrógeno, utilizando modelos calibrados como herramienta de soporte.

El diseño e implementación de las estrategias de control se puede realizar directamente mediante la experimentación. No obstante, la utilización de modelos representa una ventaja para la definición y evaluación de las estrategias, ahorrando tiempo y dinero. Por lo tanto, es necesario obtener un modelo calibrado de la planta SBR, basado en el modelo existente ASM1, que describa los procesos de eliminación de materia orgánica y nitrógeno. Para superar las dificultades del proceso de calibración y para asegurar que los estudios son de suficiente calidad han aparecido distintos protocolos sistemáticos de trabajo que pueden ser aplicados. Los aspectos más relevantes que se consideran en estos protocolos existentes se han analizado antes de empezar con la calibración del modelo del SBR. Después se han realizado dos estudios de calibración: el primero se realiza para obtener un modelo calibrado que se utilizará para evaluar estrategias de control. En este caso se utilizan sólo datos históricos y los puntos fuertes y débiles detectados se identifican para mejorar posteriores experiencias de calibración; en el segundo estudio de calibración se obtiene un modelo de fangos activados que va a ser utilizado en el desarrollo de un sistema de control y supervisión del SBR.

Normalmente la tecnología SBR funciona siguiendo un ciclo prefijado y el jefe de planta supervisa el proceso y adapta manualmente este ciclo. La flexibilidad y el alto nivel de automatización de los SBR favorecen la implementación de estrategias de control que permiten ajustar a tiempo real el ciclo prefijado. Se pueden definir distintos niveles de control dependiendo de la información necesaria y de las instrucciones de operación aplicadas. En esta tesis se han definido tres niveles de control: el bajo, el mediano y el alto.

El nivel bajo está formado por el sistema de control y adquisición de datos y por el sistema de monitorización que permiten ejecutar un ciclo definido y adquirir los datos que se obtienen del SBR. Además, se puede contribuir a la mejora del funcionamiento del SBR con el establecimiento de lazos internos de control para mantener ciertos parámetros ambientales a un valor determinado. La monitorización del proceso también permite identificar pautas de comportamiento en las variables en línea (pH, oxígeno disuelto y potencial RedOx) que se pueden relacionar directamente con las reacciones del proceso. De esta forma, se han analizado diferentes casos de estudio históricos para identificar las pautas de comportamiento y más en concreto detectar los puntos finales de las reacciones aeróbicas y anóxicas. Se presta especial atención al control del oxígeno disuelto durante las fases aeróbicas ya que éste tiene influencia sobre otras variables, y por lo tanto puede tener efectos sobre niveles de control superiores.

En el nivel medio de control la duración de las fases aeróbicas y anóxicas es ajustada para minimizar el consumo de energía e incrementar la capacidad de la planta. El objetivo es finalizar las fases aeróbicas cuando la nitrificación acabe y las fases anóxicas cuando el proceso de desnitrificación sea completado. La finalización de estas etapas es posible gracias al conocimiento adquirido anteriormente de las pautas de comportamiento de las variables en línea. De este modo, se ha diseñado una estrategia de control basada en los datos de velocidad de consumo de oxígeno (OUR) y RedOx, que se ha evaluado primero utilizando un modelo calibrado y posteriormente se ha implementado en una planta piloto semi-industrial.

El nivel más alto de control realiza la supervisión del proceso. El objetivo es asegurar que el SBR sea capaz de adaptar las condiciones de operación a la variabilidad del agua residual sin la necesidad de una continua supervisión del jefe de planta. Por esta razón se propone un módulo supervisor que es capaz de identificar el estado del proceso y adaptar el ciclo mediante la utilización de herramientas de inteligencia artificial.

Los niveles de control bajo y medio se han implementado en planta piloto. El nivel alto se ha diseñado y los distintos módulos se están desarrollando. El trabajo futuro se centra en la finalización y validación de éste sistema de control supervisor.

Summary

Within the scope of the New Water Culture there is pressure to comply with environmental requirements. Hence, regarding the field of wastewater treatment a decrease in nutrients being discharged into surface waters is required as pointed by the Urban Water Directive (91/271/CE). There is an increasing need to improve the effluent quality of domestic wastewater treatment processes. Treatment of contaminated wastewater by means of biological processes has been widely implemented from classical urban wastewater to industrial wastewaters for simultaneous carbon and nitrogen removal. Establishing aerobic and anoxic conditions in a controlled manner permits the development of microbial communities capable of executing organic matter and nitrogen removal.

The Sequencing Batch Reactor (SBR) is a fill-and-draw activated sludge system for wastewater treatment. While in continuous systems the reaction and settling occur in different basins, in SBR all the processes are conducted in a single reactor following a sequence of fill, reaction, settling and draw phases. SBR technology has proved to be an effective system to treat the wastewater of small communities mainly because less space is required as all operations occur in one basin and it provides the flexibility needed to treat a variable wastewater (load and composition).

The suitable operating conditions for the SBR have already been studied for both synthetic and real wastewater. A step further consists in increasing the productivity of the plant, decrease the personnel necessities, reduce the energy consumption, and increment the reliability on the process, which can be achieved by making use of control procedures. Hence, the general objective of this thesis is to design a control system for the SBR technology removing organic matter and nitrogen, using a calibrated model as an operation support tool.

The design and implementation of control strategies can be conducted directly with experimentation. However, using model-based approaches represents an advantage when defining and evaluating the control strategies, saving time and money. Therefore, it is necessary to obtain a calibrated model of the pilot plant SBR, based on the existing ASM1, removing organic matter and nitrogen. To overcome the difficulties of the whole calibration experience and to ensure studies of enough quality different existing systematic working procedures can be applied. The most important aspects considered in these calibration procedures are analyzed separately for each existing protocol, before starting the calibration of the model for the SBR. Then, two calibration experiences are conducted: The first one is for obtaining a calibrated model to be used for evaluating control strategies. Only historical data is used to calibrate the model, and the possible modifications or improvements are identified to improve further calibration experiences. The second calibration study is to obtain calibrate an activated sludge model to support a supervisory control system of the SBR.

Normally the SBR operates with fixed cycle configuration and the plant manager is in charge of supervising the process and manually adapting the cycle. The flexibility and the high automation degree of the SBR technology favor the implementation of control strategies that permit adjusting at real-time the fixed cycle. Different levels of control can be defined depending on the information needed and the operating instructions applied. In this thesis, three levels of control have been defined: The low level, the medium level and the high level.

The low level is the Data Acquisition and Control (DAC) and monitoring system which permits executing a defined cycle recipe and acquiring all the data coming from the SBR. Moreover, it can contribute to the improvement in the SBR performance establishing internal control loops to maintain environmental parameters at a desired level. The monitoring of the process permits also identifying possible patterns in the on-line variables (pH, dissolved oxygen and ORP) that are directly related to the process reactions. Hence, different historical case studies are analyzed to identify patterns and to detect the endpoints for the aerobic and anoxic reactions. Special attention is given to the control of the dissolved oxygen during the aerobic phases since it can influence other variables and hence, to higher levels of control.

In the medium level the length of the aerobic and anoxic phases is adjusted in order to minimize the energy consumption and increase the capacity of the plant. The objective is to end with the aerobic phases when nitrification is finished and with the anoxic phases when denitrification process is completed. This is possible with the knowledge acquired previously regarding the patterns in the on-line variables. Therefore, a control strategy has been designed mainly based on the Oxygen Uptake Rate (OUR) and the ORP data, and it has been first evaluated using the first calibrated model, and afterwards it has been implemented on the semi-industrial pilot plant.

The high level of control is related to the supervision of the process. The objective is to ensure that the SBR is able to adapt the operating conditions to the wastewater variability without the need of a continued supervision of the plant manager. For this reason a supervisory module is proposed which is able to identify the process status and adapt the cycle definition by using artificial intelligence tools.

The lower and medium levels of control have been implemented in the pilot plant. The higher level has been designed and the different modules are under development. The future work is focused on finishing and validating the supervisory control system.

Table of contents

Notation and Abbreviations

AE	Aeration Energy	MLSS	Mixed Liquor Suspended Solids
AOB	Ammonium Oxidizer Bacteria	MLVSS	Mixed Liquor Volatile Suspended Solids
ARD	Average Relative Deviation	MPCA	Multiway Principal Component Analysis
ASM	Activated Sludge Model	MSPC	Multivariable Statistical Process Control
AV	Ammonia Valley	N	Nitrogen
BSM	Benchmark Simulation Model	NA	Nitrate Apex
BIOMATH	Department of Applied Mathematics, Biometrics and Process control	NK	Nitrate Knee
BNR	Biological Nutrient Removal	NOB	Nitrite Oxidizer Bacteria
BOD	Biochemical Oxygen Demand	NUR	Nitrate Utilization Rates
BSM	Benchmark Simulation Model	OED	Optimal Experiment Design
CBR	Case Based Reasoning	ORP	Oxidation Reduction Potential
CFD	Computational Fluid Dynamics	OUR	Oxygen Uptake Rate
COD	Chemical Oxygen Demand	RCMP	Residual Carbon Manipulation Point
DAC	Data Acquisition and Control	SBR	Sequencing Batch Reactor
DME	Dehydrated Meat Extract	SRT	Sludge Retention Time
DO	Dissolved Oxygen	SSE	Sum of Squared Errors
DSVI	Diluted Sludge Volumetric Index	STOWA	Dutch Foundation of Applied Wat. Res.
EPA	Environmental Protection Agency	SWOT	Strengths, Weaknesses, Opportunities and Threats
ES	Expert System	SYCOTIN	Intelligent Control System
EWFD	European Water Framework Directive	TKN	Total Kjeldalh Nitrogen
HRT	Hydraulic Retention Time	TSS	Total Suspended Solids
HSG	Hochschulgruppe guidelines	VSS	Volatile Suspended Solids
ICA	Instrumentation, Control and Automation	WERF	Water Environment Research Foundation
IWA	International Water Association	WEST	World wide Engine for Simulation, Training and Automation
LFS	Flowing gas Static Liquid	WWTP	Wastewater Treatment Plant

S_{ALK}	Alkalinity of the wastewater	X_{BA}	Autotrophic organisms
S_I	Inert soluble organic material	X_{BH}	Heterotrophic organisms
S_{ND}	Soluble organic nitrogen	X_I	Inert particulate organic material
S_{NH}	Ammonium plus ammonia nitrogen	X_{ND}	Particulate biodegradable organic nitrogen
S_{NO}	Nitrate plus nitrite nitrogen	X_P	Organic particulate products arising from the biomass decay
S_O	Dissolved oxygen	X_S	Slowly biodegradable substrate
S_S	Readily biodegradable substrate		

f_P	Fraction of biomass yielding particulate organics	K_La AX	Oxygen mass transfer coefficient for anoxic phases
μ_A	Autotrophic maximum growth rate	K_{NH}	Ammonium substrate saturation constant for nitrifiers
μ_H	Heterotrophic maximum growth rate	K_{NO}	Nitrate half-saturation coefficient for denitrifying heterotrophic biomass
b_A	Autotrophic decay coefficient	K_{OA}	Nitrifiers oxygen substrate saturation constant
b_H	Heterotrophic decay coefficient	K_{OH}	Heterotrophic oxygen substrate saturation constant
i_{XB}	g N(g COD)$^{-1}$ in biomass	K_S	Half-saturation coefficient for heterotrophic biomass
i_{XP}	g N(g COD)$^{-1}$ in endogenous mass	K_X	Half-saturation coefficient for hydrolysis of slowly biodegradable substrate
k_a	Ammonification rate	Y_A	Autotrophic yield
k_d	Traditional heterotrophic decay coefficient	Y_H	Heterotrophic yield
k_H	Hydrolysis rate	η_g	Correction factor for μ_H under anoxic conditions
K_La	Oxygen mass transfer coefficient (1st aerobic phase)	η_H	Correction factor for hydrolysis under anoxic conditions

$BCOD_{inf}$	Influent biodegradable COD	t_{AE}	Aerobic time
BOD_U	Ultimate BOD	t_{AX}	Anoxic time
$COD_{0.1\mu m, inf}$	Influent 0.1µm filtered COD	t_C	Total cycle
$COD_{P, inf}$	Influent particulate COD	t_D	Draw time
$COD_{S, inf}$	Inflluent soluble COD	t_F	Fill time
$COD_{S, effl}$	Effluent soluble COD	Temp	Temperature
$COD_{T, inf}$	Influent total COD	t_{max}	Maximum phase time
F/M	Food/Microorganisms	t_{min}	Minimum time
f_E	Effective fraction	t_R	Reaction time
K_La	Oxygen transfer efficiency	t_S	Settling time
M	Number of filling events applied during a cycle.	t_{wait}	Waiting time
N_C	Cycles per day	V_E	Volume of water drawn
N_{EF}	Total nitrogen concentration in the effluent	V_F	Filled volume every cycle
NH_4^+ (NH_4-N)	Ammonium nitrogen concentration	V_{MIN}	Minimum volume
N_{IN}	Total nitrogen concentration in the influent	V_T	Maximum volume
NO_2^- (NO_2-N)	Nitrite nitrogen concentration	V_t	Treated volume
NO_3^- (NO_3-N)	Nitrate nitrogen concentration	V_W	Volume of MLSS wastaged
NO_X^- (NO_X-N)	Oxidized nitrogen concentration	X	MLSS concentration at maximum volume
Q_I	Influent flow	X_E	MLSS concentration in the effluent
R_E	Volumetric exchange ratio	X_W	MLSS concentration in the wastage

1 INTRODUCTION

1. INTRODUCTION

1.1. TOWARDS A NEW WATER CULTURE

Human manipulation of the environment and especially the non-sustainable exploitation of natural resources has led to the equilibrium breaking of different natural ecosystems, which affects the soil, water and atmosphere environments. Focusing on the water resources, fresh water comprises less than 1% of the global water volume. Of that volume, groundwater makes up by far the largest quantity. Rivers and fresh-water lakes constitute about 1% of the world's fresh-water resources (Turner *et al.*, 1990). Although water is a renewable resource human activities have directly and indirectly altered the quality of fresh-water resources, and in some areas reduced the quantity of these resources.

In the last decades, the awareness of environmental issues has increased in society considerably. A New Water Culture is appearing, and the prevailing notion that water is a resource is changing towards the idea of managing rivers as ecosystems. Water policies in Europe and the world have shifted towards "demand management" and have incorporated new technologies in depuration and reuse. They prime the protection of aquatic ecosystems and point towards sustainable development. The European Water Framework Directive (EWFD, 2000/60/CE) represents these tendencies.

Within the scope of the New Water Culture there is pressure to comply with environmental requirements. Hence, regarding the field of wastewater treatment a decrease in nutrients being discharged into surface waters is required as pointed by the Urban Water Directive (91/271/CE). There is an increasing need to improve the effluent quality of domestic wastewater treatment processes. New investments and recent research is growing and human knowledge is applied to anticipate effects and to avoid or at least mitigate possible deleterious effects before they occur. One of the examples is the research in the field of nitrogen removal from wastewater. The anthropogenic production of fertilizers has increased the nitrogen pollution load, endangering the aquatic ecosystems with the eutrophication process.

Treatment of contaminated wastewater by means of biological processes has been widely implemented from classical urban wastewater to industrial wastewaters for simultaneous carbon and nitrogen removal (Metcalf & Eddy, 2003). Thus, from an economical and operational point of view, biological treatment has proved to be robust and more efficient in energy use for treating biodegradable wastewaters (Grady *et al.*, 1999; Watts and Garber, 1995). The combination of the knowledge acquired and the advances in the technologies permits more control over the biological wastewater treatment process. This permits us to improve the quality of rivers and optimize the process, which is in accordance with the sustainability concept.

1.2. THE ACTIVATED SLUDGE SYSTEM

Since its beginnings in 1914, the activated sludge process developed by Arden and Lockett has increasingly gained popularity, and today it is the most widely used biological treatment process for both domestic and industrial wastewater.

The activated sludge process is a biological process in which the activity of a microbial species community under controlled operating conditions permits the biodegradation of organic matter and nutrients from wastewater. The community is composed of about 95% bacteria and the other 5% is protozoa, metazoa, fungi, algae and viruses (Richard, 1989). The composition of the community is not constant and the competition in a specific biochemical environment selects the best-adapted microbes which determine the biological reactions conducted (Grady *et al.*, 1999).

In activated sludge systems different environment conditions can be applied by regulating key process parameters such as the concentration of electron donors and electron acceptors. Establishing aerobic, anoxic and anaerobic conditions in a controlled manner permits the development of microbial communities capable of executing organic matter removal, nitrogen removal (nitrification and denitrification) and phosphorus removal (Wilderer *et al.*, 2001).

When aerobic conditions are maintained (supplying oxygen to the system) then organic substrates can be oxidized, providing energy and a carbon source for the growth of heterotrophic bacteria (see Figure 1-1-Left).

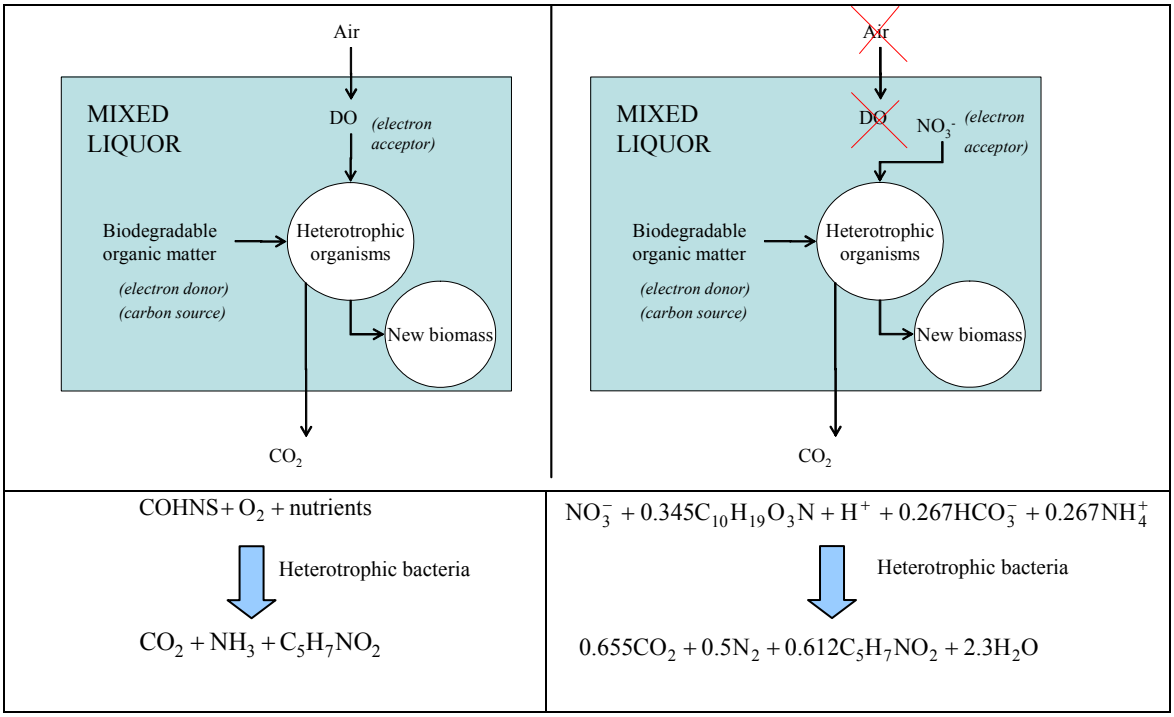


Figure 1-1. Biochemical degradation of biodegradable organic matter. Left: aerobic conditions; Right: anoxic conditions. (Reactions obtained from Metcalf & Eddy (2003)).

Moreover, autotrophic bacteria can grow obtaining energy from ammonia and nitrite oxidation using bicarbonate as the carbon source. This process is called nitrification and occurs in two steps: i) the aerobic oxidation of ammonium to nitrite by the ammonium oxidizer bacteria (AOB) and ii) the aerobic oxidation of nitrite into nitrate by the nitrite oxidizer bacteria (NOB) (see Figure 1-2).

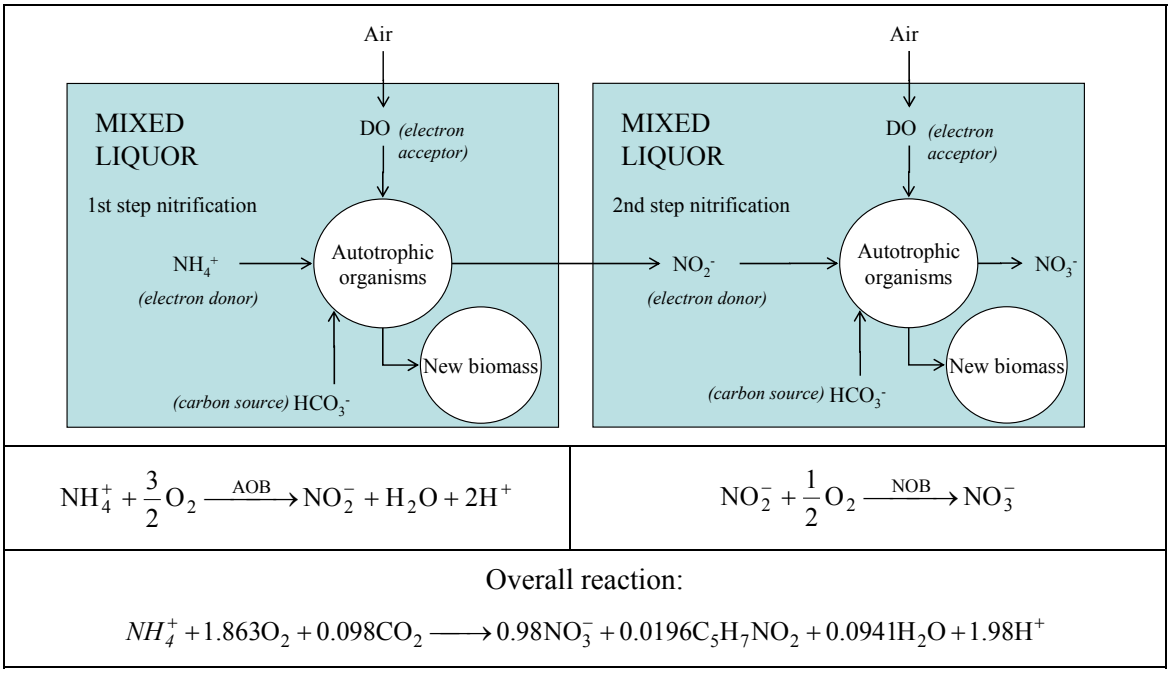


Figure 1-2. Nitrification process. Left: nitritation; Right: nitratation. (Reactions obtained from Metcalf & Eddy (2003)).

Introducing an anoxic zone (in another bioreactor or in the same) allows the nitrate formed by the autotrophic organisms to be used as an electron acceptor by the facultative heterotrophic bacteria, converting it into nitrogen gas (Denitrification process), thus removing the soluble nitrogen from the system (see Figure 1-1-Right).

Hence, the classical nitrogen removal system requires the combination of aerobic and anoxic conditions in which the processes of nitrification and denitrification occur respectively.

An important property of the activated sludge process is the capability of growing in well formed aggregates when the composition of floc-forming and filamentous bacteria is balanced. This permits their gravity sedimentation, separating the sludge to the treated wastewater that can be discharged to the receiving media. Part of the separated sludge is wasted and part is recycled back into the system.

This sedimentation process is normally conducted in a settler located after the reaction basins in continuous flow systems. However, for batch technologies it is possible to conduct the reactions and the settling in the same reactor. The Sequencing Batch Reactor (SBR) system is time-driven and permits alternating anoxic and aerobic phases easily.

1. 3. SBR TECHNOLOGY

1.3.1. Characteristics of the SBR technology

The SBR is a fill-and-draw activated sludge system for wastewater treatment. While in continuous systems the reaction and settling occur in different reactors, in SBR all the processes are conducted in a single reactor following a sequence of fill, reaction, settling and draw phases (see Figure 1-3).

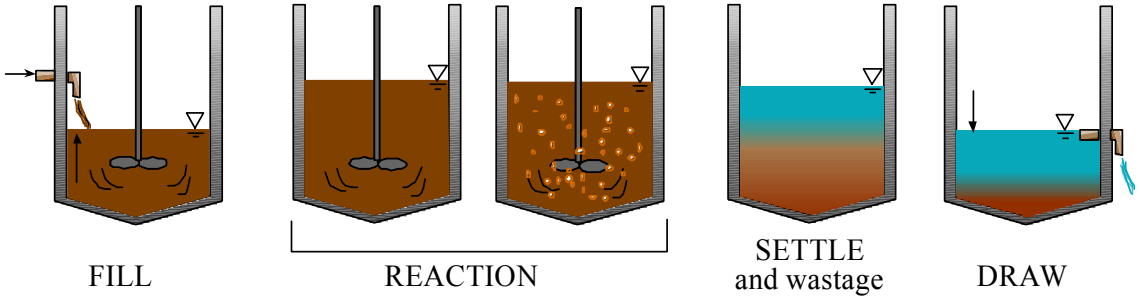


Figure 1-3. Sequence of phases in the SBR operation.

Fill: The wastewater to be treated is introduced into the reactor. Filling can be conducted under mixing or quiescent conditions and with aerobic, anoxic or anaerobic conditions, depending on the aim of the process.

Reaction: During the reaction period, the suspended biomass consumes the substrate under controlled environmental conditions. Aerobic and anoxic periods can be combined within this reaction phase.

Settle and wastage: Mixing and aeration are stopped to allow the sludge to decant and hence obtain a clarified effluent. The efficiency is normally higher than in continuous treatments because the mixed liquor is under quiescent conditions. The excess of sludge can be wastaged in this phase.

Draw: The clarified and treated water is drawn from the reactor, and then the system is ready to start a new cycle.

In some cases an idle phase is considered between executing cycles in which maintenance or other operations can be conducted.

The SBR technology was first used in 1914 (Ardern and Locket, 1914). During the 20th century this technology has gained popularity mainly due to its operating advantages and flexibility. In

addition, the automation of SBR operations has made their implementation much easier and has definitely contributed to the development of this technology.

The SBR technology has proved to be an effective system and a viable alternative to continuous flow systems for carbon and nutrient removal from domestic and industrial wastewaters. In Mace and Mata (2002) a complete review of experiences using SBR with different kinds of wastewater is presented. Finally, when dealing with treating wastewater from small communities, SBR has proved to be an effective system in terms of performance (Torrijos and Moletta, 1997; Torrijos *et al.*, 2001; Battistioni *et al.*, 2003; Lee *et al.*, 2004) and even in terms of treatment costs (Nowak and Lindtner, 2003).

As a final remark about the SBR process description the advantages and disadvantages of using this technology are listed below.

ADVANTAGES OF THE SBR TECHNOLOGY

The SBR has advantages regarding the variability of the treated wastewater, the control and operation, the design and even the microbiology of the process.

Influent treatability:

- The SBR system provides the flexibility needed to treat different kinds of wastewater in terms of load and composition (Mace and Mata, 2002).

Operation and control:

- The SBR is also a flexible system in terms of operation and control. There is no need for sludge recirculation and settling occurs during complete quiescent conditions. Moreover, the SBR operation can be easily adjusted for different treatment requirements by changing the time phase scheduling. Hence, different strategies for filling can be easily applied and different combinations of operating conditions depending on the finality of the process.

- Implementing a Data Acquisition and Control (DAC) system permits the SBR to work automatically by repeating the defined cycles and getting data about the process from the on-line probes and/or on-line analyzers. Since the batch reactor is always in a transient state the dynamics give valuable information about the state of the process. More information is obtained in this way than from continuous flow systems under almost stationary conditions (Olsson and Newell, 1999).

Design:

- The SBR process converts the conventional wastewater treatment processes from space-course to time-course, which substantially reduces the space occupation. Less space is required as all operations occur in one basin (Metcalf & Eddy, 2003). This feature makes the SBR especially suitable for small community wastewater treatment (EPA, 1999).
- Lower investment and recurrent cost is necessary because secondary settling tanks and sludge return systems are not required (Nowak and Lindtner, 2003; EPA, 1999).

Microbiology:

- It has been hypothesized that the SBR configuration would provide a strong substrate gradient that would favor the floc-forming bacteria and thus minimize bulking in accordance with the kinetic selection theory (Liao *et al.*, 2004).
- Alternating high and low substrate concentrations induce the selection of robust bacteria (Wilderer *et al.*, 2001).

DISADVANTAGES

The disadvantages are mainly related to the hydraulic limitation of the process and to the need for more sophisticated equipment.

- The hydraulic limitation of the batch processes makes it necessary to build two or more reactors working in parallel, and/or a pre-equalization tank for process operation (EPA, 1999).
- More sophisticated equipment is necessary for operation and automation (Olsson and Newell, 1999), which also implies a higher level of maintenance associated with these sophisticated controls, automated switches and automated valves.

1.3.2. Operating parameters

The operation of the SBR can be set up by defining key parameters related to the timing of the SBR operations (e.g. cycle definition) and to the volumes introduced and extracted from the reactor during the operation.

These operating parameters are presented in Table 1-1 with the symbol used, the equation and the description.

Table 1-1. Operating parameters.

Parameter	Units	Equation	Description
The total cycle time	hours	$t_C=t_R+t_S+t_D$	Sum of the length of all the phases t_R: reaction time (min) t_S: settling time (min) t_D: draw time (min)
Reaction time	hours	$t_R=t_{AE}+t_{AX}+t_F$	Sum of aerobic (t_{AE}), anoxic time (t_{AX}) and filling time (t_F)
Effective fraction	-	$f_E=t_R/t_C$	Fraction of the reaction time with respect to the total cycle time.
Number of cycles per day	cycles·d^{-1}	$N_C=24/t_C$	Determined from the total cycle time (t_C)
Maximum volume	L	$V_T=V_{MIN}+V_F$	V_{MIN}: minimum volume V_F: filled volume every cycle
Volumetric exchange ratio	-	$R_E=\frac{V_F}{V_T}$	Ratio between the fill volume and the maximum reactor volume
Influent flow	L·d^{-1}	$Q_I=V_F \cdot N_C$	Liters of water treated per day
Hydraulic Retention Time	d	$HRT=\frac{V_T}{Q_I}=\frac{1}{R_E \cdot N_C}$	Residence time of a liquid particle
Solids Retention Time	d	$SRT=\frac{V_T \cdot X}{V_W \cdot N_c \cdot X_W + V_E \cdot N_c \cdot X_E}$	Residence time of a sludge particle X: MLSS concentration at V_T V_W: volume of MLSS wastaged X_W: MLSS concentration in the wastage $V_E=V_F-V_W$: volume of water drawn X_E: MLSS concentration in the effluent (volumes are from one cycle, in L) (concentrations in mg·L^{-1})

The SBR operates cyclically repeating cycles composed of the previously defined phases (see Figure 1-3) and performing a number of cycles per day (N_C). The total length of the cycle is t_C. Part of the t_C is spent on the reaction (t_R) and the rest is used for the settle (t_S) and draw (t_D) phases. An effective fraction (f_E) can be defined as the fraction between the reaction time and the total time. Care should be taken since in some cases during settling the ongoing reactions cannot be neglected. The reaction time is divided into the aerobic time (t_{AE}), the anoxic time (t_{AX}) and the filling time (t_F) which can be conducted under either aerobic or anoxic conditions but must be considered separately regarding its importance. The volume in the SBR is variable and the total working volume (V_T) can be divided into the minimum volume (V_{MIN}) and the volume added and discharged every cycle (V_F). The fraction between V_F and V_T is defined as the volumetric exchange ratio (R_E). Two critical parameters for activated sludge design are the

Hydraulic Retention Time (HRT), the time spent by a molecule of water in the system, and the Solids Retention Time (SRT), the average period of time during which the sludge has remained in the system (Metcalf & Eddy, 2003). An effective HRT or SRT can be obtained when considering the effective fraction.

1.3.3. Cycle definition for carbon and nitrogen removal

The SBR operates by repeating a defined cycle which is composed of the 4 main operations described in Figure 1-3. The configuration of the filling and reaction phases is determined by the objective of the treatment (in this case, organic matter and nitrogen removal) and different combinations are possible. The settle and draw phases are always the last ones in the cycle structure.

Different reaction configurations are possible to remove carbon and nitrogen from the wastewater. As explained before, alternating aerobic and anoxic phases is necessary to perform nitrification and denitrification. Thus, the most common cycle structure is based on first an anoxic phase and then an aerobic phase, finishing with the settling and draw phases. At the beginning of the anoxic phase the influent is fed into the reactor and the readily biodegradable substrate is used to denitrify the nitrate remaining from the last cycle (Keller *et al.*, 1997; Johansen *et al.*, 1997).

In order to improve the SBR performance variations in this basic structure have been applied. One way of doing this is by applying multiple combinations of alternating aerobic and anoxic phases (Demuynck *et al.*, 1994; Demouling *et al.*, 1997; Artan *et al.*, 2002).

In addition, the filling strategy can also improve the performance. The filling can be conducted at the beginning of the cycle, during the whole cycle, and also split into different events distributed along the cycle. The COD/N ratio of the influent determines the best influent strategy to apply. When the COD/N ratio is high (more than 7) it is better to fill during the whole cycle, in spite of wasting part of the denitrification potential (Artan *et al.*, 2002). For low COD/N ratios (below 7) the step-feed strategy can be applied, alternating anoxic and aerobic phases and filling at the beginning of each anoxic phase (Figure 1-4). This strategy permits high nitrogen removal efficiency to be obtained with low nitrate levels during the discharge phase (Tilche *et al.* 1999; Hvala *et al.*, 2001; Lin and Jing, 2001; Puig *et al.*, 2004).

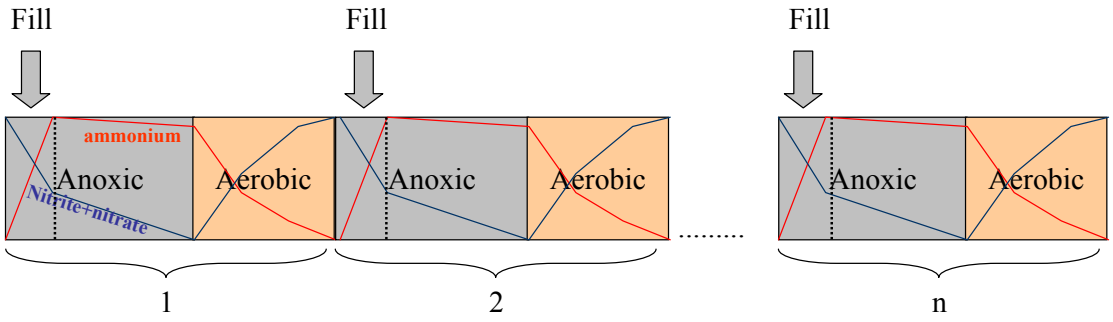


Figure 1-4. Step-feed strategy.

In the step feed strategy, the number of filling events depends on the influent nitrogen concentration and the desired effluent nitrogen concentration for a fixed R_E. The complex procedure for defining a cycle structure can be simplified to Equation 1-1 (Vives, 2004). This equation has been obtained assuming that all the filling events have the same volume, complete nitrification in aerobic phases and complete nitrification in anoxic phases.

$$N_{EF} = N_{IN} \cdot \frac{V_F}{V_T} \cdot \frac{1}{M} \qquad \text{Equation 1-1}$$

where: N_{EF}: total nitrogen concentration in the effluent (mg/L)
N_{IN}: total nitrogen concentration in the influent (mg/L)
V_F/V_T: volumetric exchange ratio
M: number of filling events applied during a cycle.

More specific studies on the cycle definition have been conducted. For instance in Coelho *et al.* (2000) the effect of filling on the process performance depending on different filling rates was studied. Hvala *et al.* (2001), Artan *et al.* (2002) and Sin *et al.* (2004) evaluated the filling distribution and different cycle configurations in order to determine the best performance with a combination of experimental and model-based approaches.

Thus, by taking advantage of the SBR's flexibility different strategies can be applied depending on the influent COD/N ratio. Correctly defining the operating strategy can overcome the problem of lack of readily biodegradable substrate for denitrification, leaving the use of external carbon source (Bernardes and Klapwijk, 1996) or the use of an intracellular electron donor as last options, both of which increase the treatment costs.

1.3.4. Controlling SBR operation

1.3.4.1. The benefits of control

Instrumentation, Control and Automation (ICA) has increased the capacity of Wastewater Treatment Plants (WWTP) that remove organic matter and biological nutrients by 10-30% (Olsson, 2005). The increasing knowledge of the processes involved in nutrient removal together with the improvements in the developed technologies (sensors, actuators, computer power…) permits better control over the process. Different potential benefits of using dynamic control presented in Vanrolleghem (2003) are summarized in Table 1-2.

Table 1-2. Benefits of control.

Benefit	Description
Performance	Maintaining plant efficiency closer to its maximum
Productivity	Increasing the amount of waste that can be treated per unit process capacity
Reliability	Decreasing the frequency of gross process failures
Stability	While appearing to be highly stable processes, occasional upsets may have important consequences that could be avoided by increased process control
Personnel	Running plants with less skilled personnel or decreasing time devoted to plant management
Operation	Reducing chemical and energy consumption
Start-up	The procedure for starting-up new treatment plants can be shortened
Variable Efficiency	Integrating the dynamics of the receiving waters within the control of the treatment plant so as to match the assimilative capacity of the receiving waters
Dynamic operation	Improving performance by taking advantage of process dynamics

Ways of controlling the activated sludge process have been widely presented with different examples and applications in the ICA conferences. Nevertheless, there is more to do in this subject. The main objective pointed out in the 2005 ICA conference as the new challenge for the coming years is the development of systems that are able to work autonomously and that combine most of the benefits presented above. Another important point is implementing the control strategies in real plants, which is slowly being achieved, and finally the plant wide control with the integrated plant operation in real-time.

The control of the activated sludge process can be conducted by regulating key process parameters such as the concentration of electron donors and electron acceptors. The controlled shifting of aerobic and anoxic conditions permits the process to be optimized.

1.3.4.2. Levels of control in SBR operation

SBR technology requires a high degree of automation. In order to take advantage of this particularity, control strategies can easily be implemented in the system. These strategies can be used to control the nitrification and denitrification processes, to optimize the functioning of the SBR and even to increase the reliability and stability of the process.

An adaptation of the hierarchical control described in Olsson and Newell (1999) is presented in Figure 1-5 for the SBR. Different levels of control can be defined for the SBR technology: a low level contributes to improving the performance in the SBR operation. A medium level is in charge of increasing the productivity, optimizing the operation and decreasing the necessary personnel. Finally, a high level is responsible for providing stability and reliability to the process.

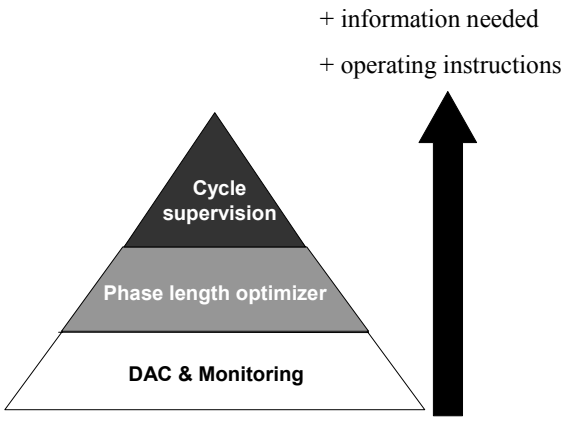


Figure 1-5. Levels of control applied to the SBR operation.

In Figure 1-5 these levels are presented as a pyramid considering that at the top more information and more operating instructions are needed.

a) LOW LEVEL CONTROL

Having a defined cycle with fixed phases length a first level of control can be established to maintain environmental or operating parameters at a desired level, for instance by 1) using a Dissolved Oxygen (DO) set-point to control the nitrification process, 2) using a low DO set-point for simultaneous nitrification-denitrification, 3) adjusting the SRT of the system by controlling the wastage, 4) adding an external carbon source to the anoxic phase to improve denitrification and 5) applying different filling strategies to maintain the electron donors and acceptors at desired concentrations.

1) Control of the DO

Conventional: The DO control in aeration phases is of primary importance in the activated sludge process. It has been practiced for many years in order to maintain the aerobic depletion of organic matter, nitrogen and other substances, without supplying an excess of oxygen. The

complexity can increase from the On/Off to the continuous controllers such as PID or Fuzzy. Different examples controlling the DO in the reactor can be found in Olsson and Newell (1999).

Advanced: Instead of using a fixed DO set-point, the DO set-point can be manipulated in order to control the ammonium concentration. Different experiences can be found in Nielsen and Lyngaard-Jensen (1993), Lindberg and Carlsson (1996), Olsson and Newell (1999), Suescun *et al.* (2001), Serralta *et al.* (2002), and Ingildsen *et al.* (2002), among others, all of which are applied to continuous flow systems.

2) Simultaneous nitrification and denitrification

The simultaneous nitrification and denitrification during aerobic phases can be achieved by applying low dissolved oxygen levels in the reactor. This phenomenon has been studied in Munch *et al.* (1996) and Artan *et al.* (2002), and it is suitable when nitrification is not limiting. Extra denitrification conducted during the aerobic phase can help in the overall denitrification capacity.

3) SRT control

SRT is an operating parameter that permits controlling the establishment of determined microbe communities. The SRT determines a maximum time for the microbes to be in the system, and therefore the species which grow slower are washed out from the system. Since the autotrophic bacteria have a lower growth rate than the heterotrophic a minimum SRT is necessary to ensure nitrification. The SRT can be calculated and controlled manually or automatically. The last option is possible when a suspended solids analyzer and flow rate meters are available and then it can be easily adjusted to a desired value by manipulating the wastage flow rate. An example is presented in Wiese *et al.*, (2005).

4) Adding an external carbon source

The denitrification process can be limited by the available organic matter. Adding an external carbon source can be used to control the denitrification process (Bernardes and Klapwijk, 1996; Cheng and Liu, 2001).

5) Fill strategy

As explained in point 1.3.3, different filling strategies can be applied within the SBR operation. The COD/N ratio determines the suitable strategy to follow, and different possibilities permit the denitrification capacity to be improved.

b) MEDIUM LEVEL CONTROL

The common practice used in SBRs is based on executing a predefined cycle over time. However, it is possible to take more advantage of the flexibility of the SBR technology by finding the correct duration of aerobic and anoxic phases to achieve complete nitrification and

suitable denitrification respectively. This medium level of control permits the functioning of the system to be adapted to the influent composition and flow variability, optimizing the performance (saving energy and increasing the capacity of the plant) without affecting the effluent quality.

6) Adjusting the aerobic and anoxic phase lengths

If the system can detect the end of the nitrification process it makes no sense to continue with the oxygen supply and thus the aerobic phase can be finished changing to the next phase. A similar reasoning can be applied to the anoxic phases changing to the next phase when the end of denitrification is detected. The methodology to detect the end of the nitrification and denitrification processes determines two different control strategies:

i) Using direct measurements

This is based on using ammonium and oxidized nitrogen on-line analyzers that measure the concentrations at a reasonable time interval. This output measurement permits a feed-back control to be established, which can be as simple as continuing aerating or stopping aerating. With these on-line analyzers the efficiency of the plant can be maintained at a desired level.

Several applications of the aerobic phase length adjustment for intermittently aerated systems can be found in the literature (Sorensen *et al.*, 1994; Oennerth *et al.*, 1996; Potter *et al.*, 1996). An example regarding SBR technology can be found in Wiese *et al.* (2005).

ii) Using indirect measurements

This control is based on the on-line measurements from the sensors or variables calculated from them, obtained at very short time intervals (order of seconds). Nevertheless, there is less flexibility in the control and the definition of the desired level of efficiency.

Abstracting knowledge from simple on-line probes (DO, pH and Oxidation-Reduction-Potential-ORP) can be used as an indicator of the SBR cycle phase status. The degree of nitrogen depletion can be characterized by observing endpoints in the probes' signal profiles. Figure 1-6 shows the nitrogen removal endpoints that can be observed during a cycle.

There are many endpoints of the nitrification process in the aerobic phase:

> α_{O2} point (Figure 1-6-A): An inflexion point in the DO profile with time, at the end of ammonia nitrification. When the ammonia is consumed the oxygen demand decreases what causes an increase in the DO concentration inside the reactor (Plisson-Saune *et al.*, 1996; Battistoni *et al.*, 2003).

> Residual Carbon Manipulation Point (RCMP point) (Figure 1-6-B): An inflexion point in the ORP profile (Yu *et al.*, 1997; Ra *et al.*, 1998).

> **Ammonia Valley** (Figure 1-6-C): The Ammonia Valley appears as a consequence of the equilibrium between proton production during the nitrification process (decreases pH) and stripping of CO_2 (increases pH). Before the end of nitrification the pH decreases because proton production in the nitrification process is higher than the stripping effect, but once nitrification is finished no more protons are produced and the stripping effect is considerably large, representing an increase in the pH (Al-Ghusain and Hao, 1995).

> α_{OUR} or Average Viability (Figure 1-6-D): Sharp decrease in the OUR profile related to the diminution in the microbial activity once the substrate (ammonium) is finished (Watts and Garber, 1995).

In the anoxic phase, two endpoints can indicate the end of denitrification:

> **Nitrate Knee** (Figure 1-6-E): This is an inflexion point in the ORP profile, which is related to the change of the electron acceptor from nitrate to sulfates or other components (Al-Ghusain and Hao, 1995; Plisson-Saune *et al.,* 1996).

> **Nitrate Apex** (Figure 1-6-F): A maximum in the pH caused by the equilibrium between the OH^- production during denitrification and the alkalinity of the system (Al-Ghusain and Hao, 1995).

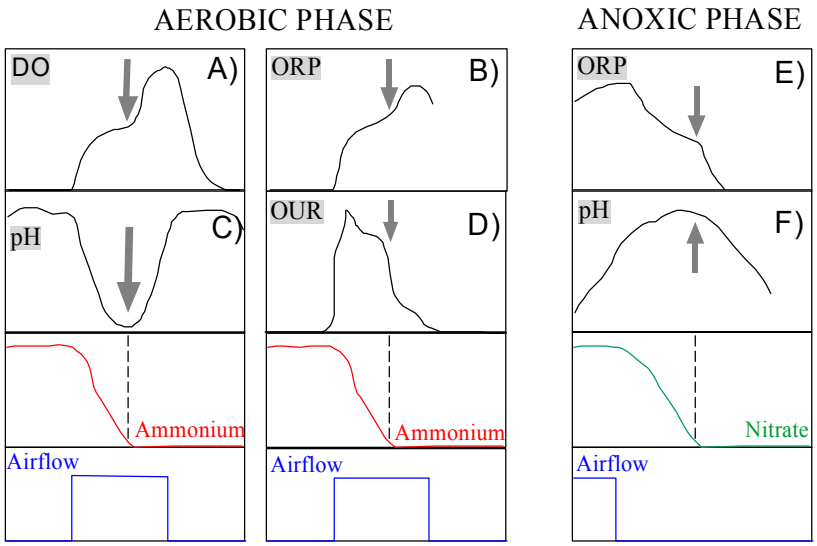


Figure 1-6. Patterns in the DO, ORP, pH and OUR profiles during aerobic and anoxic phases.

Based on these patterns open loop control can be applied to adjust the length of aerobic and anoxic phases when the endpoints are detected.

Different literature references applied to SBR technology can be found in this subject using different measured variable signals (Chang and Hao, 1996; Yu *et al.*, 1997; Cho *et al.*, 2001; Kishida *et al.*, 2003). A complete review can be found in Puig (2004). Moreover, two patented systems have been developed in this subject: INFLEX© (Mauret *et al.*, 2001) based on ORP and DO profiles and OGAR© (Klapwijk *et al.*, 1998) based on ORP profiles.

HIGH LEVEL CONTROL

A higher level of control is necessary when the system faces abnormal situations (e.g. significant changes of wastewater quality or quantity, environmental shifts, equipment faults…). This control level is related to the supervisory control defined in Olsson and Newell (1999), and is based on analyzing and diagnosing the process performance in order to take decisions. Hence, a supervisory control system can increase the reliability and stability of the system.

7) Supervisory control

One step forward in the optimal management of activated sludge systems involves supervision at a higher level to monitor, evaluate and diagnose these systems, actuate the system, and finally detect problems faster and provide problem solving procedures (Comas, 2000).

For this supervision it is necessary to use expert knowledge combined with artificial intelligence tools such as expert systems (Comas, 2001), case-based reasoning systems (R-Roda *et al.*, 2001; Wiese *et al.*, 2004), Fuzzy logic (Lardon *et al.*, 2004) and also multivariable statistics (Rosen and Yuan, 2001; Rosen and Lennox, 2001). In terms of SBR performance the supervisory control can be in charge of defining all the operating conditions and manage the whole cycle structure.

Table 1-3 summarizes all the strategies presented above for the low, medium and high levels of control. This table also includes the benefits of each type of control.

Table 1-3. Summary of the control strategies for SBR operation.

<table>
<tr><th>Level of control</th><th colspan="2">Strategy</th><th>Benefits</th></tr>
<tr><td rowspan="6">a) Low</td><td rowspan="2">1) DO set-point</td><td>Conventional</td><td rowspan="6">Performance</td></tr>
<tr><td>Advanced</td></tr>
<tr><td colspan="2">2) Simultaneous nitrification-denitrification</td></tr>
<tr><td colspan="2">3) SRT</td></tr>
<tr><td colspan="2">4) External carbon source addition</td></tr>
<tr><td colspan="2">5) Fill strategy</td></tr>
<tr><td rowspan="2">b) Medium</td><td rowspan="2">6) Aerobic and anoxic phase length adjustment</td><td>Direct</td><td rowspan="2">Productivity
Operation
Personnel</td></tr>
<tr><td>Indirect</td></tr>
<tr><td>c) High</td><td colspan="2">7) Automatic configuration of the cycle operating conditions (supervisory control)</td><td>Reliability
Stability</td></tr>
</table>

1.4. MODELING AND CALIBRATION OF THE ACTIVATED SLUDGE PROCESS

1.4.1 Activated sludge models

A model is a description of the processes occurring in a system, and is used to understand and predict certain aspects of reality (Meijer, 2004). In this case the complexity of the activated sludge process for organic matter and nutrients is simplified and transferred into i) differential equations obtained through the mass balances (white box models-deterministic models), or ii) relationships between inputs and outputs without reflecting physical, biological or chemical process knowledge (black box models). The combination of the two previously mentioned models leads to the grey-box models.

Deterministic models are most commonly used to describe the activated sludge process. To describe the overall functioning of a WWTP different sub-models are considered: the biological conversions, the mass transport and hydraulic behavior and the settling of the sludge.

Regarding the biological models, the international Association on Water Pollution Research and Control (since 2000 the International Water Association, IWA) introduced the first Activated Sludge Model for biological carbon and nitrogen removal (ASM1) in 1987. Further extensions and improvements of the ASM1 have been developed in the research community, although this model is still being used. The ASM2 was developed to include enhanced phosphorous removal, and then the ASM2d was developed, build on the basis of ASM2 adding the denitrifying activity of phosphorus accumulating organisms (PAOs). Then, the ASM3 appeared to overcome some limitations of ASM1. Two important differences can be noted in ASM3 compared to ASM1: 1) it recognizes the importance of storage polymers in the heterotrophic activated sludge conversions, and 2) the death and regeneration concept has changed to the endogenous respiration concept, which ensures better parameter identifiability (Gernaey *et al.*, 2004). More information about these models can be found in Henze *et al.* (2000).

Other models have appeared that also describe the nitrification, denitrification and Bio-P processes (see Table 1-4). The complexity of the model can be associated with the number of state variables and the reactions considered. For instance, when describing not only the nitrification and denitrification processes but also the biological phosphorus (bio-P) removal process the number of reactions is more or less doubled. This is also related to an increase in the number of parameters which leads to a more complex model calibration.

Recently, the calculation of the pH has been included in the model. This calculation can be based on mass balances (Serralta *et al.*, 2004) or on charge balances (Magrí *et al.*, 2005).

Table 1-4. Overview of the activated sludge models (adapted from Gernaey *et al.* (2004).

Models	Nitrification+ denitrification	Bio-P	State variables	Processes	Reference
ASM1	X		13	8	Henze *et al.* (1987)
ASM2	X	X	19	19	Henze *et al.* (1995)
ASM2d	X	X	19	21	Henze *et al.* (1999)
ASM3	X		13	12	Gujer *et al.* (1999)
ASM3+BioP	X	X	17	23	Rieger *et al.* (2001)
B&D	X	X	19	36	Barker and Dold (1997)
TUDP	X	X	17	21	Brdjanovic *et al.* (2000)
ASM2d+pH	X	X	23	23	Serralta *et al.* (2004)
ASM1+pH	X		16	10	Magrí *et al.* (2005)

Although different models of the activated sludge process for carbon and nitrogen removal have been developed in recent years, the ASM1 has been widely accepted and applied by the scientific community, e.g. in the continuous flow reactor (Carucci *et al.*, 1999; Petersen *et al.*, 2002; Moussa *et al.*, 2004) and also in the case of SBR technology (Oles and Wilderer, 1991; Andreottola *et al.*, 1997; Novák *et al.*, 1997; Melcer *et al.*, 2003). ASM3 is still under study and its application is not widespread.

1.4.2. ASM1

1.4.2.1 State variables in ASM1

COD is selected as the most suitable parameter for defining the carbon substrates as it provides a link between electron equivalents in the organic substrate, the biomass and oxygen used. In ASM1 the components are divided based on solubility, biodegradability, biodegradation rate and viability (biomass). The organic matter and nitrogen components are presented in Figure 1-7 and Figure 1-8. The components of ASM1 are listed below.

Definition of organic components:

S_S: Readily biodegradable substrate. This is relatively small molecules which can be used for growth directly.

S_I: Inert soluble organic material. This is biologically inert (cannot be further degraded in the treatment plants) and passes through the activated sludge system in an unchanged form. This material is assumed to be part of the influent and it is also assumed to be produced in the context of hydrolysis of particulate substrates X_S.

X_S: Slowly biodegradable substrate: The slowly biodegradable substrate (X_S) is considered to be more complex material (e.g. larger molecules), which requires extra cellular breakdown prior to uptake and utilization

X_{BA}: Nitrifying organisms. They are responsible for nitrification; they are obligate aerobic, chemo-litho-autotrophic. It is assumed that nitrifiers oxidize ammonium S_{NH} directly to nitrate S_{NO}.

X_{BH}: Heterotrophic organisms. They are generated by growth on the readily biodegradable susbtrate, and can grow aerobically and anoxically.

X_I: Inert particulate organic material. This material is not degraded. It is flocculated onto the activated sludge. X_I may be a fraction of the influent.

X_P: Organic particulate products arising from the biomass decay. This material is not degraded. It is flocculated onto the activated sludge. X_P may be produced in the context of biomass decay.

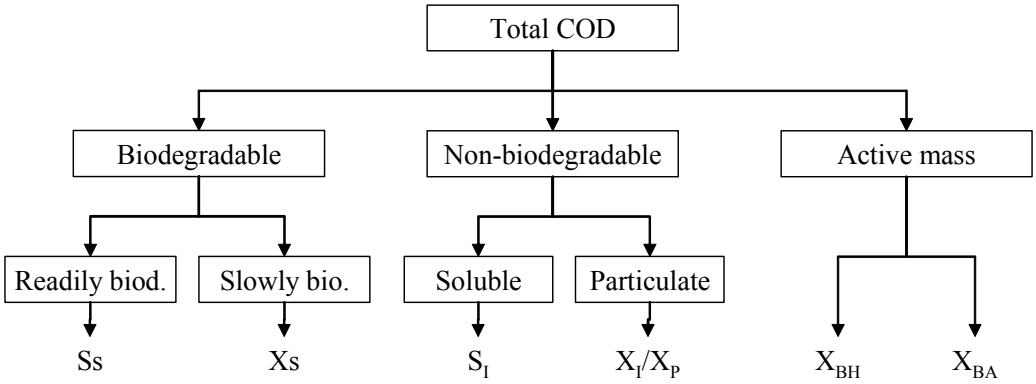


Figure 1-7. Organic matter components.

Definition of nitrogen components:

X_{ND}: Particulate biodegradable organic nitrogen. This is generated from decay of both heterotrophic and autotrophic biomass, and is lost by ammonification.

S_{ND}: Soluble organic nitrogen. This is formed by hydrolysis of particulate organic nitrogen and converted to ammonia nitrogen by ammonification.

S_{NH}: Ammonium plus ammonia nitrogen. For the balance of the electrical charges, S_{NH} is assumed to be NH_4^+.

S_{NO}: Nitrate plus nitrite nitrogen (NO_3^-+NO_2^-). S_{NO} is assumed to include nitrate as well as nitrite nitrogen, since nitrite is not included as a separate model component. For all stoichiometric computations (COD conservation), S_{NO} is considered to be NO_3^- only.

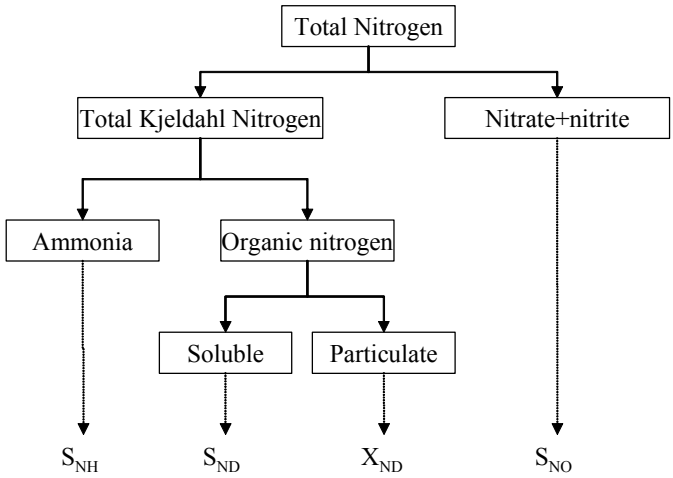


Figure 1-8. Nitrogen components.

Definition of other components:

S_O: Dissolved oxygen. Dissolved oxygen may be subject to gas exchange.

S_{ALK}: Alkalinity of the wastewater. This is used to approximate the continuity of electrical charges in biological reactions. Alkalinity is introduced in order to obtain an early indication of possible low pH conditions, which might inhibit some biological processes. For all stoichiometric computations, S_{ALK} is assumed to be bicarbonate, HCO_3^- only.

1.4.2.2. Processes in ASM1

Basically there are four different main processes defined in ASM1: growth of biomass, decay of biomass, ammonification of organic nitrogen and hydrolysis. These are subdivided into a total of 8 processes. The relationship between the state variables and the processes is presented in Figure 1-9.

As presented in Figure 1-9 two groups of microorganisms are considered in ASM1: heterotrophic (X_{BH}) and autotrophic organisms (X_{BA}). Heterotrophic organisms can grow under aerobic (1) or anoxic conditions (2), using S_S as substrate, which can either come with the wastewater or originate from the hydrolysis (7) of slowly biodegradable substrate (X_S). Autotrophic organisms only grow under aerobic conditions (3) consuming the ammonium (S_{NH}) coming from the influent wastewater or originating from the consecutive processes of hydrolysis of organic nitrogen (8) and ammonification (6).

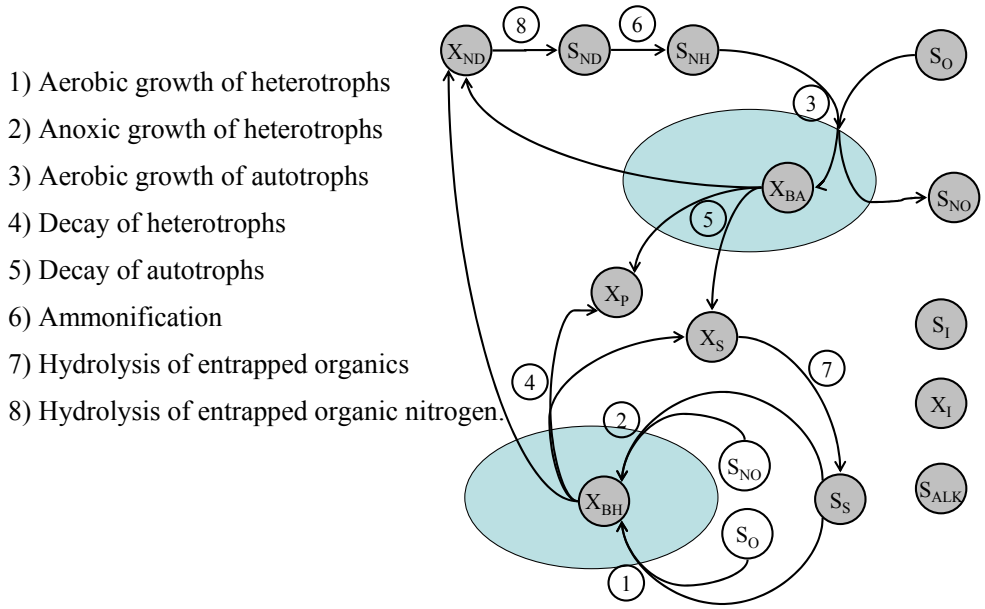


Figure 1-9. ASM1 state variables and process relationships.

These organisms die (4 and 5) generating X_P, X_S and X_{ND}. The X_P are organic particulate products which don't react further and are eliminated from the system with the wastage. The other two (X_S and X_{ND}) are again available for further reactions according to the concept of death and regeneration.

The variables S_I, X_I are inert and thus they are not involved in any conversion processes. Their origin is the influent wastewater and they are considered since they are important to the performance of the process (they are considered in the total COD balance). The variable S_{ALK} is considered in all the reactions involving adding or removing species with a proton accepting capacity, and/or adding or removing protons that cause changes in alkalinity.

The biological models are normally presented in the matrix notation for chemical reactions as used by Petersen (1965). Table 1-5 shows the ASM1 Petersen matrix, with the state variables in columns and the processes in rows. The process rates are located in the last column, and the generation term can be calculated following the conversion tax expression presented in the last row.

Table 1-5. Matrix representation of the ASM1 model (Henze *et al.*, 1987).

Component V_{ij} i / j Process	S_I	S_s	X_I	X_s	X_{BH}	X_{BA}	X_p	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	Process rate, ρ_j
1.Aerobic heterotrophic growth		$-\frac{1}{Y_H}$			1			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{xB}}{14}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}\right)X_{BH}$
2.Anoxic heterotrophic growth		$-\frac{1}{Y_H}$							$\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14*2.86Y_H}-\frac{i_{XB}}{14}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{BH}$
3.Aerobic autotrophic growth						1		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\mu_{mA}\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\frac{S_O}{K_{OA}+S_O}\right)X_{BA}$
4.Heterotrophic death				$1-f_p$	-1		f_p					$i_{XB}-f_p.i_{XP}$		$b_H X_{BH}$
5.Autotrophic death				$1-f_p$		-1	f_p					$i_{XB}-f_p.i_{XP}$		$b_A X_{BA}$
6.Ammonification										1	-1		$\frac{i_{XB}}{14}$	$k_a S_{ND} X_{BH}$
7.Hydrolisis of organics		1		-1										$k_H\frac{X_S/X_{BH}}{K_X+X_s/X_{BH}}\left(\frac{S_O}{K_{OH}+S_O}+\eta_h\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\right)X_{BH}$
8.Hydrolisis of organic nitrogen											1	-1		$P_7(X_{ND}/X_s)$
Conversion tax	$r_j=\sum_j v_{ij}\rho_j$													

Stoichiometric parameters:

Heterotrophic yield: Y_H

Autotrophic yield: Y_A

Fraction of biomass yielding particulate products: f_P

Mass N/Mass COD in biomass: i_{XB}

Mass N/Mass COD: i_{XP}

Kinetic parameters:

Heterotrophic grwoth and decay: μ_{mH}, K_S, K_{OH}, K_{NO}, b_H

Autotrophic growth and decay: μ_{mA}, K_{NH}, K_{OA}, b_A

Correction factor for anoxic growth of heterotrophs: η_g

Ammonification: k_A

Hydrolysis: k_H, K_X

Correction factor for anoxic hydrolysis: η_H

1.4.3. Calibration of ASM1

Model calibration is understood as the estimation of the model parameters to fit a certain set of data obtained from the WWTP under study (Gernaey *et al.* 2004). The purpose of the modeling task determines the effort needed for the calibration. For instance, for activated sludge models to be used for educational purposes or for simulating non-existing plants, no calibration is necessary and the default parameter values presented in Henze *et al.* (2000) can be used. However, when the model is to be used in the field of optimization, control and process performance evaluation, an accurate calibration is necessary to properly describe the behavior of the state variables.

Important steps in the activated sludge model calibration are the data collection, the characterization of the influent wastewater and the kinetic/stoichiometric parameter estimation. The determination of the model parameters can be achieved by applying mass balances or conducting lab-scale experiments. However, some of them have to be adjusted during the calibration procedure, normally using a trial and error method. Within the calibration procedure, first a steady state calibration is conducted in which the parameters responsible for long-term behavior are determined, which serves to establish the initial conditions prior to the dynamic model calibration. In order to describe dynamic situations a dynamic model calibration is then conducted using data obtained from an intensive monitoring campaign. The parameters responsible for short-term behavior are determined in this step.

With the purpose of standardizing the calibration procedure, different calibration protocols have been presented and accepted by the scientific community. They are the BIOMATH protocol (Vanrolleghem *et al.*, 2003), the STOWA protocol (Hulsbeek *et al.*, 2002), the Hochschulgruppe (HSG) guidelines (Langergraber *et al.*, 2004) and the WERF protocol (Melcer *et al.*, 2003). They are presented and compared in Chapter 4 of this thesis.

Two of the key points for calibration are characterizing the state variables of the influent wastewater and estimating the kinetic and stoichiometric parameters. They are both considered in more or less detail in the above-mentioned calibration protocols.

1.4.3.1. Characterization of influent state variables

An important part of the model calibration is the characterization of influent state variables. Different analytical measurements (COD, BOD, TN…) from the influent wastewater can be performed, but these data are converted into the state variables of the ASM1 to be introduced in the model.

The methods for characterizing the wastewater are not standardized. There is still no consensus on this subject, especially regarding the organic fractions. This characterization is directly related to the goal of the calibration and also to the calibration protocol itself. The wastewater characterization protocols can deal with physical-chemical and BOD analysis, and respirometry approaches. The main disagreement is in determining the readily biodegradable substrate, and the convenience of determining the X_I fraction performing COD mass balance (BOD tests are needed), or calibrating the fraction of X_I directly.

Different procedures have been proposed for the influent characterization (see Figure 1-10). Henze *et al.* (1987) used mass balances for the soluble COD and for the particulate COD and X_I was calibrated. The STOWA protocol introduced a long BOD test to estimate the biodegradable organic matter (X_S+S_S), and therefore no calibration of X_I is needed.

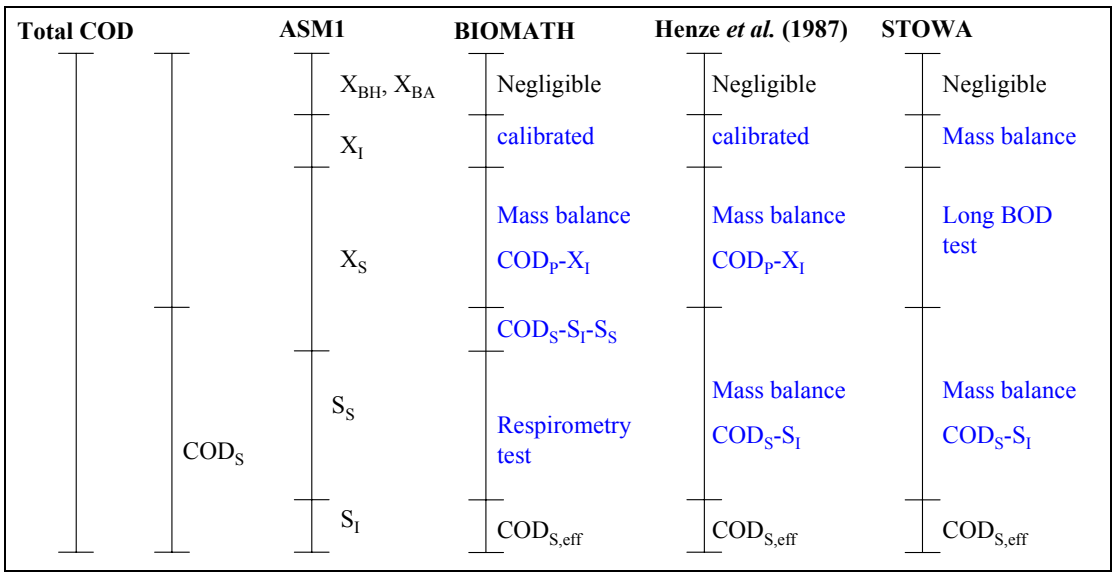


Figure 1-10. Different ASM1 based influent wastewater characterization approaches.

With the BIOMATH protocol a respirometric test was proposed to determine the S_S fraction directly and therefore take into account that there is a part of soluble COD which is slowly biodegradable. Figure 1-10 shows a comparison of the different protocols.

1.4.3.2. Kinetic and stoichiometric parameter estimation

Different approaches have been applied for the estimation of the kinetic and stoichiometric parameters of the activated sludge models. Mass balances have been used for this purpose, and using respirometry techniques is also gaining ground in this subject. Moreover, also other methods such as nitrate utilization rates, titrimetry and ammonium uptake rate are powerful to estimate some of the kinetic and stoichiometric parameters.

The results of mass balances can be used directly for the estimation of model parameters since ASM1 is based on balances for COD and nitrogen. By means of mass balances only the state of equilibrium can be described and therefore, only parameters responsible for long-term behavior can be estimated, i.e. the heterotrophic yield Y_H, the fraction of biomass yielding particulate organics f_P, the heterotrophic decay rate b_H and the concentration of particulate inert organics X_I in the influent (Nowak *et al.*, 1999).

The respiration rates of the microorganisms under non-limiting dissolved oxygen concentration is related to the kinetics and stoichiometry of the processes involved in the respiration. The conduction of respirometry assays under controlled conditions permits estimating (directly or indirectly) these parameters of the model. Different experiences for both long and short term behavior parameters can be found in Spanjers *et al.* (1999), Vanrolleghem *et al.* (1999) and Gutierrez (2003).

Other methodologies have to be applied for estimating parameters that do not involve oxygen consumption. For instance, the Nitrate Utilization Rates (NUR) or titrimetry can provide useful information for the determination of parameters related to the denitrification process.

1.4.3.3. Calibration experiences

A review of the calibration experiences dealing with ASM1 can help to face a new calibration work, especially for new practitioners. Table 1-6, Table 1-7 and Table 1-8 present this review for SBR applications and continuous systems. The purpose of the calibration is presented and divided into the processes which are described and the application of the model. Moreover, the source of characterization of the influent wastewater, the biomass and the kinetic and stoichiometric parameters are given. The model parameters presented in the table are those strictly specified in the papers and which have a clear origin. The parameters that are not mentioned may have a value obtained from the literature (e.g. default values of ASM1).

In the majority of cases the processes described in the model are COD removal combined with N removal. The models described are based on ASM1, and modifications on it are sometimes implemented, such as the description of two step nitrification (Andreottola *et al.*, 1997; Moussa *et al.*, 2004), modification of the ammonification process (Thayalakumaran *et al.*, 2003), conversion to the endogenous decay concept (Murat *et al.*, 2002), or inclusion of inhibiting terms (Andreottola *et al.*, 1997).

The influent wastewater has been conducted using the full-scale data combined with mass balances and lab-scale experiments. These experiments have been performed to determine for instance the combination of S_I and S_S (Carucci *et al.*, 1999; Thayalakumaran *et al.*, 2003;

Moussa *et al.*, 2004; Nuhoglu *et al.*, 2005), the inert fractions S_I and X_I (Lesouef *et al.*, 1992), S_S and X_{BH} (Xu and Hultman, 1996) or single parameters (S_S in Murat *et al.*, 2002; X_I in Siegrist and Tschui, 1992; S_S in Kristensen *et al.*, 1998). Furthermore, the X_I fraction is adjusted by trial and error during calibration in some examples.

The kinetic and stoichiometric parameters are normally determined by calibrating the model. Nevertheless, some studies also include lab-scale experiments. For instance the maximum growth rates are determined (Pedersen and Sinkjaer,1992; Stokes *et al.*,1993; Kristensen *et al.*, 1998; Carucci *et al.*, 1999; Murat *et al.*, 2002; Petersen *et al.*, 2002; Thayalakumaran *et al.*, 2003), the decay coefficients (Stokes *et al.*, 1993; Kristensen *et al.*, 1998; Murat *et al.*, 2002; Petersen *et al.*, 2002), and finally the heterotrophic yield (Murat *et al.*, 2002; Nuhoglu *et al.*, 2005). In general, when the calibrated model is applied with the purpose of optimizing or upgrading, more parameters are calibrated and estimated.

The kinetics and stoichiometry of the reactions are influenced by the origin of the wastewater. When non-domestic wastewater is treated the parameter values may differ from the default suggested in the ASM1, which makes it worth while to perform the lab-scale experiments (e.g. Murat *et al.*, 2002; Thayalakumaran *et al.*, 2003; Moussa *et al.*, 2004).

Table 1-6. Information sources for the calibration of ASM1 for SBR applications (adapted from Petersen *et al.*, 2003).

Reference	Purpose		Characterization						
			Influent Wastewater				*Biomass*	*Kinetic and stoichiometric*	
	Processes	Application	Full-scale data	State variables			Lab-scale analyses	Model calibration	Lab-scale experiments
				Lab-scale experiments	Mass balances	Calibration			
AN97	COD removal N removal (2 step nitrif + nitratation inhibition)	Lab-scale (5L). Optimization	Piggery WW. 1, 2, 3, 6, 7					μ_H, μ_A, Y_H, Y_A, B_H, K_X, k_A, η_g, η_a, f_p, i_{XB}, i_{XP}	
NO97	COD removal N removal	Full-scale 228m^3 Description	Domestic 3, 5			No information		No information	
ME03	COD removal nitrification	Lab-scale (10L) Description	Synthetic 1, 2, 3, 6, 7			X_I	N of VSS	μ_A	
TH03	COD rem. N rem. (Ammonification modif)	Lab-scale (15L). Description	Meat process WW 2, 3, 6, 7, 8, 9	S_I , Ss				μ_H, K_S, b_H, K_{OA}, b_A, k_A, Y_H, Y_A	μ_{mA} (Sözen et al, 1996)
MU02	COD removal N removal (End.decay)	Lab-scale (844L). Description	Tannery WW 1, 2, 3, 5, 6, 8	S_S	X_S, S_H	X_I, S_I	Inbm*, i_{NSI}*, i_{NXI}*,	k_H, K_X	μ_{Hmax}, b_H, K_S*, μ_{Amax}*, Y_H*,

AN97: Andreottola *et al.*, 1997
NO97: Novák *et al.*, 1997

ME03: Melcer *et al.*, 2003
TH03: Thayalakumaran *et al.*, 2003
MU02: Murat *et al.*, 2002

1 : SS
2: VSS
3 : COD tot – COD sol
4: COD floculated
5: BOD_5

6: TN and TKN
7: NH_4^+
8: NO_x^-
9: P

* values obtained in similar studies with the same wastewater

Table 1-7. Information sources for the calibration of ASM1 for continuous flow system applications (adapted from Petersen *et al.*, 2003). Continues in Table 1-8.

Reference	Purpose		Characterization						
			Influent Wastewater				*Biomass*	*Kinetic and stoichiometric*	
	Processes	Application	Full-scale data	State variables			Lab-scale analyses	Model calibration	Lab-scale experiments
				Lab-scale experiments	Mass balances	Calibration			
XU96	COD removal N removal (Modified ASM1)	Full-scale Description (1750m3)	Municipal WW 3, 4, 6, 7, 8	S_S, X_{BH},	S_I, S_S, X_S	X_I,	1	K_{OH}, K_{NH}, η_g	
ST92	COD rem Nitrification	Description	3,6,7,8	X_I	S_I				
L92	N-removal	Optimization	3,4,7,8	S_I, X_I	S_S, X_S, X_{BH}			Y_H, μ_H, K_S, k_H, K_X, b_H,μ_A, K_{NH}	
PS92	N-removal	Description	3,4,5,6,7,8		S_S, S_I, X_I		1,2,3,6	K_X, k_H	b_A,μ_A,
DS94	N-removal	Optimization	3,4,5,6,7,8					μ_A, K_S, η_g	
S93	COD rem Nitrification	Description	1,3,5,6,7					K_S, η_g	b_A,μ_A, K_{NH}, K_{OA}
dS94	All processes	Optimization	3,5,6,7,8,9			all	1,2,3	μ_H, μ_A, K_S	
K98	COD & N-removal	Description	1,2,3,4,6,7,8	S_S			1,2	k_H, K_X,b_H, K_{OH}, η_g	b_H, μ_H, μ_A, K_{OA}
C99	COD & N-removal	Optimization	3, 8	S_S, S_I	X_S	X_I	Not available		μ_H, μ_A, η_g

XU96: Xu and Hultman (1996)
ST92: Siegrist and Tshui (1992)
L92: Lesouef *et al.* (1992)
PS92: Pedersen and Sinkjaer (1992)
DS94: Dupont and Sinkjaer (1994)

S93: Stokes *et al.* (1993)
dS94: de la Sota *et al.* (1994)
K98: Kristensen *et al.* (1998)
C99: Carucci *et al.* (1999)

1 : SS
2: VSS
3 : COD tot – COD sol
4: COD floculated
5: BOD_5

6: TN and TKN
7: NH_4^+
8: NO_x^-
9: P

Table 1-8. Information sources for the calibration of ASM1 for continuous flow system applications (adapted from Petersen *et al.*, 2003). Continuing from Table 1-7.

Reference	Purpose		Characterization						
			Influent Wastewater				*Biomass*	*Kinetic and stoichiometric*	
	Processes	Application	Full-scale data	State variables			Lab-scale analyses	Model calibration	Lab-scale experiments
				Lab-scale experiments	Mass balances	Calibration			
PE02	COD removal N removal	Full-scale. Optimization (2400m3)	Municipal WW 1, 3, 6, 7	S_S	S_I, X_S	X_I	1,2,3,5	b_A, b_H, μ_H, μ_A, K_S, K_{OH}, η_g	b_H, μ_H,μ_A
MO04	COD removal N removal (Two step nitrification)	Full-scale. Upgrading (8000m3)	Tannery WW 1, 2, 3, 6, 7, 8, 9	S_I, S_S	X_S	X_I	Batch tests	K_{OA}, K_{OH}, b_{A1}, b_{A2},	Nitrification batch tests
NU05	COD removal Nitrification	Full-scale. Upgrading. (5000m3)	Municipal WW 1, 2, 3, 6, 7, 8	S_I, S_S, X_S				μ_{mH}, K_S, μ_{mA}, K_{NH}	Y_H
PE02: Petersen *et al.*, 2002 MO04: Moussa *et al.*, 2004 NU05: Nuhoglu *et al.*, 2005			1 : SS 2: VSS 3 : COD tot – COD sol 4: COD floculated 5: BOD_5	6: TN and TKN 7: NH_4^+ 8: NO_x^- 9: P					

1.4.4. Using models in the wastewater treatment field

Mathematical modeling of the activated sludge processes provides a powerful tool for understanding the processes better and also for designing, managing and operating these systems. Within the framework of control, simulations can help in upgrading activated sludge plants by defining and testing control strategies, testing scenarios rather than performing time consuming laboratory experiments, and even for directly controlling the process.

1) Upgrade and design of the activated sludge plant

Models can be used to evaluate possibilities of design and upgrading WWTPs, considering minimal supplementary investments. The upgrading process is normally related to improving nutrient removal since the legislation is becoming more restrictive. Sometimes predicting the future performance of a plant by using models can help in the current decision making.

Different solutions for process upgrading have been obtained based on simulation studies for particular cases. The extrapolation is limited by the model itself and the particularities of the plant. Upgrading the plant might imply improving the nitrification or denitrification capacity. Thus, different scenarios are normally simulated to choose the best plant configuration (Coen *et al.*, 1996; Cheng and Rivarova, 1999; Carucci *et al.*, 1999; Flores *et al.*, 2005).

Simulation can also be a tool for reproducing and anticipating the behavior of the WWTP. A prediction of the performance of the plant when working at full loading is presented in Hatziconstantinou *et al.* (1995). An evaluation of future performance considering the increase in the treated flow due to population growth is carried out in Van Veldhuizen *et al.* (1999) and Ladiges *et al.* (1999). In Printemps *et al.* (2004) a simulation tool to be used directly by managers, also with prediction purposes, is presented. Moreover, the potential for augmenting the endogenous nitrifying population (BABE system) was tested using simulation procedures (Salem *et al.*, 2002).

Thus, mathematical modeling can efficiently bridge the gap between lab-scale tests and full-scale application of the available and new technologies saving time and money (Salem *et al.*, 2002).

2) Definition and testing of control strategies

a) The Benchmark

Simulations provide a cost-effective way of testing and evaluating control strategies prior to implementing them. In order to be able to compare different control strategies a platform for simulation purposes was developed by the different Working Groups of COST Actions 632 and

624 and presented in Copp (2001). It is called Benchmark Simulation Model nº1 (BSM1). It consists of a comprehensive simulation model of the plant, plant layout, influent files, controllers, sensors, procedure for performing the simulations, and includes several evaluation criteria for plant performance. Currently, the IWA Task Group on Benchmarking of Control Strategies for WWTPs is developing an upgrade of the BSM1. First of all BSM1_LT attempts to extend the applicability for evaluation of process monitoring methods by providing a long term influent model/file (Gernaey *et al.*, 2005). The BSM2 has been developed within the scope of plant-wide control including the primary clarifier, thickener unit, anaerobic digester and a dewatering unit (Jeppsson *et al.*, 2004). Moreover, the IWA/COST simulation benchmark that was extended to include expert reasoning for system performance evaluation is presented in Comas *et al.* (2005), and enables settling problems of biological origin to be detected.

More than 100 scientific papers have been presented, according to Jeppsson and Pons (2004), using the benchmark or part of it.

Moreover, a proposal of a benchmark for SBRs has been presented in Pons *et al.* (2004). Nevertheless, this is not widespread and still has to be accepted by the scientific community.

b) Real plants

Beyond the benchmark applications, real cases using model approaches to evaluate possible control strategies prior to implementing them can be found in literature. For instance the control of the DO in the aerobic reactor of a plant can be tested (Demey *et al.*, 2001). Another application is testing strategies for equalization or for dosage of chemicals (Demey *et al.*, 2001). Regarding modeling and control strategy testing for nitrogen and phosphorus removal in a WWTP, Ingildsen *et al.* (2005) extends the control scheme for N removal used by STAR® (Oennerth *et al.*, 1996) with biological and chemical phosphorus removal. In Ayesa *et al.* (2005) a model is used for testing supervisory control strategies before the implementation on a WWTP.

Another application is related to calculating the costs of controlling the system. Devisscher *et al.* (2005) presents a methodology for estimating the costs and benefits of advanced control of WWTPs.

The level of model accuracy makes detailed concept engineering of control strategies possible.

3) **SBR Optimization of the plant's performance**

From the literature different parameters or strategies have been found to have a direct influence on the SBR performance and they have been tested or applied in order to improve and optimize operation. For this purpose, model-based approaches have shown to provide a platform in which

many strategies can be tested. The best operating conditions can be found with the simulations and then applied at the lab-scale or full-scale therefore saving time and money.

The main parameters which have been demonstrated through model-based approaches to influence nitrogen removal are the fill strategy, intermittent aeration, the oxygen set-point in the aerobic phase and adjustment of the length of the phases.

Research into continuous and discrete fill strategies and different rates have been conducted in Coelho *et al.* (2000) obtaining the best results when a discrete fill strategy was applied, consisting of symmetric pulses for wastewater and oxygen supply to the system. The step-feed of the influent has been shown to improve denitrification capacity in Andreottola *et al.* (1997) and Hvala *et al.* (2001), eliminating the need to add external carbon.

Intermittent aeration has also been applied to reduce the external carbon source and also the oxygen supply in Demuynck *et al.* (1994) and in Casellas *et al.* (2002), alternating anoxic and aerobic phases after the filling phase.

The dissolved oxygen set-point in the aerobic phase can be established at low values to favor simultaneous nitrification-denitrification during the aerobic phase. This phenomena was investigated in Artan *et al.* (2002) showing that additional denitrification substantially reduced the nitrate concentration with a minor increase in the ammonium concentration due to slower nitrification, which made the strategy suitable when nitrification is not limiting.

Finally, adjusting the length of the phases is the most commonly used strategy, which is also complementary to the previous parameters in order to optimize the cycle and reduce the aeration energy during aerobic phases. This adjustment can be conducted on-line (Katsogiannis *et al.*, 1999) using an adaptive optimization algorithm, and off-line (Mikosz *et al.*, 2003) after a scenario analysis and in this case adjusting the length of the aerobic and total cycle length to improve nitrification under low temperatures.

Artan *et al.* (2002) considers phosphorus removal in the SBR and the consequent phase scheduling and proposes different scenarios to study the effect of several operational parameters which could influence the design procedure. In Sin *et al.* (2004) the phosphorus is also considered and a scenario evaluation is presented using more than 150 cycle structures containing all the above mentioned strategies. An evaluation is made not only with performance indices but also with a robustness index.

As a final remark, when the strategies have been tested based on simulations and the best strategies applied at lab-scale or full-scale to improve the plant performance, the capability of

the calibrated model to describe the new behavior can be tested as well (Hvala *et al.*, 2001; Sin *et al.*, 2004). Better performance is obtained but the model can not describe the new performance satisfactorily due to changes in the microbiological community.

4) Model-based control

Control based on models working on-line is another application of the models. It is normally based on linearized models (Anderson *et al.*, 2000; Smets *et al.*, 2003; Mazouni *et al.*, 2004) because the computational effort demanded by the complete activated sludge models for both parameter estimation and simulation is very high. The optimization of the process is based on the optimization of the model predictions. An application is presented in Kim *et al.* (2000) in which an algorithm is implemented and solved daily to determine the fraction of aeration time and the total cycle time.

2 OBJECTIVES

2. OBJECTIVES

The SBR has been demonstrated to be a flexible system capable to remove carbon and nitrogen from the wastewater. The suitable operating conditions have been already studied for both synthetic and real wastewater. A step further consists in increasing the productivity of the plant, decreasing the personnel necessities, reducing the energy consumption, and increasing the reliability on the process, which can be achieved by making use of control procedures. Hence, the general objective of this thesis is to ***design a control system for the SBR technology removing organic matter and nitrogen, using a calibrated model as an operation support tool***. This main objective is divided into more specific goals:

1) To obtain the modeling support tools by studying the calibration of activated sludge models to describe the carbon and nitrogen removal processes in the SBR. For this purpose it is necessary:
    a. To evaluate the available calibration protocols.
    b. To follow a calibration procedure for obtaining the models, that can support the design of the SBR control system. In this thesis, two calibration studies are conducted:
        i. The first one is for obtaining a calibrated model to be used for evaluating control strategies.
        ii. The second calibration study aims to calibrate an activated sludge model to support a supervisory control system of the SBR.

2) To propose a control system, with the help of the calibrated model, able to i) manage and control the length of the reaction phases of the SBR and ii) identify the process status and adapt the cycle definition. Thus, more concrete objectives can be defined:

    a. To identify the SBR control variables with a key role when removing organic matter and nitrogen.
    b. To define and evaluate control strategies to adjust the length of the reaction phases using a calibrated model.
    c. To implement the control strategy on a semi-industrial pilot plant to evaluate its effectiveness.
    d. To propose a supervisory control system design based on a three-level structure from the experience acquired.

3 MATERIALS AND METHODS

3. MATERIALS AND METHODS

3.1. MATERIALS

3.1.1. Pilot Plants

LAB-SCALE PILOT PLANT SBR

The lab-scale pilot plant located at the University of Girona is composed of three main elements. The SBR with a maximum capacity of 30L, the storage tank with a capacity of 150L and the control panel with the electronic devices. These elements are presented in Figure 3-1, with a general picture (A) and a scheme (C).

The influent wastewater storage tank is made of stainless steel and is completely mixed. It is equipped with a cooler that allows the temperature of the tank to be controlled. In this case, the influent wastewater is kept at 4ºC in order to minimize the microbiological activity.

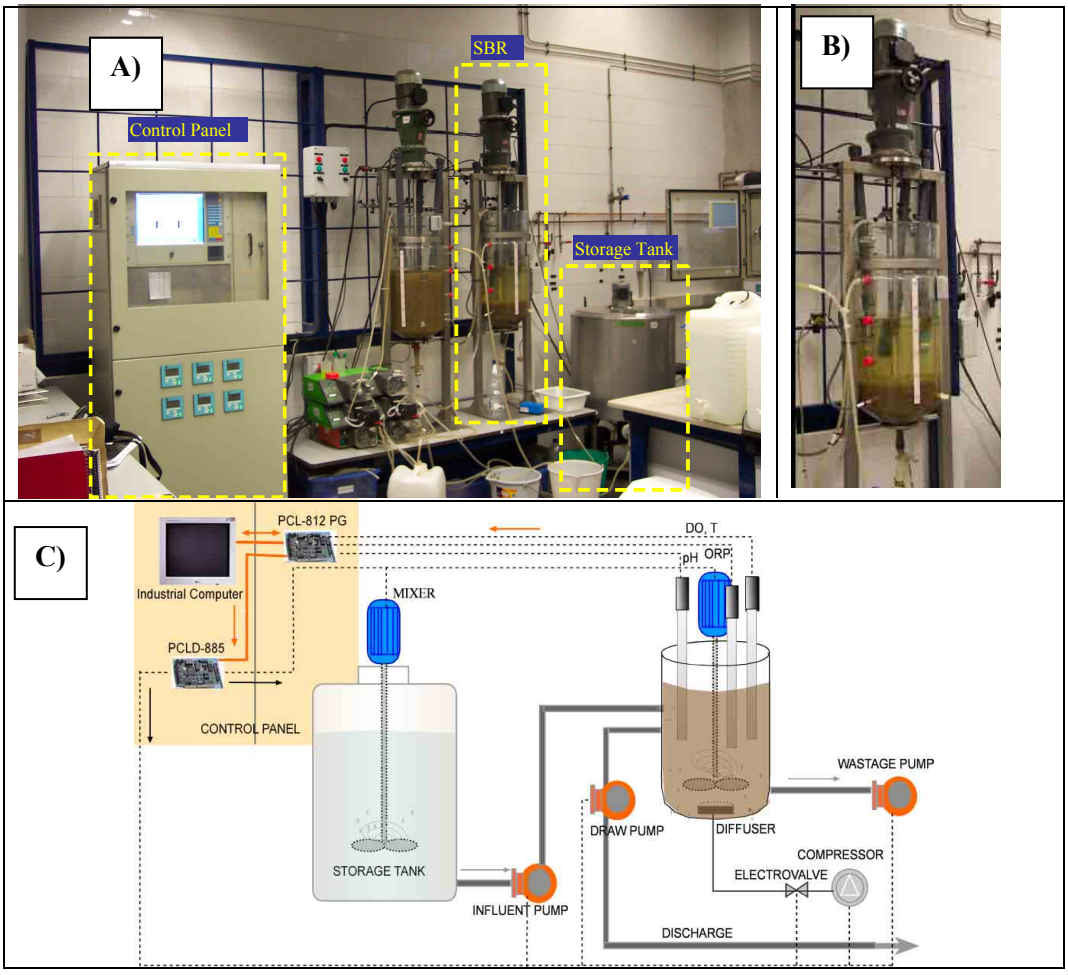


Figure 3-1. Lab-scale pilot plant. A: General picture, B: picture of the SBR, C: scheme of the plant.

The cylindrical glass SBR (Figure 3-1-B) operates as a fill-react-settle-&-draw mode. The influent peristaltic pump (Watson Marlow) allows the influent wastewater to be transferred from the storage tank to the reactor. There, the sludge and the wastewater can be completely mixed using a mixer with a marine helix turning at 400 rpm. The reactor can be operated under anoxic or aerobic conditions. In the last case compressed air is supplied and introduced into the reactor through a pierced tube located at the bottom. An electrovalve is used to control the dissolved oxygen concentration inside the reactor. The wastage pump (Watson Marlow) is used to remove sludge from the system. During the settling phase all the devices are switched off, which causes the sludge (decanted at the bottom of the reactor) to separate from the treated water. Finally the draw pump is switched on during the draw phase in order to discharge the treated water until a desired minimum volume. The reactor is equipped with DO-Temperature (OXIMAX-W COS 41), pH (CPF 81) and ORP (CPF 82) probes (from Endress-Hauser), which are connected to the control panel.

The control panel is equipped with the transmitters, the cards and the computer. The signal from the probes is filtered in the transmitter and captured by a data acquisition and control card (PCI-821PG) which converts the signal from analog to digital. This card can also send digital output signals in order to drive a power relay output board (PCLD-885) in charge of controlling the On-Off switch for the process of filling, wastage, drawing of peristaltic pumps, the mixing device, and air supply.

A self-developed software programmed in LabWindows® (from National Instruments) was installed in an industrial computer to control the process. It is based on user-friendly user interfaces (Figure 3-2) and is able to create operating cycles and make them run.

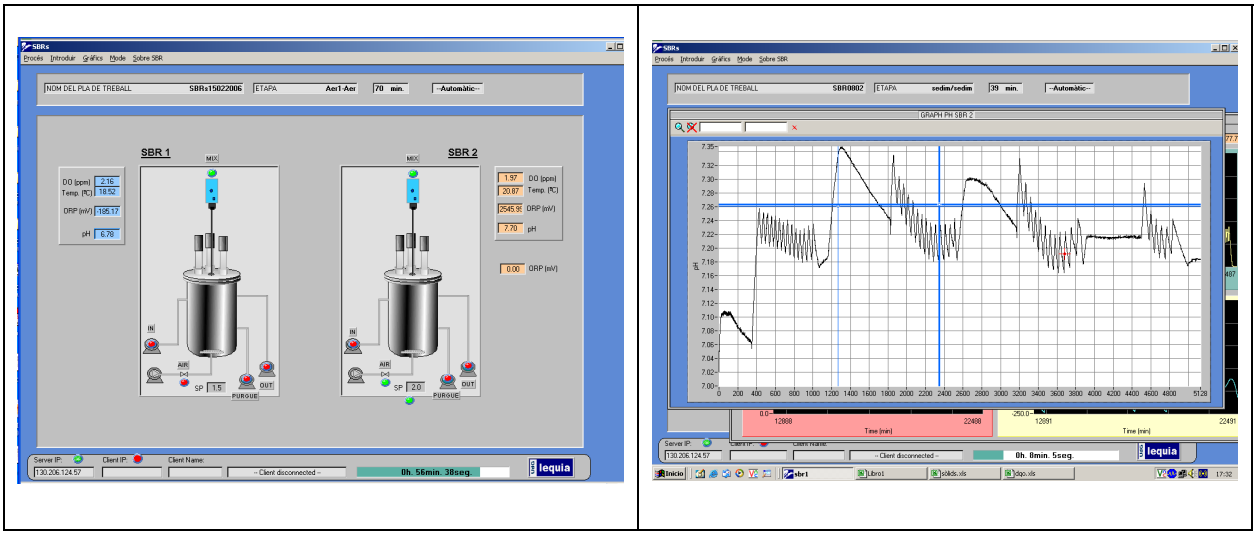


Figure 3-2. Print screen of the main user-friendly interfaces.

On-line mean values of pH, ORP, DO and temperature are obtained at each defined sampling interval (10 seconds) and stored in a simple ASCII file for further processing.

SEMI-INDUSTRIAL PILOT PLANT SBR

The semi-industrial pilot plant was designed especially to be located at Wastewater Treatment Plants to treat real wastewater. Thus, a compact structure was needed to be able to move the plant. The external structure is made of steel, and is 4 m long, 2.20 m high, and 2 m wide. The three elements which make up the plant were built inside the structure: the SBR with a maximum capacity of 1m^3, the storage tank of 300L and the control panel with the electronic devices (Figure 3-3).

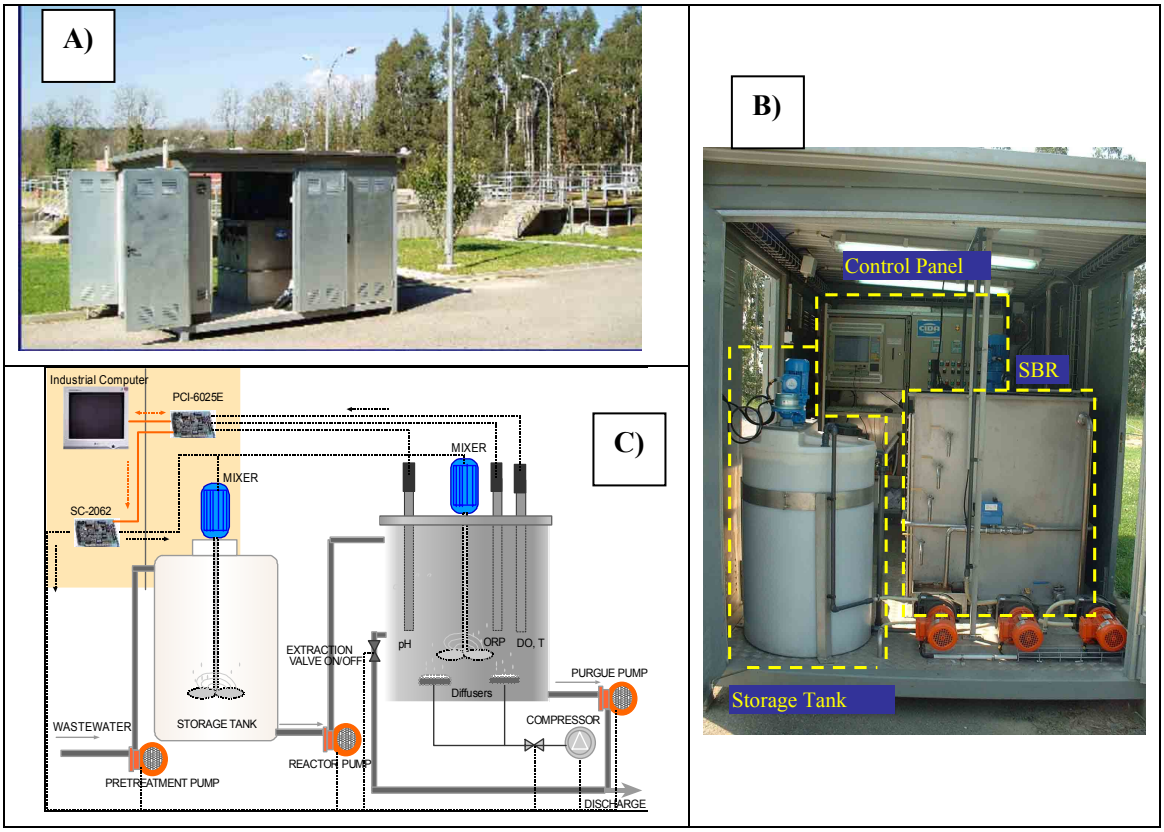


Figure 3-3. Semi-industrial pilot plant. A: Picture from outside, B: Picture from inside of the plant, C: Scheme of the plant.

The storage tank is made of plastic and is completely mixed. The wastewater coming from the influent of the wastewater treatment plant is sequentially introduced into the storage tank using the pretreatment pump (Watson Marlow 621 F/R 77 RPM, flow=0-50L·h^{-1}).

The SBR is square with a slight inclination at the bottom and made of stainless steel. The wastewater coming from the storage tank is introduced with the reactor pump with a maximum capacity of 100L•h^{-1}. A mixer has been installed at the centre of the reactor. Its capacity and the shape of the marine helix permit to maintain the mixed liquor under suspension and homogeneous conditions. A blower (SKS-80 EW) permits air to be introduced into the reactor

through 4 diffusers installed at the bottom. The air supply can be controlled with an On-Off valve or with a variable frequency engine, coupled with the blower. A wastage pump permits the sludge to be removed from the system and the extraction valve is in charge of drawing the reactor until a desired minimum volume.

The reactor is equipped with DO-Temperature (OXIMAX-W COS 41), pH (CPF 81) and ORP (CPF 82) probes (from Endress-Hauser), as well as an air flow meter (Endress-Hauser t-mass S AT70), which are all connected to the control panel. This control panel is similar to the one installed in the lab-scale pilot plant. It is also equipped with the transmitters, the cards and the computer. In this case, the probes and transmitters are the same, but the cards used are the data acquisition card PCI-6025E and the power relay output board SC-2062 from National Instruments. The same software used in the Lab-scale pilot plant has been installed in an industrial computer to control the process.

3.1.2. Fermenter (BIOSTAT B PLUS - SARTORIUS AG)

The fermenter (Figure 3-4) is a cylindrical glass reactor with a maximum capacity of 5L with a cap at the top that permits hermetic conditions to be obtained. The mixing is conducted by a stirrer. The gassing system consists of a rotameter, solenoid valves and mass flow controller. The system is thermostated with a circulation pump or dry heating with a controlled cooling water valve.

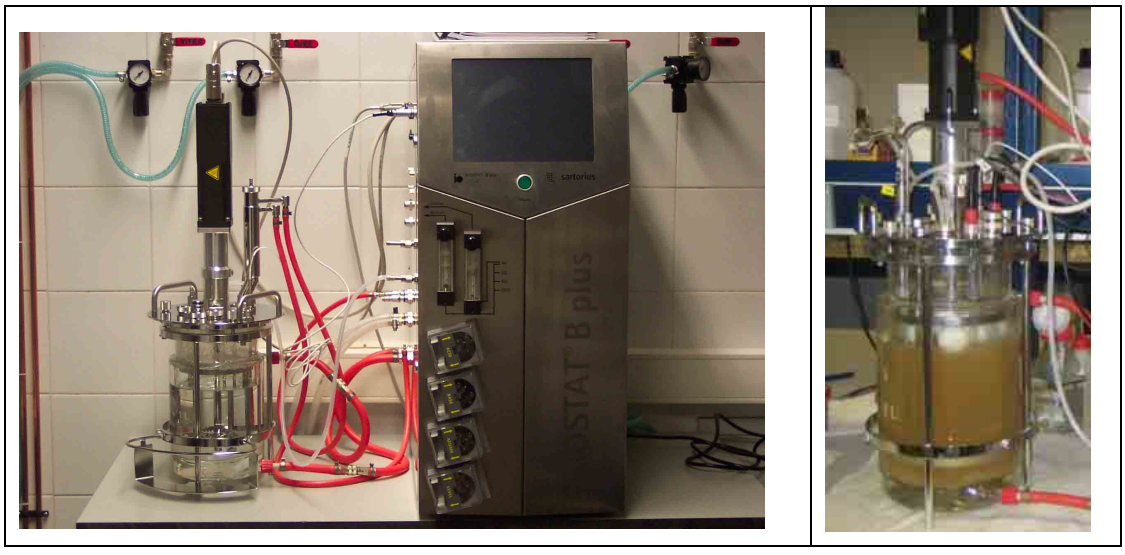


Figure 3-4. Picture of the Biostat B-plus fermenter.

It is equipped with pH, ORP, conductivity, dissolved oxygen and temperature probes. A supervisory software MFCS/DA for extended visualization, data acquisition and trend display is included. Main features include on-line data acquisition and storage, sample data management for off-line measured values, process evaluation and visualization, as well as event dependent process control, process documentation via data export and batch reporting.

3.1.3. Respirometer

An LSS respirometer (Spanjers *et al.*, 1998) was used, where the dissolved oxygen concentration is measured in the liquid phase of a continuously mixed reactor, with neither inputs nor outputs. It was designed and constructed during the research study presented in Gutierrez (2003). The respirometer is composed of two reactors. The aeration tank (the bigger one) is cylindrical and has a maximum capacity of 10L. The measurement cell (the smaller one) has a capacity of 250mL and is cylindrical and hermetically closed. The experimental set-up is presented in Figure 3-5.

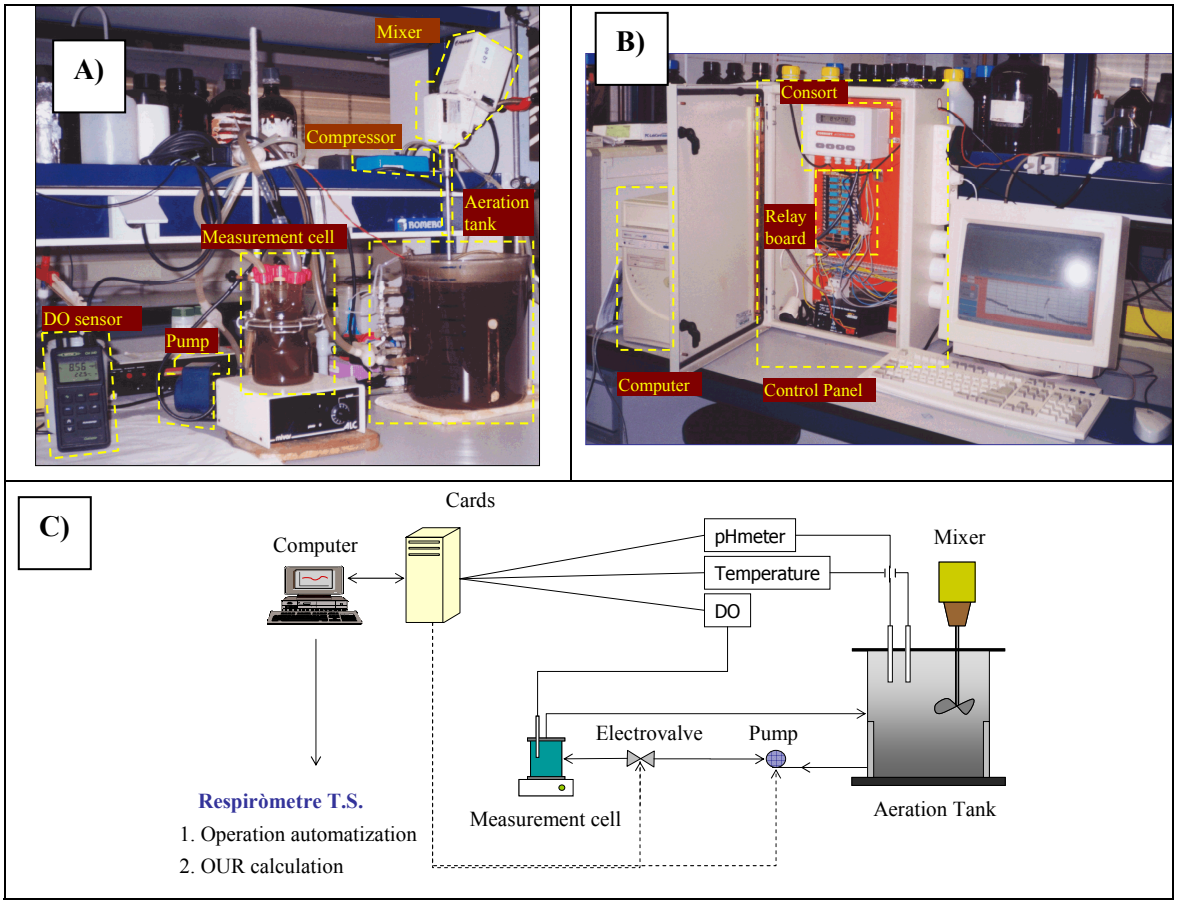


Figure 3-5. LFS respirometer: A) Experimental set-up, B) Electronic devices, C) Scheme with the respirometer devices.

In the 10L reactor the mixed liquor is constantly mixed and aerated using a mechanical stirrer (Heidolph Type RZR1), and a compressor. A pump giving a maximum flow of 10L·min^{-1} is in charge of recirculating the mixed liquor from the aeration tank to the measurement cell. The recirculation is stopped when the recirculation is considered sufficient to have replaced the 250mL volume of the small cell with aerated mixed liquor. The electrovalve stops oxygenated water being introduced into the measurement cell after the pump has stopped. The small cell is also completely mixed using a magnetic stirrer (Mivar) with a diameter of 6 cm. Then, the drop in the dissolved oxygen concentration is measured in the small reactor using a DO meter (WTW Cell OX 325).

The pH and temperature of the aeration tank and the DO of the measurement cell are measured every 5 seconds. A CONSORT® unit is in charge of receiving the data coming from the probes and sends the data to the computer. The combination of PCL-724 (located inside the computer) and a relay output board (PCLD-885) permits switching the pump and the electrovalve On and Off (Figure 3-5-B).

A software called "Respiròmetre T.S." is in charge of data acquisition and controlling the plant. It permits the operation to be automated and calculates the oxygen uptake rate. Another software called Program for Respirometry Analysis (PAR) allows us to deal with the data obtained from the data acquisition system to make interpreting the respirograms easier.

3.1.4. Simulators

WEST

WEST is the World wide Engine for Simulation, Training and Automation (Hemmis, Belgium). It is a general modeling and simulation environment that can be used together with a model base for this task. It can be used in the field of wastewater treatment using a specific model base. This simulator is described extensively in Vanhooren *et al.* (2003). The software is composed of three main elements: the model base, the configuration builder and the experimentation environment:

- Basically, a WEST model base is structured as a collection of text files (.msl) obtaining a hierarchy of model classes. The model base used in this thesis is specific for biological wastewater treatment and is written in MSL-USER which is a high-level object-oriented language.
- The configuration builder allows you to build the physical layout of the plant, and each building block can be linked to a specific model from the model base. The controls of the different objects are also defined in this element. The graphical information is then combined with the information in the model base to produce MSL-EXEC code, which can be compiled with a C+ + compiler.
- In the experimentation environment, the user can design different experiments, such as simulations and optimizations of, for instance, designs, controllers and model fits to data (calibration).

This software also includes analysis modules to make interpreting the simulation results easier, such as an optimizer and a sensitivity analysis module.

GPS-X

GPS-X is a modular, multi-purpose modeling environment for simulating municipal and industrial wastewater treatment plants. It only uses one advanced graphical user interface. The layout of the plant can be easily configured using the process table item which consists of a

collection of unit processes and control points that are used to build the model layout for a WWTP.

The layout is built by translating the GPS-X flow sheet into binary executable code. GPS-X uses a special procedure to convert the graphical images in the drawing board first into a high-level simulation language code (ACSL) and then into a FORTRAN binary executable program.

The simulation properties can be established within the same user interface using the simulation control window. Moreover, the graphs and controls can be easily established within this environment. Other modules are available to make interpreting the results easier or to perform analyses, such as the analyzer, the optimizer and the dynamic parameter estimation.

3.2. METHODS

3.2.1. Analytical methods

Different analytical methods were used for the periodic analysis of the plant, the experiments and the influent wastewater characterization. They are all based on the methods described in the Standard Methods (APHA, 1998). Table 3-1 presents the method and the instrumentation used for the different analyses. More information about the analytical measurements used in this thesis can be found in Vives (2004).

Table 3-1. Analysis methods and instrumentation.

Analysis	APHA method	Instrumentation
Mixed Liquor Suspended Solids (MLSS)	2540D	Filter of 0.45μm
Mixed Liquor Volatile Suspended Solids (MLVSS)	2450E	Filter of 0.45μm
Total Solids (TSS)	2540B	Filter of 0.45μm
Volatile Solids (VSS)	2450C.	Filter of 0.45μm
Chemical Oxygen Demand (COD)	5220B	Open reflux method (digester and titrimetry).
Ammonium (NH_4^+)	4500-NH_3.B-C	Distillation combined with titrimetry (BÜCHI B-324 distiller).
Total Kjeldahl Nitrogen (TKN)	4500-Norg.B	Digestion, distillation and titrimetry (BÜCHI B-324 distiller).
Nitrite and nitrate (NO_2^-, NO_3^-)	4110B	Ion chromatography: Metrohm 761-Compact IC 831 Compact autosampler.

SECTION 1

CALIBRATION OF ACTIVATED SLUDGE MODELS TO DESCRIBE THE CARBON AND NITROGEN REMOVAL PROCESSES IN THE SBR

General frame of section 1

The use of models can help in the field of wastewater treatment to obtain results without doing time-consuming and expensive experiments. Before using the models for operation and control purposes they have to be calibrated.

Hence, this section deals with the calibration of activated sludge models to describe the carbon and nitrogen removal processes in the SBR. First of all, in Chapter 4 the available calibration protocols are presented as a background for performing calibration experiences. Chapter 5 faces the work of obtaining a calibrated model that can be used to evaluate control strategies. In Chapter 6 a model to support the supervisory control system of the SBR is obtained.

Publications

The main part of Chapter 5 was presented as a poster in the conference BNR 2005:

- Corominas, Ll., Sin, G., Balaguer, M.D., Colprim, J. and Vanrolleghem, P.A. (2005). Calibration and validation of a N-removing SBR only using on-line measurements of DO and historical off-line data. *In proceedings: Nutrient Management in Wastewater Treatment Processes and Recycle Streams*, Krakow, Poland, 19-21 September 2005. pp. 1333-1338.

4 The existing calibration protocols

4. THE EXISTING CALIBRATION PROTOCOLS

4.1. SYSTEMATIC CALIBRATION PROTOCOLS

The use of models in the field of wastewater treatment requires a calibration procedure where the parameters of the chosen model are adjusted one by one, until the experimental values are fitted. This calibration procedure is complex and normally conducted according to the experience of the modeler resulting in different approaches followed during the recent years, what makes difficult to compare the modeling studies. Therefore, a general guideline is needed to unify working procedures and also to assess the quality of the calibrated models obtained.

Up to now, four systematic protocols from different research groups have been proposed:

i) BIOMATH - Department of Applied Mathematics, Biometrics and Process control, Ghent University, Belgium (http://biomath.ugent.be).

ii) STOWA - The Dutch Foundation of Applied Wat. Res., The Netherlands (http://www.stowa.nl).

iii) WERF - Water Environment Research Foundation, North America (http://www.werf.org).

iv) HSG (The Hochschulgruppe), a group of researchers from German speaking countries (e.g. EAWAG (Swiss), BOKU (Vienna) and IFAK (Germany)).

The existing systematic calibration protocols have a similar structure: they all begin by defining the calibration goal/s which will influence the rest of the procedure. Then the data is collected and its quality evaluated. After that, the mechanistic model is selected and then, a steady state calibration is performed followed by a dynamic calibration and finally, the results are evaluated. Some feed back loops are established in order to obtain a dynamic step wise procedure.

Nevertheless, at each step there are also differences that originate from the different points of view the protocols have on particular aspects. For instance, the methods used for the influent wastewater characterization or the kinetic and stoichiometric parameter estimation.

A Strengths, Weaknesses, Opportunities and Threats (SWOT) analysis that compares the different protocols has already been presented in Sin *et al.* (2005a). A complementary explanation is presented in this Chapter in which the most important aspects considered in the calibration procedures are analyzed separately for each existing protocol.

4.2. STATE OF THE ART OF THE CALIBRATION PROTOCOLS

As stated before, different calibration protocols have been presented and accepted by the scientific community to systematize the calibration procedure. In this chapter a comparison of these protocols is presented. First the similarities that define a common structure are identified, and then we go into detail about the four calibration protocols and detect their particularities.

A common structure can be defined by analyzing the existing protocols. The calibration procedure can be structured into five main stages:

- Stage I: Defining the objectives

All the steps of the calibration are conducted according to the goal defined at the beginning. The objective can be more or less ambitious mainly depending on time, the budget and the level of human expertise. It has to be clear which processes are going to be modeled and what the model is going to be used for.

- Stage II: Plant survey/Data analysis

Available data from the plant is collected, e.g. design information, operating conditions, off-line and on-line measurements. An accurate analysis of the data has to be performed because errors in the data would propagate in the model parameters and would affect the entire model structure. The quality of the data has influence on the whole calibration procedure. One has to make sure that errors in the data do not propagate to the model.

- Stage III: Model structure/process characterization

This stage includes defining the model structure. This accounts for the hydraulics of the plant, the aeration, the settling and the biological reactions of the process. Once the model is defined the process characterization is performed, which includes the influent wastewater fractionation and the experimental estimation of some of the activated sludge parameters.

- Stage IV: Calibration and Validation

The calibration consists in determining the values of the model parameters to fit a certain set of measurements obtained from the wastewater treatment plant. Since activated sludge models have a lot of parameters this procedure is normally systematized into sub-steps. The parameters are tuned until the simulated and the measured values are close to each other (visual inspection or numerical error quantification), and the trends of the variables are well described. The validation consists in using the model with parameter values obtained in the calibration and applying them to another independent data set, if possible obtained in other operating conditions, e.g. temperature, flow, influent load.

- Stage V: Evaluation of success.

The success of the calibration depends on whether the objective of the study is accomplished or not. It is important to take into account that an error made in the beginning stages may be detected at stages IV and V. Therefore it is necessary to use the loops established within the process which permit one to go back to earlier steps.

Although this general structure is very similar in the existing protocols, there are differences that can be observed when the stages are looked at in detail. The main structure of the calibration protocol itself is an indication of the particularities of the procedure. Moreover, some key points can be identified that can distinguish one protocol from the others. For instance, the protocols deal differently with the data quality evaluation, the methodology for the influent wastewater characterization and determining the kinetic and stoichiometric parameters. More particular aspects like the importance given to using a sensitivity analysis or to the settling characterization can increase the differences between the protocols.

It has to be stated that the development of the calibration protocols is the result of a lot of previous work. Therefore, the procedures obtained are dependent on the trajectory of the department/institution and the particular research they have conducted. The four calibration procedures discussed in this Chapter have developed differently. For instance, the BIOMATH protocol originated from a scientific background and this is the reason it gives importance to the Stage III and especially to the biological characterization and the model structure. Alternatively, the STOWA protocol appeared after interviewing practitioners with extensive experience, under the influence of Water Boards and consultants. For this reason, practical methods were preferred above scientific exactness, and therefore more importance is given to the Stages II and III focusing on the data analysis, the influent wastewater characterization and the model structure. The HSG guidelines appeared later with the purpose of systematizing the documentation of the overall calibration study, and referring to the BIOMATH and STOWA protocols for the Stages II and III considering that they have described these aspects intensively. Finally, the WERF protocol appeared also under a scientific background but giving another point of view to the calibration procedure establishing different calibration levels depending on the amount and quality of the available data.

Thus, these differences between the protocols imply that the percent time for each stage in relation to the whole study is different for each protocol. In the BIOMATH protocol the most time consuming would be the Stage III and in the STOWA protocol the Stage II. For the HSG guidelines more time should be spend in the data quality check and in the documentation, and finally in the WERF protocol, the time demand would be according to the quality of the data. Moreover, the most time consuming stages would be the ones where more expert knowledge is

required. However, the stage IV, where the adjustment of the parameters is conducted, is achieved easier and faster according to the experience of the modeler.

In the next pages, the four calibration protocols accepted by the scientific community are presented. The five common stages are identified for each protocol (to make the comparison easier) and the particular aspects of each stage are discussed.

4.2.1 BIOMATH protocol

The BIOMATH calibration protocol (Vanrolleghem *et al.*, 2003) was developed to standardize the calibration procedure based on the expert knowledge acquired in previous experiences. Scientific exactness guides the entire procedure and thus a high level of sophisticated mathematical/statistical methods is needed when applying this protocol.

The general structure is presented in Figure 4-1 with an accurate scheme with feed back loops that make the protocol dynamic. The main points of the protocol are the biological characterization (Figure 4-1-step 7), the mass transfer and settling characterization (Figure 4-1-steps 5 and 6) and the calibration (Figure 4-1-steps 8 to 12).

Stage I

Defining the goal is the first step of the calibration procedure and the decision is based on the time and/or budget necessary/available for the modeling task. Different kinds of objectives are proposed (optimization and upgrading, cost reduction in operation, development of control strategies…).

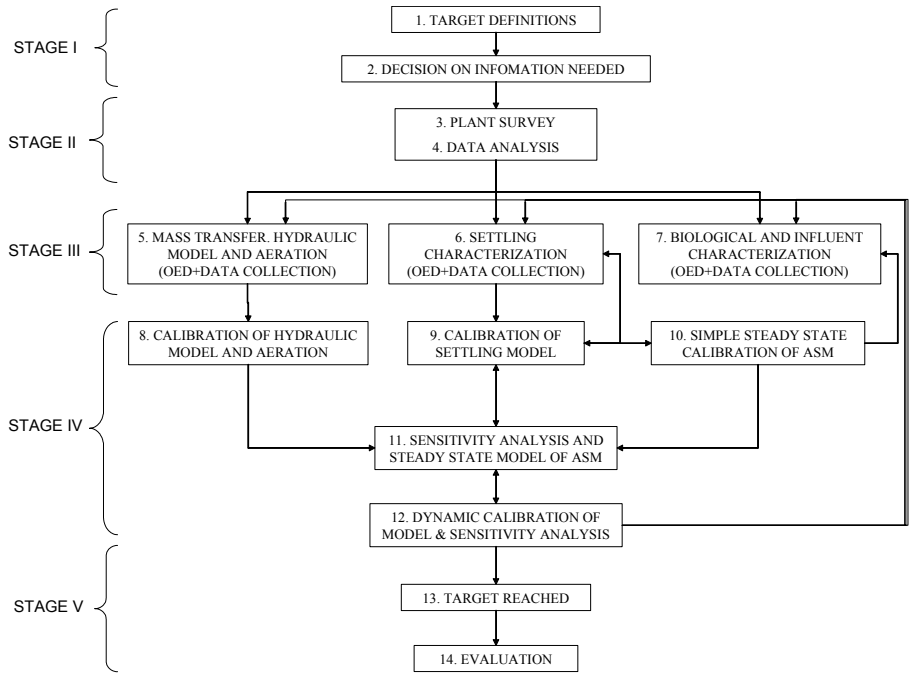


Figure 4-1. BIOMATH protocol.

Stage II

The type of data needed is divided into the design data, the operational data and the measured data, which is considered the most important issue. There is a specific description of the variables needed for characterizing the influent and effluent, the on-line measurements and the parameters from the clarifier and sludge characterization.

The data quality evaluation is included in the data analysis section and refers to the mass balances regarding the flow rate and the sludge composition, and focuses on accurately estimating the sludge age. There is no specific guide in this step and other literature references are proposed.

Stage III

This protocol divides the plant model into three sub-models: mass transfer, settling and biological. For each sub-model a detailed decision tree is defined in order to help make the decision of how complex the model should be, according to the main goal and the data available.

The biological model is selected in step 7 after the data analysis and is related to the settling model if reactions in the settler are considered. A guide to decide which model to apply is available in the protocol, including ASM1, ASM2 and ASM3 (with possible modifications when necessary). Thus, phosphorus removal is also considered in this protocol.

The influent wastewater characterization is based on biological (respirometry) and physical-chemical experiments. The BIOMATH group has conducted intensive research on this subject, focusing on respirometric experiments (Spanjers and Vanrolleghem, 1995; Vanrolleghem *et al.*, 1999).

Parameter estimation is also based on respirometry and the protocol contains a detailed explanation of the methodology, taking into account identifiable parameter combinations. In this sense, a high level of expertise on certain advanced mathematical/statistical methods is necessary when applying these techniques since interpreting the respirometric measurements is not straightforward.

The Optimal Experiment Design (OED) is presented as a useful tool for maximizing the information content of the experiments (Dochain and Vanrolleghem, 2001) and could be applied when planning the measurement campaign. Applying the OED means that once again a high level of expertise is necessary since using it is not straightforward and no specific application is presented in the protocol. More information about OED can be found in De Pauw (2005).

Stage IV

The general structure of the calibration proposes first performing a steady state calibration of the sub-models and then a dynamic calibration.

In the steady state calibration the data of full-scale wastewater are averaged assuming that this average represents a steady state. Long term behavior parameters can be tuned in this step and a proposal of these possible parameters is included.

The dynamic calibration takes the biomass composition resulting from the steady state calibration as a starting point, and uses dynamic influent data to describe the dynamics of the process properly. This protocol does not propose which parameters to tune as this is case specific. Nevertheless, in other studies (Insel *et al.*, 2004) a dynamic calibration through a more specific step wise procedure with special mention of the processes and parameters is presented.

Importance is given to the sensitivity analysis as a part of both the steady state calibration and dynamic calibration, since it can help for selecting the more influencing parameters to be adjusted.

For the calibration different options are possible: trial and error (manually) or using an optimizer (or parameter estimation). The first approach is based on expert knowledge and the second requires system identification, practical identifiability analysis (Weijers and Vanrolleghem, 1997).

Stage V

The final evaluation is proposed and the solutions when no success is achieved can be found by re-evaluation of the plant data, the sub-models or even the targets defined in the first step. In addition, the possibility of modifying the model structure or using an alternative one is described.

Complementary information

BIOMATH group has been and is currently involved in the development of the software (WEST). This cooperation reflects on the user-friendly interface of the software for performing the calibration and carrying out the complex sensitivity analysis and parameter estimation.

4.2.2. STOWA protocol

The STOWA calibration protocol (Hulsbeek *et al.*, 2002) was developed after interviews with experienced practitioners, and the main purpose was to structure the experience and knowledge acquired in order to improve the quality of the simulation studies. In this protocol easiness is preferred to scientific exactness.

It has an accurate calibration structure, presenting a general scheme (see Figure 4-2) and with particular sub-schemes for the different stages of the calibration. Extensive guidance is given at each step in terms of the data needed, the process to follow and even an estimation of the time required. The main points are the data verification (Figure 4-2-step 3), the model structure (Figure 4-2-step 4) and the influent wastewater characterization (Figure 4-2-step 5).

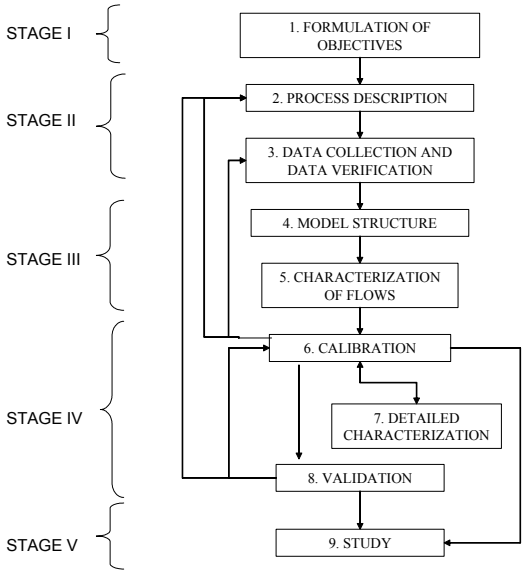


Figure 4-2. STOWA protocol.

Stage I

The protocol structure depends on the objectives of the study. The possible goals of the calibration rely on three different model studies that are defined: the system chosen during the basic design, optimization studies for existing WWTPs and the development of control strategies. This objective determines the level of specification of the model, and the necessary monitoring frequency of relevant flows.

Stage II

First of all a process description is required that defines the relevant process components. An accurate review of the required data is presented. It is advised to first use the available data, and later (if needed) perform extra monitoring.

Special attention is given to the data quality evaluation since the reliability of the model is clearly dependent on the quality of the data. Mass balance calculations are proposed as the tool for doing this data reconciliation and even the equations are included in the calibration protocol. The calibration cannot continue until the mass balances are fitted.

Stage III

The model structure is defined according to the number of compartments estimation, the aeration configuration, the settling characterization and the control implemented in the plant. There is little guidance for determining the compartments and the aeration configuration but more guidance is available for the settling characterization and the process control.

The protocol is developed entirely for using ASM1 and therefore phosphorus removal is not considered. Nevertheless, a good complement to the protocol is the work presented in Meijer (2004), in which calibration experiences are presented for nitrogen and phosphorus removal using the TUDP model in lab- and full-scale plants.

The influent wastewater characterization is described in a specific protocol (Roeleveld and Van Loosdrecht, 2002). It is based on combining physical-chemical methods to characterize the soluble and particulate fractions, and BOD measurements to determine the biodegradable fraction of the total COD. Five years of experience are summarized, with successful calibrations using this protocol. Nevertheless, some weaknesses have been described in Weijers (1999), especially regarding the reproducibility of the BOD analysis, and the assumption of the inert particulate (f_P).

There is no reference to estimating kinetic or stoichiometric parameters, performing lab-scale experiments or to the biomass characterization because the protocol considers the lab-scale experiments not necessary.

The sampling depends on the objective. Daily average concentrations of influent and effluent are enough for description purposes. For optimization studies, dynamic data from 4- or 2-hourly composite samples are required. In this case, recirculation should also be sampled. The OED is not considered in this protocol.

Stage IV

There is no division between a steady state and a dynamic calibration. It aims to perform a pre-calibration trial to check the model structure. If the results show that a major adjustment of the model parameters is necessary then it recommends that you modify the model structure or check the operational data itself rather than continue with the calibration.

Once the model structure is considered to be correct then the kinetic and stoichiometric parameters are adjusted. A specific guideline is given beginning with the calibration of the sludge production, then the nitrification process, denitrification and finally internal flows. General advice is given and also the set of parameters to be tuned at each step. This is risky as each calibration is case specific. Phosphorus removal is not considered in this protocol. Nevertheless, this subject is dealt in Meijer (2004), what could be considered as an extension of the STOWA calibration protocol.

A sensitivity test for process parameters (e.g. flow rates, set-points) is proposed to detect inconsistencies in the model structure.

Stage V

There is no specific mention of evaluating the whole calibration procedure, and therefore no solutions proposed for when bad calibration results are obtained. This protocol recommends performing the validation with data obtained under different operating conditions from the calibration.

4.2.3. The Hochschulgruppe (HSG) guidelines

The HSG guidelines (Langergraber *et al.*, 2004) were developed to define a reference quality level that helps to make the results of simulation studies comprehensible and comparable. They are not focused only on the simulation, but also on the entire study process in order to make it easier, minimizing time and cost effort and giving reliable results.

It has an accurate structure (see Figure 4-3) but it does not systematize each step. There are no feed-back loops, which makes the procedure static. The main points of the protocol are quality control of the data (Figure 4-3-step 3) and careful documentation (Figure 4-3-step 7).

Stage I

The possible objectives are not specified, but it is stated that they have to be defined in collaboration with the client and the plant operator.

Stage II

The layout of the plant is considered to be easy to determine, in contrast to operational data and performance data which are often unclear. The data needed are not specified.

Special importance is given to the data and its quality evaluation, since this control is needed whenever new information is incorporated into the procedure. It is suggested to perform mass balances especially for phosphorus and nitrogen. In addition, it points out the necessity to check

the accuracy of the measurements in the laboratory. The protocol refers to Meijer *et al.* (2001) for more information about data quality evaluation, which is affiliated with STOWA protocol.

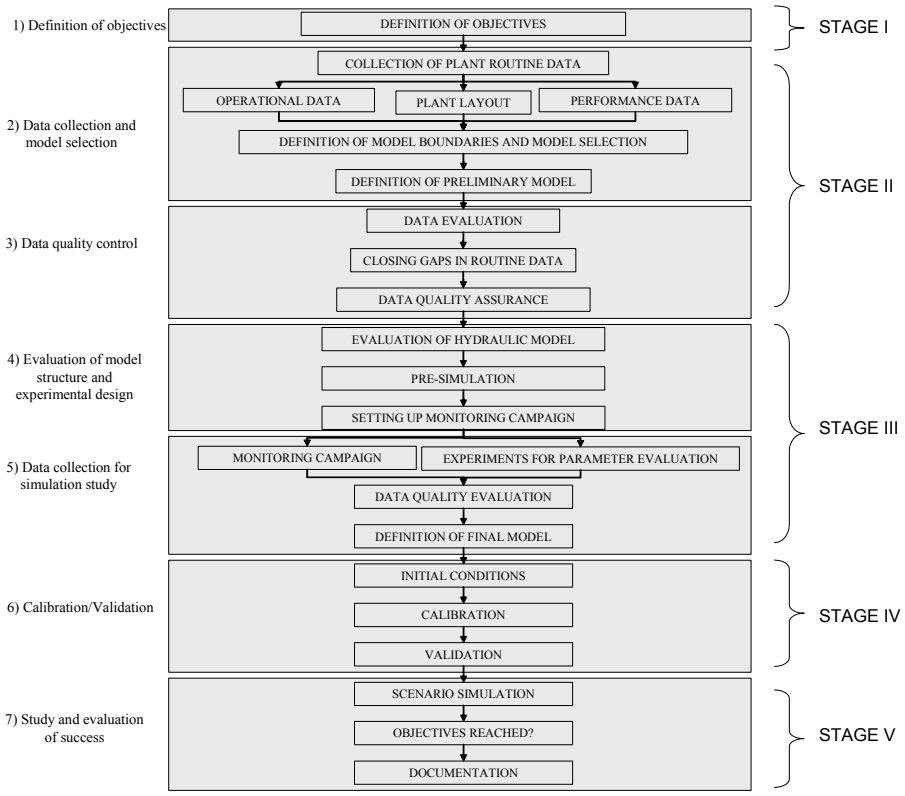


Figure 4-3. HSG guidelines.

Stage III

In order to set up a plant model the protocol proposes defining the model boundaries, sub-systems and operational units, and the interaction between them. It is aimed to evaluate the hydraulic model using tracer experiments or Computational Fluid Dynamics (CFD). Little guidance is given in the sedimentation modeling.

Selecting the model is considered together with collecting data and a guide is available as in the BIOMATH protocol.

Influent wastewater characterization, biomass characterization and parameter determination are not specifically described. The influent wastewater characterization refers to the STOWA protocol and the parameter estimation to the BIOMATH procedure. In Sin *et al.* (2005a) it is pointed out that too much freedom for the modelers to decide which experimental methodologies to employ questions the level of standardization of this protocol.

Regarding the monitoring campaign and experiments for parameter evaluation the protocol recommends performing an intensive sampling program of about 10 days. Mass balances should be performed after the monitoring campaign. No OED is considered.

Stage IV

Before the calibration task, there is an evaluation of the hydraulic model and then a pre-simulation using a steady state model. There is no division between steady state and dynamic calibration

The calibration begins with the correct estimation of the initial conditions obtained after simulating several weeks of operation (similar to a steady state calibration).

For the dynamic calibration a similar procedure to the STOWA guideline is proposed, but the parameters to be tuned are not assessed. It is proposed to follow a step-wise procedure, in which phosphorus removal is also considered. This protocol proposes evaluating the quality of the fit by using mathematics criteria.

The guidelines consider the possibility of using a sensitivity analysis to identify the parameters with major influence on the model.

Stage V

As stated before, this protocol aims for quality not only of the calibration but also of the whole simulation study. Thus, the results are evaluated after the simulations are finished. As a final remark, the HSG guidelines are the only protocol that proposes a standardized documentation for the calibration studies to improve the comparability of different studies.

Complementary information

It is planned to complete this protocol with different case-studies that apply this methodology.

4.2.4. Water Environmental Research Foundation (WERF) protocol

The WERF calibration procedure (Melcer *et al.*, 2003) is part of a book which focuses on wastewater characterization methods where a compendium of peer-reviewed procedures for measuring important parameters involved in calibrating the models is provided.

The structure of the calibration protocol is not clearly presented and no scheme is available. An approach of the procedure is presented in Figure 4-4. The main points are the influent wastewater characterization and the concept of guiding the study not only according to the objective of the simulation but also with the available data.

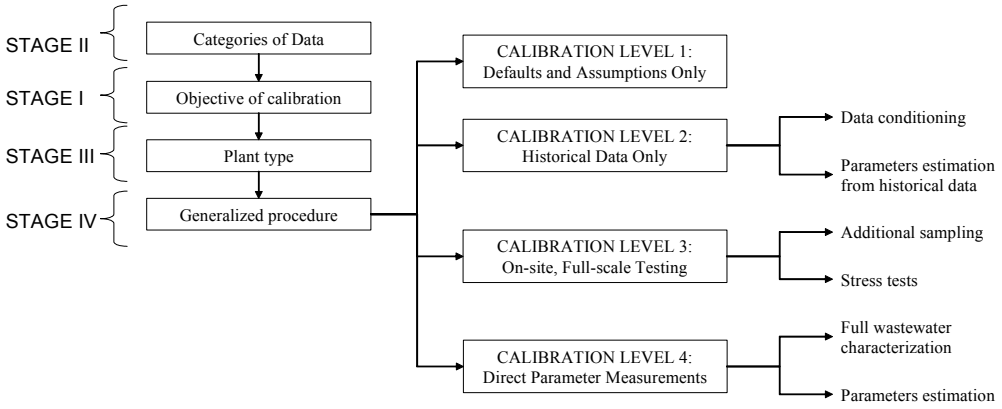


Figure 4-4. WERF protocol.

Stage I

A description of the general calibration objective is presented. It does not specify the final aim of the model but intends to establish the field of validity and the expected accuracy of the model in specific circumstances.

Stage II

The information to be collected is divided into four groups: physical plant data, plant operational data, influent loading data and kinetic and stoichiometric model parameters. A complete review of the required data is presented for different types of plants.

Data conditioning is an important step in the calibration. This is based on applying a statistical analysis for identifying outliers and data entry errors.

Stage III

There is no reference to the model structure and few explanations about methods for hydraulic and settling characterization.

A review of the Activated Sludge Models is presented in the document but no special guidance is given for selecting the model within the calibration procedure.

Special attention is given to the influent wastewater characterization, which is conducted by using SBR based methods and combining OUR measurements with physical-chemical analyses. The lab-scale SBR method is preferred since it allows more accurate control and less specialized equipment is required.

Parameter estimation is focused on nitrification dependent parameters (μ_A and b_A), since they are identified as the critical kinetic parameters. Three methods for estimating the nitrifier decay rate are presented: low F/M SBR based-method, high F/M test and washout test. Nevertheless, the SBR experimental approaches presented in this protocol should not be applied when taking

sludge from continuous flow systems (Sin *et al.*, 2005a). The batch process may provoke physiological changes causing kinetic and stoichiometric behavior that is not representative of the original system.

The monitoring campaign is performed when working only with historical data is not enough to achieve the objectives of the study. A proposal of the monitoring campaign is presented.

Stage IV

The calibration procedure is presented at different levels of complexity depending on the data sources. The first level considers using default values and assumptions only. The second level is based on historical data and conditioning the data and estimating some parameters from the historical data. The third level is applied when more testing in the plant is possible by conducting additional sampling or stress tests. Finally, the fourth level is based on estimating parameters directly and performing full wastewater characterization.

The document presents a list of steps for a "typical" plant, and "typically available" data to provide an initial blueprint for a calibration exercise, using a similar approach to the STOWA protocol, but also considering phosphorus removal (see Figure 4-5).

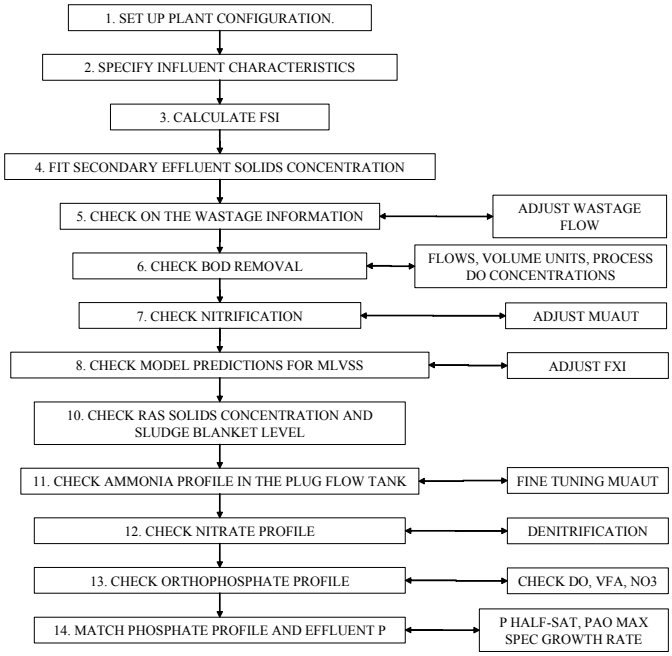


Figure 4-5. Case-specific calibration procedure of WERF.

The sensitivity analysis is presented in a separate chapter of the whole document with an example, but it is not located in a specific part of the calibration protocol.

Stage V

The final evaluation of the process is not specified. Nevertheless, it is mentioned that the final fit obtained will influence the expected accuracy of the model under certain circumstances.

Complementary information

Common pitfalls in calibration are presented, including sampling and analysis problems, misleading results from deficiencies in plant operation and the waste activated sludge measurements and sludge age.

After dealing with the different protocols separately, a summary of the most important aspects is presented in Table 4-1. The four protocols are located in the columns, and the rows show the most remarkable aspects of the five stages.

Table 4-1. Summary of the main aspects of the four calibration protocols.

		BIOMATH	STOWA	HSG	WERF
Stage I	General structure	* Accurate general structure * Feed-back loops are considered	* Accurate structure with specific information at each step * Feed-back loops are considered * Duration estimation of the different calibration steps	* Accurate structure but does not go into detail at each step * No feedback loops	* No accurate structure
	Main points	* Biological characterization, calibration, model structure	* Data verification, model structure, influent wastewater characterization	* Data quality control, careful documentation	* Biological characterization
	Definition of objectives	Six model objectives: 1) Optimization and upgrading 2) cost reduction 3) development of control strategies 4) Meeting the effluent criteria 5) Reuse of effluent wastewater 6) Design of the treatment plant	Three model studies: 1) system choice during basic design 2) Optimization studies 3) Development of control strategies	* No specification of possible objectives * The objectives defined in collaboration with the client and plant operator.	* No specification of possible objectives * Establish field of validity and expected accuracy
Stage II	Plant Survey	* Specific description of the variables needed	* Accurate review of required data * 1st use available data, then perform extra monitoring	* No specification of required data	* Complete review of required data
	Data quality evaluation	* Based on mass balances (sludge age). No guidance * No especific guidance. Referred to Barker and Dold 1995 and Nowak et al., 1999	* Mass balances, equations available * More info referred to Meijer *et al. (* 2001) and Nowak et al., 1999	* Based on mass balances and measurements accuracy * No specific guidance. Referred to Meijer (2001)	* Based on statistical analysis for identifying outliers
Stage III	Model structure	* Three submodels considered: 1) Mass transfer 2) settling 3) biological and influent characterization * Review of used biological models. * Phosphorus removal is considered	* Four elements considered: 1) compartments number 2) aeration 3) settling 4) Control structure * No guidance for selecting the biological model. * No phosphorus removal considered	* No specification of model structure * Review of the existing biological models * Phosphorus removal is considered	* Not specified * Review of the existing biological models * Phosphorus removal is considered
	Settling	* Decision chart on settling characterization	* Decision chart on settling characterization	* Little mention	* Not emphasized
	Influent wastwater characterization	* Combination of biological (respirometry) and physical-chemical methods	* Combination of physical-chemical methods and BOD measurements * Ref: Roeleveld 2001; STOWA, 1996; STOWA 1999	* It referres to Roeleveld and Vanloosdrecht (2002)	* Comparison of different methods
	Parameter estimation	* Respirometry methods (μ_{mH}, μ_{mA}, K_S, K_{NH}, b_H) * Identifiability analysis also considered * OED also considered, although no guidance is available	* Experimental evaluation of model parameters considered not usefull	* It refers to Vanrolleghem *et al* . (1999)	* Comparison of three methods * Foccused on μ_{mA}, b_A, η_g, η_H
Stage IV	Calibration procedure	* Iterative procedure: 1) Steady state calibration. (X_I, Y_H, b_H) 2) Dynamic calibration * No proposal of parameters to be tuned	* Iterative procedure: 1) Sludge age 2) Effluent ammonia 3) Effluent nitrate * Parameters to be tuned are proposed	* Iterative procedure: 1) Sludge age 2) Effluent ammonia 3) Effluent nitrate 4) Effluent phosphate * No prosal of parameters to be tuned	* Iterative procedure * case-specific calibration procedure * Common pitfalls are presented * Parameters to be tuned are proposed
	Sensitivity analysis	* Both in steady state and in dynamic calibration	* Sensitivity test for process parameters	* In a pre-simulation, before monitoring campaign	* Not specifically included in a part of the calibration protocol
Stage V	Evaluation	* Solutions when there is no success have to be found by re-evaluation of the plant data, the sub-models or even the targets defined in the first step	* No mention of evaluation	* Evaluation of the results is performed after the study	* No mention of evaluation

4.3. ADAPTING THE CALIBRATION PROTOCOLS TO SBR APPLICATIONS

Different calibration protocols have been described above which, in the context of providing general guidelines, aim to fulfill particular purposes e.g. scientific exactness, applicability, quality control, etc. All the available calibration protocols have a similar structure, but when going into detail one can see that they are focused on different aspects which depend on the purpose of the calibration procedure itself.

Moreover, after analyzing the available calibration protocols one can see that they are focused on continuous flow activated sludge systems. When dealing with batch systems, the methodology must be adapted taking advantage of some particularities that can led to easier calibrations, which is the case in SBR systems.

When calibrating an SBR model the major advantage is that during one cycle, composed of filling, reaction, settle and draw phases, it is possible to observe a huge variation in the state variables. This variation in a system that alternates aerobic and anoxic phases gives an indication of the nitrification and denitrification processes and thereby provides rich-information for model-calibration/identification. As pointed out in Vanrolleghem and Coen (1995), dealing with the SBR technology, data from the plant alone may be sufficient for a dynamic model calibration since some reaction kinetics can be readily obtained. Thus, the model calibration applied to SBRs is focused on the calibration at the cycle level, in which the dynamic of the biological reactions is clearly described by means of analytical measurements. Therefore, the nitrification and denitrification parameters can be adjusted without performing extra lab-scale experimental assays. This implies performing a measurement campaign for the calibration and another one for the validation. This measurement campaign consists in taking samples at short time intervals during one cycle evolution and analyzing the desired variables. Another advantage of SBR model calibration is the hydraulic characterization, which is not normally needed and the SBR can be modeled as a single reactor tank. Nevertheless, a tracer test can be performed to ensure that no mixing problems occur in the reactor. Finally, the SRT in the SBR can be better controlled, and this can help in the calibration.

In the next chapters (5 and 6) two calibration experiences are presented. The objective of the first calibration is to obtain a model to properly describe carbon and nitrogen removal to be applied for evaluating control strategies. The experience acquired in this calibration has also been used to detect the limitations in the process which make some steps complicated. The second calibration study is focused on obtaining a calibrated model to support a supervisory control system. Hence, a more accurate procedure is followed and some improvements detected

in the first calibration have been incorporated. Special attention is paid to the influent wastewater characterization and also to the long term parameters which influence sludge production. At the end of the studies two calibrated models have been obtained which can be used for different purposes according to the objective of the model application and the final evaluation of the results.

5

Calibration of the nitrogen-removing SBR using historical data

5. CALIBRATION OF THE NITROGEN-REMOVING SBR USING HISTORICAL DATA

5.1. MOTIVATION

The motivation of this chapter is to obtain a calibrated model to be used for evaluating control strategies. Hence, the requirements of the model rely in the correct description of the nitrogen and dissolved oxygen trends during the SBR cycles. Historical data is considered enough to achieve these requirements. Moreover, this experience is also a learning exercise to detect the critical points of the calibration, determining the advantages and weaknesses of the followed procedure. This is translated into knowledge that can be used to improve further calibration experiences.

5.2. DESCRIPTION OF THE SBR PILOT PLANT

The historical data was obtained from Vives (2004) using the lab-scale pilot plant described in point 3.1.1. The operating conditions, cycle configuration and influent wastewater for this particular study are described in the next paragraphs.

5.2.1. Operating conditions and cycle description

The lab-scale pilot plant operated for three months treating 10L of wastewater per cycle and using a cycle of 8 hours divided into reaction, settling and discharge. The step-feed strategy described in point 1.3.3 was used and anoxic and aerobic reaction phases were alternated, with a constant air supply during the aerobic phases. The study consisted in two periods in which the number of filling events and minimum volume were different: Period 1 with two filling events and 14L of minimum volume and Period 2 with six filling events and 20L of minimum volume (see Figure 5-1).

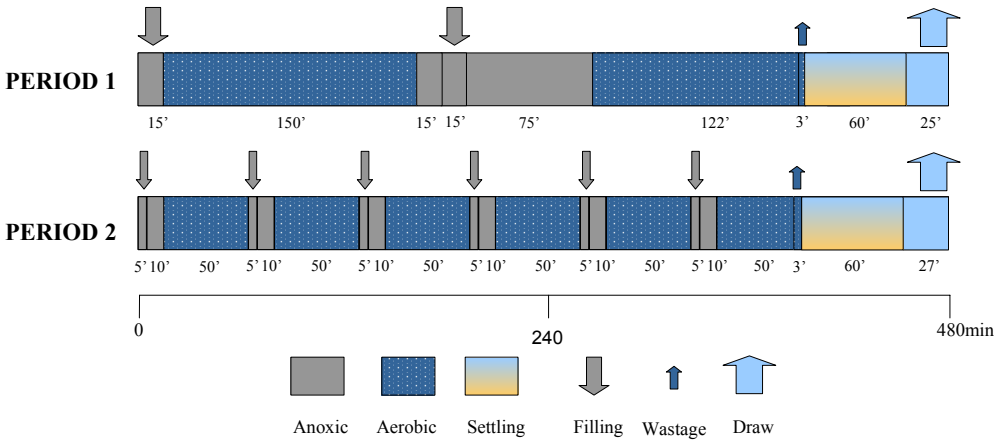


Figure 5-1. SBR cycle definition indicating anoxic, aerobic and filling phases for Periods 1 and 2.

Period 1 served as the first approach for defining the cycle for removing carbon and nitrogen and Period 2 represented the redefinition of the cycle to improve the efficiency of the process. The operating conditions are summarized in Table 5-1.

Table 5-1. Operating conditions applied in the lab-scale SBR

Description	Symbol	Units	Period 1	Period 2
Influent flow	Q_I	$L \cdot d^{-1}$	30	
Total cycle time	tc	H	8	
Volumetric exchange ratio	R_E	-	0.42	0.33
Minimum volume	V_{MIN}	L	14	20
Reaction time	t_R	H	6.58	6.55
Anoxic reaction time	%ANOXIC *	%	30.4	22.9
Aerobic reaction time	%AEROBIC *	%	69.6	77.1
Hydraulic Retention Time	HRT	d	0.8	1
Sludge Retention Time	SRT	d	18	18
Temperature	Temp	ºC	21	17.5

(* % Aerobic and Anoxic reaction times are calculated over the reaction time)

5.2.2. Synthetic wastewater

The synthetic wastewater was basically composed of a mixed carbon source, an ammonium solution, a phosphate buffer, alkalinity control ($NaHCO_3$) and a microelements solution (adapted from Dangcong *et al.*, 2000). The synthetic wastewater was prepared twice a week with a concentration of 650 $mg \cdot L^{-1}$ COD, 80 $mg \cdot L^{-1}$ TKN-N and 70 $mg \cdot L^{-1}$ NH_4-N. The composition is described in Table 5-2.

Table 5-2. Synthetic water composition

Concentration	Formula	Name	Solution
1.9 $mg \cdot L^{-1}$	CH_3COONa	Sodium acetate	Carbon source (~650 mg $COD \cdot L^{-1}$)
1.9 $mg \cdot L^{-1}$	CH_3CH_2COONa	Sodium propionate	
1.9 $mg \cdot L^{-1}$	$(C_6H_{10}O_5)n$	Starch	
1.9 $mg \cdot L^{-1}$	-	Tryptone	
0.14 $mL \cdot L^{-1}$	CH_3CH_2OH	Ethanol	
0.84 g	-	Dehydrated Meat Extract (DME)	
183 $mg \cdot L^{-1}$	NH_4Cl	Ammonium chloride	Ammonium source (~70 $mgNH_4$-$N \cdot L^{-1}$, ~80 mg TKN-$N \cdot L^{-1}$)
280 $mg \cdot L^{-1}$	$NaHCO_3$	Sodium bicarbonate	Alkalinity
0.19 $mg \cdot L^{-1}$	$MnCl_2.4H_2O$	Manganese (II)chloride tetrahydrate	Microelements solution
0.0018 $mg \cdot L^{-1}$	$ZnCl_2.2H_2O$	Zinc chloride dehydrate	
0.022 $mg \cdot L^{-1}$	$CuCl_2.2H_2O$	Copper (II) chloride dehydrate	
5.6 $mg \cdot L^{-1}$	$MgSO_4.7H_2O$	Magnesium sulphate heptahydrate	
0.88 $mg \cdot L^{-1}$	$FeCl_3.6H_2O$	Iron (III) chloride hexahydrate	
1.3 $mg \cdot L^{-1}$	$CaCl_2.2H_2O$	Calcium chloride dehydrate	
7.0 $mg \cdot L^{-1}$	KH_2PO_4	Potassium dihydrogen phosphate	Phosphate buffer
18 $mg \cdot L^{-1}$	K_2HPO_4.	Dipotassium hydrogen phosphate	
14 $mg \cdot L^{-1}$	$Na_2HPO_4 \cdot 7H_2O$	Disodium hydrogen phosphate heptahydrate	

5.3. CALIBRATION OF THE SBR PILOT PLANT

5.3.1. Simulation software

The model calibration and validation was conducted using the WEST software (Hemmis, NV, Kortrijk). The differential equations were integrated by means of a variable step-size 4th order Runge Kutta algorithm.

5.3.2. Calibration procedure

The BIOMATH protocol presented in Vanrolleghem *et al.*, (2003) and an extended version for SBR systems (Insel *et al.*, 2004) were adapted to systematize the calibration procedure.

The calibration protocol used in this study was divided into five stages: i) defining the target, ii) plant survey, iii) process characterization, iv) calibration, and v) evaluating the results. The main structure is very similar to the BIOMATH protocol. Nevertheless, modifications were applied in two of the stages:

- For the process characterization (stage iii) an alternative influent wastewater characterization was defined because respirometric analysis were not available.
- For the calibration step (stage iv) a methodology for obtaining better initial conditions for the dynamic calibration was applied.

In the stage iv, as in the BIOMATH protocol, two calibration steps were considered: the steady state and the dynamic. The steady state calibration is called stable-state calibration since the SBR is not considered to be in a strictly steady state because the variables change with time during the batch. In the SBR, stable-state means that the final conditions of one batch are equal to the final conditions of the next ones. The dynamic calibration is called cycle-evolution calibration because it is conducted using the data from a cycle measurement campaign.

The simulation procedure for the calibration is presented in Figure 5-2. First of all, a stable-state period was simulated using averaged concentrations and flows. This simulation was iteratively conducted until the long-term behaviour parameters related to both the sludge model and the settler were adjusted. Afterwards a daily evolution period was simulated where the dynamics of influent composition, flow and process performance were considered. The simulation of these two periods permitted obtaining proper initial conditions for the cycle evolution calibration. The longer this daily evolution period the closer to the reality can be the initial conditions. In this case, seven days of dynamic data were applied. Therefore, the history of the previous days to the cycle evolution period was transferred into the model.

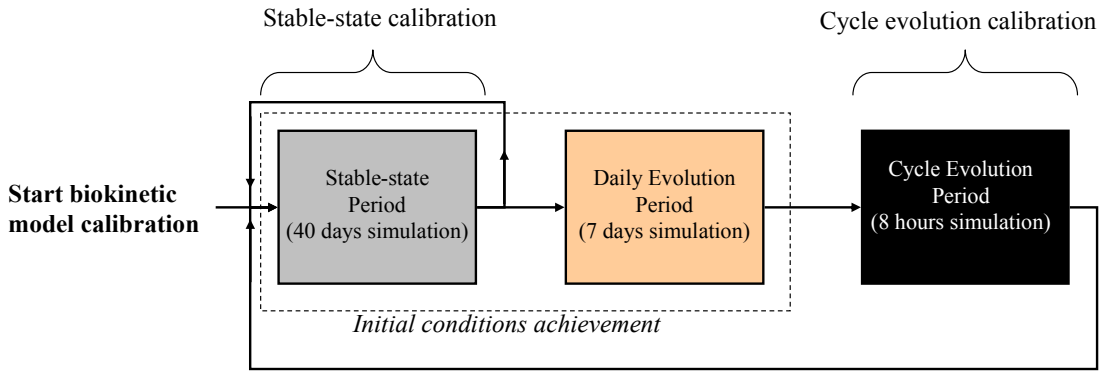


Figure 5-2. Simulation procedure for the calibration

Finally, the cycle evolution period was simulated and the parameters responsible for the dynamic behaviour of the plant performance were adjusted. Whenever a parameter was changed during this cycle evolution calibration the whole simulation for the three periods was conducted obtaining an iterative calibration procedure.

5.3.3. Step-wise model calibration

The different stages of the calibration procedure described above were followed in order to obtain a calibrated model of the lab-scale SBR. In the next pages the step-wise model calibration is presented in detail.

STAGE I

Defining the target

In the calibration protocol the first step is to define the target of the calibration, which will influence the other following steps. Therefore, what is going to be modeled and the application of the calibrated model should be clear.

In this work, the aim of the calibration was to obtain a model for evaluating control strategies for optimizing the SBR operation. The model was focused on carbon and nitrogen removal and therefore it was expected to describe the ammonia, the oxidized nitrogen and also the oxygen dynamics in the system.

STAGE II

Plant survey

Two data sets were available, thus one (obtained from Period 1) was used for the calibration and the other (obtained from Period 2) for the validation. These data sets included the operating conditions (see Table 5-1), the periodic analytics (from the influent, effluent and reactor or wastage) and the intensive monitoring during the measurement campaign, which consisted in obtaining the dynamic evolution of the nitrogen compounds and the physical-chemical parameters during one cycle of the SBR operation (see Table 5-3).

Table 5-3. Available analytical data for the two data sets.

Measurement	Influent	Effluent	Reactor/ wastage	Measurement campaign
COD	total, soluble	soluble	total	-
Nitrogen	TKN_T, NH_4^+, NO_2^-, NO_3^-	NH_4^+, NO_2^-, NO_3^-	-	NH_4^+, NO_2^-, NO_3^-
Solids	TSS	TSS	TSS, VSS	-
On-line measurements	-	-	pH, DO, ORP, Temp	pH, DO, ORP, Temp

STAGE III. Model structure and process characterization

Mass transfer

In the mass transfer characterization two main aspects have to be considered. The first one is determining the oxygen transfer efficiency (K_La) and the second aspect is the hydraulic characterization of the plant. This second aspect is not considered when dealing with the lab-scale SBR since ideal mixing can be assumed in this rigorously mixed small reactor.

As there is no dedicated experiment performed for determining K_La, then regular on-line dissolved oxygen measurements, which are available, can be used (Sin, 2004). In this way, the K_La values can be calibrated to fit the data during plant model calibration. As a first approach, the K_La value can be calculated using the following equations:

In a well-mixed region of a batch biological reactor the mass balance for dissolved oxygen without influent and effluent flow can be written as:

$$V\frac{dS_O}{dt} = K_La(S_{O,sat} - S_O)V + r_OV \qquad \text{Equation 5-1}$$

where: V=volume (m^3); S_O=dissolved oxygen concentration in the reactor ($gO_2 \cdot m^{-3}$); Q=influent flow rate ($m^3 \cdot d^{-1}$); $S_{O,in}$=dissolved oxygen concentration in the influent ($gO_2 \cdot m^{-3}$); K_La=oxygen transfer efficiency (d^{-1}); $S_{O,sat}$=saturation dissolved oxygen concentration ($gO_2 \cdot m^{-3}$); r_O=respiration rate ($gO_2 \cdot m^{-3} \cdot d^{-1}$).

Under aeration conditions the balance is expressed in Equation 5-2.

$$\left.\frac{dS_O}{dt}\right|_{ON} = K_La(S_{O,sat} - S_O) + r_O \qquad \text{Equation 5-2}$$

If the aeration is turned off, Equation 5-2 yields:

$$\left.\frac{dS_O}{dt}\right|_{OFF} = r_O \qquad \text{Equation 5-3}$$

Thus, assuming that just after aeration is stopped r_o remains unvaried, combining Equations 5-2 and 5-3 the K_La values can be calculated as presented in Equation 5-4.

$$K_La = \frac{\left.\frac{dS_O}{dt}\right|_{ON} - \left.\frac{dS_O}{dt}\right|_{OFF}}{S_{O,sat} - S_O} \qquad \text{Equation 5-4}$$

Since K_La is considered to be dependent on the volume (Makinia and Wells, 1999) and the SBR operating with the step-feed strategy changes the volume with time, it is necessary to correct K_La with the volume in the mass transfer model. Hence, a correction for the working volume was applied following Equation 5-5, in which $K_La(V)$ is the K_La for a given reactor volume, and $K_La(Vref)$ the K_La calculated at a reference volume.

$$K_La(V) = K_La(Vref)\cdot\frac{Vref}{V} \qquad \text{Equation 5-5}$$

K_La was also corrected in relation to the temperature in the mass transfer model following the Arrhenius expression presented in Equation 5-6 using the temperature correction coefficient (θ) of 1.024 which is typical for diffused aeration devices (Metcalf & Eddy, 2003).

$$K_La(V)^T = K_La(V)^{Tref}\cdot\theta^{(T-Tref)} \qquad \text{Equation 5-6}$$

In this case-study the oxygen profile obtained in the measurement campaign (presented in Figure 5-3) could be used for calculating K_La since:

- Continuous air was supplied during the aerobic phase.
- At the end of the aerobic phase all the substrates (COD, NH_4^+ and NO_2^-) were depleted.
- After the first aerobic phase there was an anoxic phase without filling, in which the oxygen concentration decreased due to endogenous respiration (r_O).

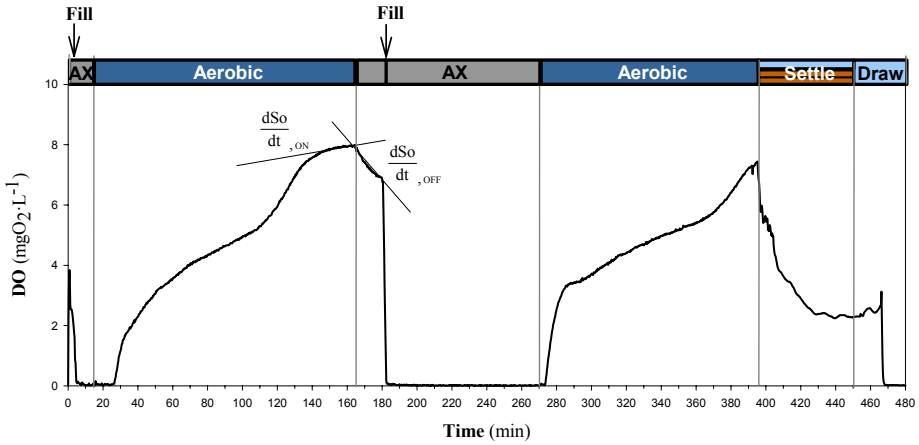


Figure 5-3. Dissolved oxygen profile during the measurement campaign.

Thus, the calculation of K_La was performed by applying Equation 5-4 to the first aerobic phase at a reference volume of 25L and a reference temperature of 21ºC.

$$K_La(25L)^{21ºC} = \frac{\left.\frac{dS_O}{dt}\right|_{ON} - \left.\frac{dS_O}{dt}\right|_{OFF}}{S_{O,sat} - S_O} = \frac{7.88gO_2 \cdot m^{-3} \cdot d^{-1} - (-358gO_2 \cdot m^{-3} \cdot d^{-1})}{(9.28-8)gO_2 \cdot m^{-3}} = 285d^{-1}$$

The value obtained for K_La also includes the effect of surface aeration. In small reactors with a high area/volume ratio this can have an important effect. This also implies that during the anoxic phases a small amount of K_La can be applied.

Settling characterization

The settling performance can influence the system's overall behavior. Therefore, modeling the settler has to be performed as close as possible to reality, but always considering the simplest solution. The most important aspects are the solids concentration in the effluent (related to the SRT of the system) and the reactions that can occur during the settling phase. The model for the settling phase is chosen depending on the need for a detailed settling characterization and on the necessity to consider biological reactions. In Figure 5-4 a decision tree for choosing the suitable settling model is presented.

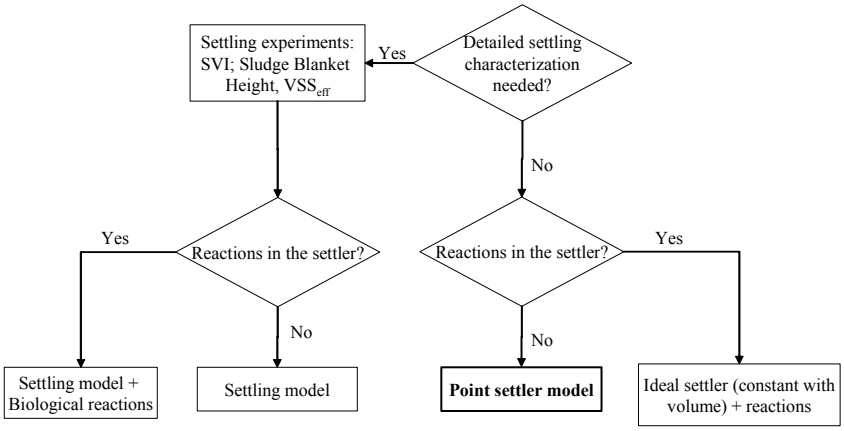


Figure 5-4. Decision tree for selecting the settling model (source: Vanrolleghem *et al.*, 2003).

In this study some problems were detected during the settling which made it advisable to perform a detailed settling characterization. Nevertheless, within the historical data there were no sedimentation experiments. Thus, it was decided to use the simplest settling model which is the point settler and check whether this was enough to describe the reality. On the other hand no indication of biological reactions was observed during settling and therefore the point settler was modeled without reaction.

Biological and influent wastewater characterization

- Selecting the biological model

The activated sludge models proposed by the IWA task group on mathematical modeling for design and operation of biological wastewater treatment (Henze *et al.*, 2000) have been successfully applied for modeling the biological reactions that occur in wastewater treatment plants. Selecting the model depends on the biological activity observed in the reactor and the processes and variables to be considered. A decision tree for choosing the model to use is presented in Figure 5-5.

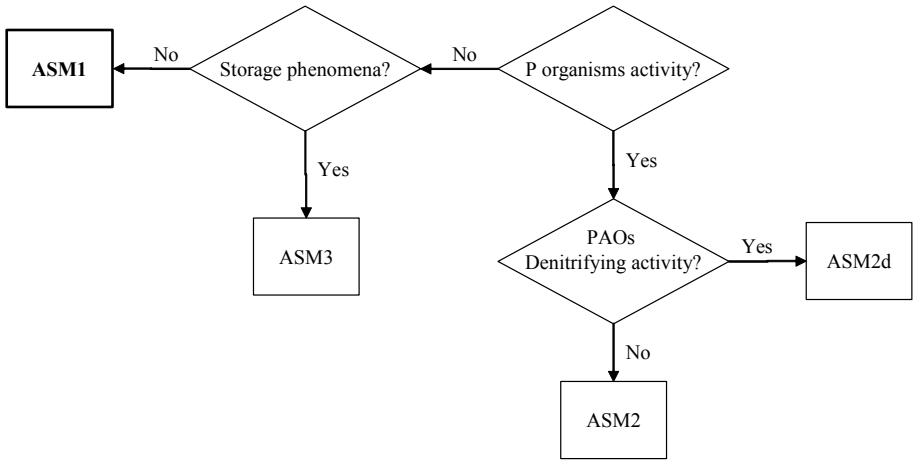


Figure 5-5. Decision tree for selecting the biological model (source: Vanrolleghem *et al.*, 2003).

The decision tree for selecting the biological model was followed. The objective of this study was focused on carbon and nitrogen removal and the operating conditions were established for this purpose. No experiments were available to observe storage phenomenon. Nevertheless, Koch *et al.* (2000) concluded that ASM1 and ASM3 are both capable of describing the dynamic behaviour in common municipal WWTPs. The ASM3 performs better in situations where the storage of readily biodegradable substrate is significant (industrial wastewater) or for WWTPs with substantial non-aerated zones. As this is not the case, it was decided to use the simplest model which is ASM1.

When implementing the model the effect of temperature on the kinetic parameters was considered by applying the Arrhenius equation. The default temperature coefficient factors of ASM1 were used.

- Influent wastewater characterization:

A physical-chemical approach (STOWA) combined with the sludge balance method by Henze *et al.* (1987) was used for the influent wastewater characterization. Figure 5-6 shows the relationship between the state variables and the analytical measurements for the organic matter fractionation. It has to be emphasized that the influent inert particulate COD, X_I, was adjusted during the calibration, as proposed by Henze *et al.*, (1987), by fitting the solids content of the reactor (MLSS).

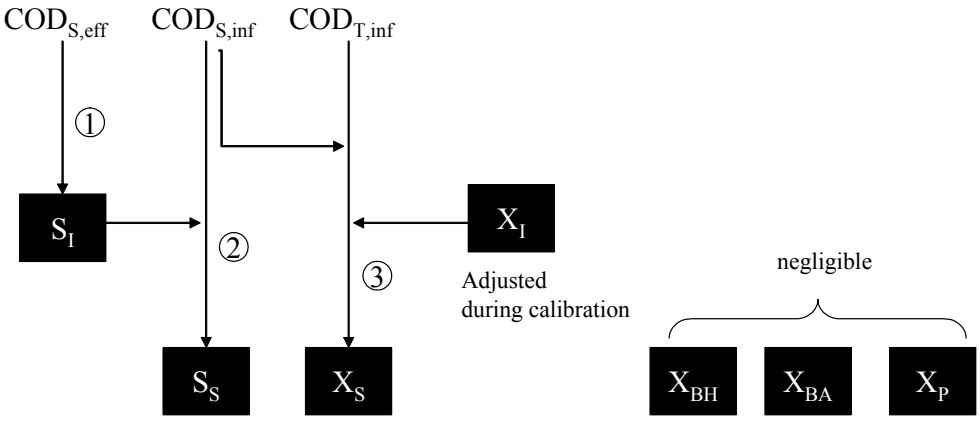


Figure 5-6. Organic matter fractionation.

The relationship between the nitrogen state variables and the analytical measurements is presented in Figure 5-7. The nitrogen fractionation is straightforward. S_{NH} is obtained directly from the ammonium measurement. The difference between TKN and ammonium is the organic nitrogen, which is divided into soluble organic nitrogen and particulate organic nitrogen. The division is done assuming the same percentage of soluble/particulate as in the organic matter fractionation.

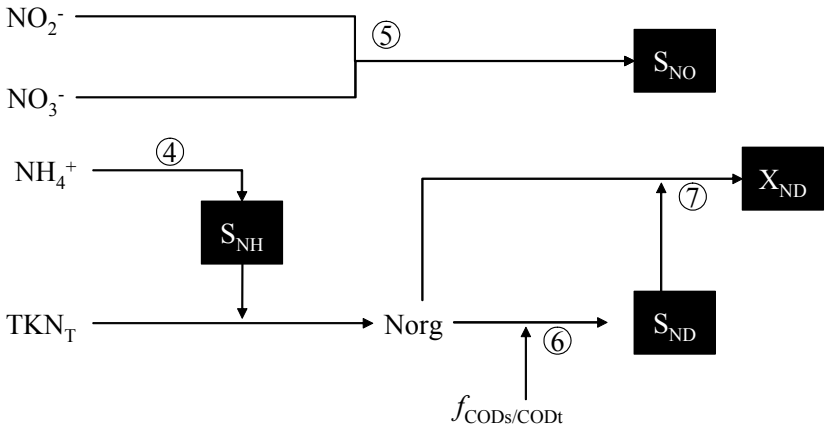


Figure 5-7. Nitrogen fractionation.

The equations used for the organic matter and the nitrogen fractionation are presented in Table 5-4.

Table 5-4. Equations used for the organic matter and nitrogen fractionation.

Definition (compounds)	Symbol	Units	Equation
Inert soluble organic	S_I	$gCOD \cdot m^{-3}$	$S_I = COD_{S,eff}$ (1)
Readily biodegradable organic	S_S	$gCOD \cdot m^{-3}$	$Ss = COD_{S,inf} - S_I$ (2)
Inert particulate organic	X_I	$gCOD \cdot m^{-3}$	X_I= adjusted
Slowly biodegradable organic	X_S	$gCOD \cdot m^{-3}$	$Xs = COD_{T,inf} - COD_{S,inf} - X_I$ (3)
Ammonium	S_{NH}	$gN \cdot m^{-3}$	$S_{NH} = NH_4^+$ (4)
Oxidized nitrogen	S_{NO}	$gN \cdot m^{-3}$	$S_{NO} = NO_2^- + NO_3^-$ (5)
Soluble organic nitrogen	S_{ND}	$gN \cdot m^{-3}$	$S_{ND} = (f_{CODs,inf/CODT,inf}) \cdot (TKN_T - NH_4^+)$ (6)
Particulate organic nitrogen	X_{ND}	$gN \cdot m^{-3}$	$X_{ND} = (TKN_T - NH_4^+) - S_{ND}$ (7)

(The numbers of the equations are related to Figures 5-6 and 5-7)

Based on this procedure the influent wastewater characterization of the calibration and validation periods in terms of average organic matter and nitrogen fractions for ASM1 is summarized in Table 5-5 and Table 5-6.

Table 5-5. ASM1 based influent wastewater characterization for the organic compounds.

	CALIBRATION		VALIDATION	
Analytical data	**Concentration ($mgCOD \cdot L^{-1}$)**	**(%)***	**Concentration ($mgCOD \cdot L^{-1}$)**	**(%)***
$COD_{T, inf}$	627.2	100.0	692.5	100.0
$COD_{S, inf}$	557.4	88.9	597.6	86.0
$COD_{P, inf}$	69.8	11.1	94.9	13.7
$COD_{S, eff}$	35.0	5.6	35.0	5.1
$BCOD_{inf}$	570.7	91.0	630.2	91.0
State variables				
S_S	522.4	83.3	562.6	81.2
S_I	35.0	5.6	35.0	5.1
X_S	48.4	7.7	67.6	9.8
X_I	21.4	3.4	27.3	3.9

* The percentage is with respect to the total influent COD.

It can be seen that the fraction of biodegradable organic matter is very high due to the large presence of readily biodegradable components in the synthetic wastewater (basically ethanol).

Table 5-6. ASM1 based influent wastewater characterization for the nitrogen compounds

	CALIBRATION		VALIDATION	
Analytical data	**Concentration ($mgN \cdot L^{-1}$)**	**(%)***	**Concentration ($mgN \cdot L^{-1}$)**	**(%)***
NH_4^+	71.59	90.10	67.70	87.69
TKN_T	79.05	99.50	76.80	99.48
NO_X^-	0.40	0.50	0.40	0.52
State variables				
S_{NH}	71.59	90.10	67.70	87.69
S_{ND}	6.63	8.30	7.85	10.17
X_{ND}	0.83	10	1.25	1.62
S_{NO}	0.40	0.50	0.40	0.52

* The percentage is with respect to the total nitrogen

STAGE IV. Calibration

The calibration procedure was divided in two parts: the stable-state calibration in which the volatile suspended solids (VSS) were fitted and the cycle evolution calibration in which nitrification and denitrification processes were adjusted. This process was structured in a step-wise methodology (Figure 5-8) refined from Insel *et al.* (2004). The default parameter values of ASM1 were taken as a starting point for the iterative calibration procedure.

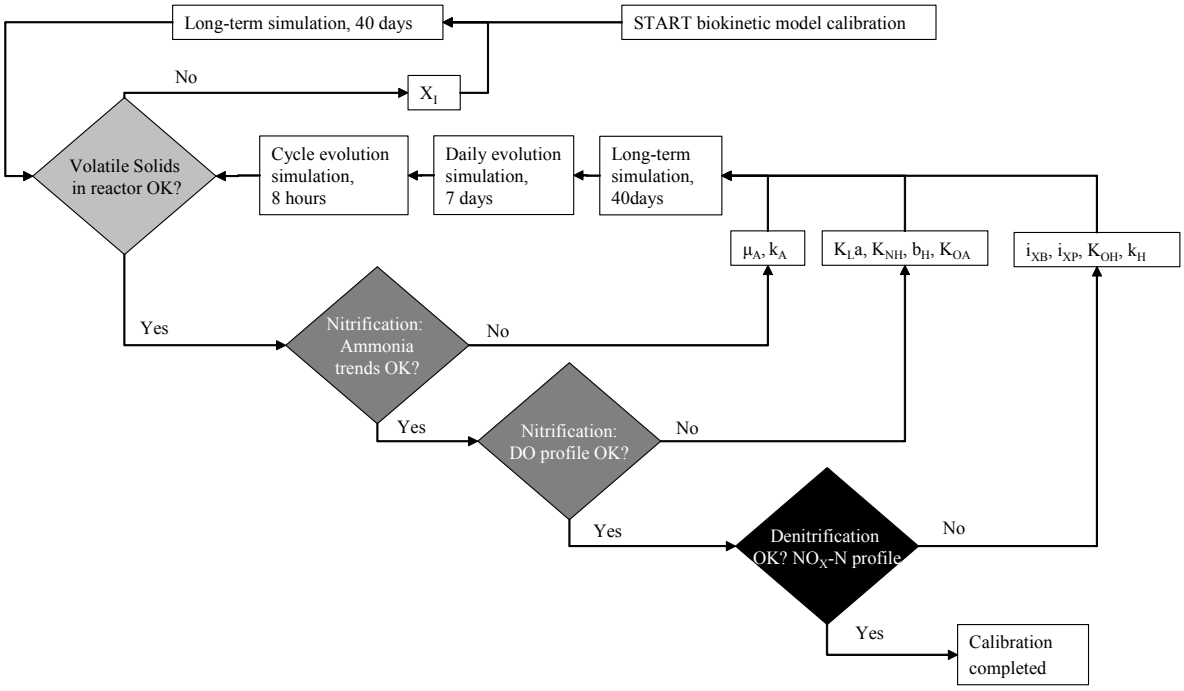


Figure 5-8. Calibration methodology for the ASM1 model (Adapted from Insel *et al.*, 2004).

Stable-state calibration

The objective of the stable-state calibration is to adjust the solids concentration of the reactor and effluent. This was done by simulating the stable-state period (Figure 5-2), in which influent composition and flows were averaged and the long-term behavior parameters were adjusted.

In this case, three parameters were implied in this stable-state calibration: the non-settleable fraction (f_{ns}), influent particulate inert fraction (X_I) and the heterotrophic decay rate (b_H). First of all, the f_{ns} was fixed using the experimental values of the effluent VSS concentration. Then, for a fixed value of b_H the X_I was adjusted until a good fit to the reactor MLVSS concentration was achieved. If the b_H was modified (see cycle evolution calibration) the X_I was readjusted. Thus, in order to fit the solids concentration in the SBR, which was around 2300 mg VSS·L^{-1} in stable conditions, an f_{ns} of 0.035 had to be applied and the X_I was adjusted to 21.4 mg COD·L^{-1} (3.4% of the total influent COD), for a final b_H value of 0.25.

After adjusting the solids concentration the iterative procedure could continue. Thus, the daily evolution simulation was done (see Figure 5-2) in this case with the purpose of adjusting a phenomenon of solids washout. During the daily simulation the f_{ns} was changed according to the experimental data because there was a decrease in the solids concentration due to problems in the settling 7 days before the measurement campaign. Therefore, an f_{ns} of 0.2 was used for 4 days and then the value of 0.035 was applied for the three days before the measurement campaign to allow the solids concentration to recover. This daily evolution period permitted us to achieve proper initial conditions for the cycle evolution calibration. Therefore, it was possible to describe the process taking into account the importance of the settling, which influenced the overall system behavior.

Cycle evolution calibration

The objective of the cycle evolution calibration is to adjust the parameters related to the short-term behavior of the plant (e.g. parameters of the nitrification and denitrification processes). This was done through the simulations conducted in the cycle evolution period after performing the stable-state period simulation and the daily simulation to achieve proper initial conditions (see Figure 5-2).

In the cycle evolution period the simulated dynamics of ammonium, oxidized nitrogen and dissolved oxygen were fitted to the experimental values following the methodology presented in Figure 5-8.

Before going into detail about the parameters adjusted during the cycle evolution calibration it should be mentioned that the biological model had to be modified in order to describe the

ammonium dynamics of the system properly. This was observed after the first simulations with the ASM1 default values. The modifications were the following:

1) Both heterotrophic aerobic and anoxic growth rates were dependent on the ammonium concentration. Low concentrations of ammonium are achieved inside the SBR during aerobic phases and the lack of ammonium to be assimilated represents a limitation for the growth of the microorganisms.

Aerobic heterotrophic growth rate:

ASM1	This model
$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{S_o}{K_o+S_o}\right)X_{BH}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{S_o}{K_o+S_o}\frac{\mathbf{S_{NH}}}{\mathbf{K_{NH}}+\mathbf{S_{NH}}}\right)X_{BH}$

Anoxic heterotrophic growth rate:

ASM1	This model
$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{K_O}{K_O+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{BH}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{K_O}{K_O+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\frac{\mathbf{S_{NH}}}{\mathbf{K_{NH}}+\mathbf{S_{NH}}}\right)\eta_g X_{BH}$

2) Hydrolysis was assumed to be independent from the electron acceptor as in ASM3 (Henze *et al.*, 2000). In the second anoxic phase of the measurement campaign it was observed that hydrolysis should continue, even when the oxidized nitrogen was finished. Otherwise, the ammonium profile decreased too much because the assimilation was not compensated by the hydrolysis of nitrogen released after decay.

Hydrolysis rate:

ASM1	This model
$K_H\frac{X_S/X_{BH}}{K_X+X_s/X_{BH}}\left[\left(\frac{S_O}{K_{OH}+S_O}\right)+\eta H\left(\frac{K_{OH}}{K_{OH}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\right]X_{BH}$	$K_H\frac{X_S/X_{BH}}{K_X+X_s/X_{BH}}X_{BH}$

After modifying the biological model, the cycle evolution calibration could continue iteratively as part of the model calibration. The next step was to adjust nitrification (see Figure 5-8). Hence, the ammonium and oxidized nitrogen trends during the aerobic phases were fitted. First of all, the ammonification process was accelerated by increasing k_A, to make the organic nitrogen in the influent available for nitrification. This increase is normal since in ASM3 this process is not considered because it is very fast. During the aerobic phases the measured ammonia oxidation and the NO_X-N production rates, i.e. derivative of the change of the measured concentrations, were adjusted by increasing the maximum specific nitrification rate

(μ_A). In this case the absolute measurements of the NO_X-N concentration at the end of the phase were trusted more than the absolute measurements of ammonium, which were used for qualitative comparison reasons with the model predictions.

The next step in order to adjust the nitrification was to check the oxygen profile (see Figure 5-8), as it contains significant information. The importance of the DO profile has already been presented by Olsson and Andrews (1978). First of all, the K_La of the first aerobic phase was adjusted by fitting the magnitude of the DO profile using the experimentally obtained value of $285d^{-1}$ as the initial approach. A small value of K_La was also applied during the anoxic phases to account for the superficial aeration effect. Then, the K_{OA} was reduced because nitrification was observed to be less limited by oxygen when low values of oxygen were detected. Afterwards, the K_{NH} was increased in order to properly describe the nitrification process at the end of the aerobic phase, when the ammonia as substrate was limiting. The value of b_H was adjusted taking into account the drop in dissolved oxygen concentration during the second anoxic phase before the second feeding (see Figure 5-3). During this short period, there was no presence of organic matter and ammonium, therefore oxygen consumption was mainly related to endogenous respiration. In this case, the b_H was decreased because the oxygen drop was too sharp. This modification in the b_H, implied that the value of X_I had to be modified accordingly, to adjust the solids concentration during the stable-state simulation (see stable-state calibration).

Denitrification was adjusted through the NO_X-N profile in the anoxic phases. The main limitation in the denitrification process is the availability of readily biodegradable substrate, which depends on the influent wastewater characterization and on the hydrolysis process. In this case the NO_X-N trends were properly described, especially because the hydrolysis and heterotrophic anoxic growth were predicted well using the ASM1 default values.

Nevertheless, to adjust the oxidized nitrogen profile (NO_x-N) it was found that more nitrogen was needed in the reactor and this was directly related to the nitrogen content of the biomass. The nitrogen content of the reactor biomass was also checked showing that the assimilation was too high. Therefore, the nitrogen content assimilated during microbial growth was decreased by reducing the values of the nitrogen content of the biomass (i_{XB}) and the nitrogen content of the biomass that comes from endogenous products (i_{XP}). In principle, the BIOMATH protocol (similarly to the others) recommends performing this check during the stable-state calibration when the initial sludge composition of the plant is estimated. However, since no total nitrogen measurement was available, this check could not be performed in the steady state calibration.

Finally, Figure 5-9 presents the experimental and simulated values of the cycle evolution period after applying the calibration procedure explained above. The evolution of nitrogen compounds is presented in the upper part, and the dissolved oxygen evolution in the lower part of the graph.

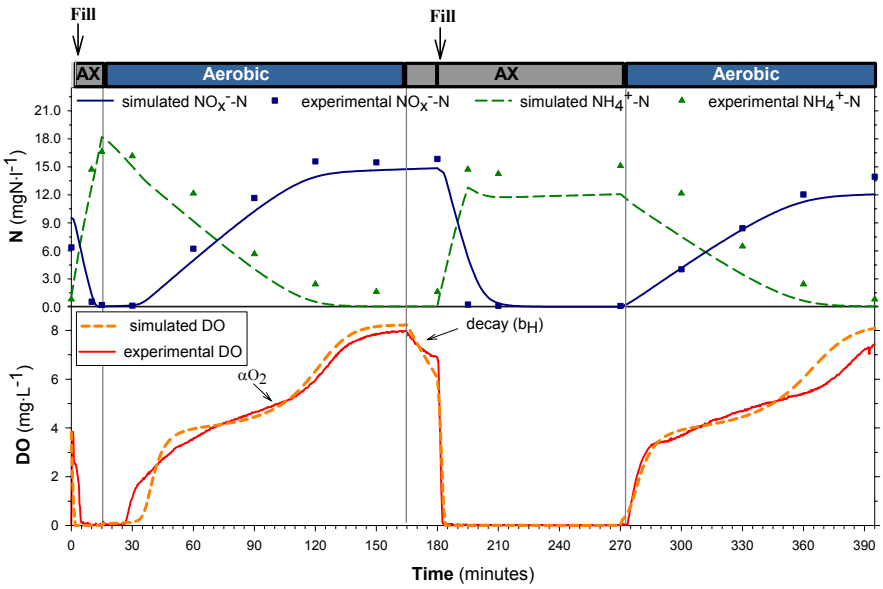


Figure 5-9. Experimental vs. simulation results of the cycle evolution calibration during reaction.

An evaluation of the fit shown in Figure 5-9 is now presented. Good matches were observed for the ammonium and oxidized nitrogen profiles, particularly between the experimental and simulated oxidized nitrogen (NO_X-N). However, the simulated ammonium was always found below the experimental data (see Figure 5-9-Top). In fact, in this study, NH_4-N measurements during aerobic phases of the cycle were felt to be inaccurate because the initial NH_4-N at the beginning of the aerobic phase was not recovered as NO_X-N at the end of the aerobic phase. Therefore, as stated before, the absolute measurements of the NO_X-N concentration at the end of the aerobic phase were trusted more and used when calibrating the nitrification process, whereas the ammonium measurements were used for qualitative comparison reasons with the model predictions.

The simulated oxygen dynamics closely followed the measured oxygen dynamics in the reactor, particularly in the first aerobic phase (see Figure 5-9-bottom). In the second aerobic phase, the model mismatch between the measurements increased slightly, although the model remained capable of following the dynamic dissolved oxygen trends.

In Table 5-7 the calibrated parameters are presented and compared with the ASM1 default values. All calibrated values are in the range reported in the literature. Only the b_H is low, but it is within the range between 0.05 and 1.6 reported in Hulsbeek *et al.* (2002). In addition, it has been demonstrated that the kinetics and stoichiometry may vary drastically in SBRs in comparison with continuous feeding reactors (Oles and Wilderer, 1991). Similar low values of b_H have been obtained in similar studies. For instance, Avcioglu *et al.* (1998) presented a value of 0.235 d^{-1} and in Wichard (2001) a value of 0.17 d^{-1} was obtained. Thayalakumaran *et al.* (2003) used a value of 0.24 for calibrating ASM1 in an SBR.

Table 5-7. ASM1 parameters: default (20ºC) and calibrated values.

Parameter	Symbol	Unit	default	calibration
Ammonification rate	k_a	L/(mgCOD·d)	0.08	0.1
Heterotrophic decay coefficient	b_H	d^{-1}	0.62	0.25
Autotrophic maximum growth rate	μ_A	d^{-1}	0.80	0.95
Ammonium substrate saturation constant for nitrifiers	K_{NH}	mg NH_3-N/L	1.0	1.3
Heterotrophic oxygen substrate saturation constant	K_{OH}	mgO_2/L	0.2	0.15
Nitrifiers oxygen substrate saturation constant	K_{OA}	mg O_2/L	0.4	0.1
Hydrolysis rate constant	k_H	d^{-1}	3	2
g N(g COD)$^{-1}$ in biomass	i_{XB}	mg N/mg COD	0.086	0.06
g N(g COD)$^{-1}$ in endogenous mass	i_{XP}	mg N/mg COD	0.06	0.05
Oxygen mass transfer coefficient (1st aerobic phase)	K_La	d^{-1}	-	266
Oxygen mass transfer coefficient for anoxic phases	K_La AX	d^{-1}	-	12

Validation

The data set used for the validation was taken from Period 2 (see Table 5-1) in which the SBR system was operated using a strategy that is fundamentally different from the one used in the calibration period. A six step-feed strategy cycle was applied alternating anoxic and aerobic phases. The volumetric exchange ratio was decreased to 0.33 and the temperature decreased to a mean value of 17.5ºC. Due to changes in the aeration system and in the minimum volume the K_La for the first aerobic phase was decreased to 170 d^{-1}. Thus, 40 days were simulated taking as the initial conditions the final values of the cycle-evolution calibration using an averaged influent (see Table 5-5 and Table 5-6). Then, using a second measurement campaign of a cycle the experimental and simulated NO_x-N and DO profiles could be compared (see Figure 5-10).

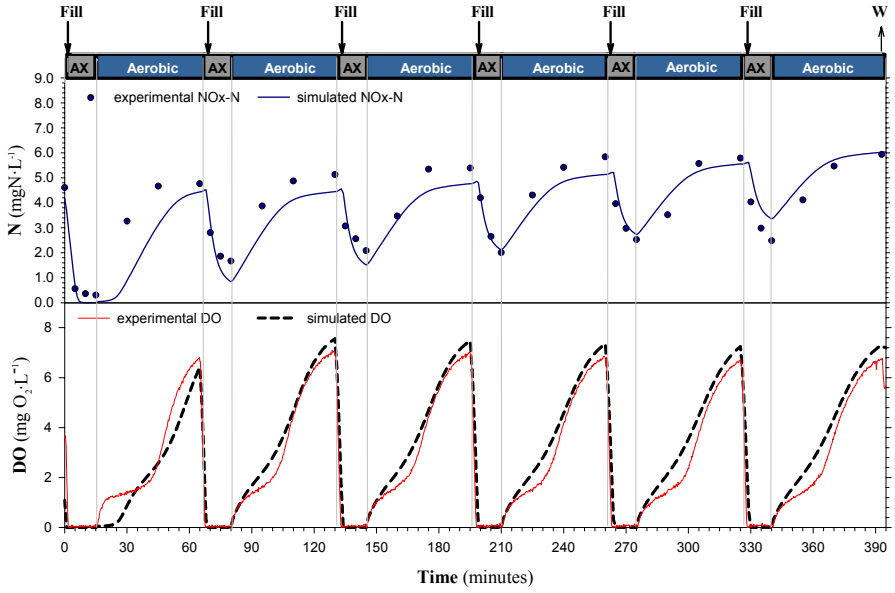


Figure 5-10. Experimental versus simulations for the model validation step.

It can be seen in the validation that there is a very good fit between the experimental and simulated values not only for the NO_X-N profile but also for the oxygen profile.

The influence of reactor volume on K_La

The oxygen profile is very sensitive to the values of K_La and DO saturation. The SBR operation cycle used for the validation had six feeding steps and thus the volume increased by 33%. In this operation mode it was observed that the effect of the changing reactor volume became pronounced in the K_La of the system. This is further illustrated in Figure 5-11 in which the simulated DO profiles with a constant value of K_La and K_La with volume correction ($K_La(V)$) together with the volume are presented. From a parameter identification point of view, this makes it necessary to correct the K_La value in the model. Otherwise the error of an incorrectly modeled K_La would most probably be propagated to other parameters of the model (Dochain and Vanrolleghem, 2001) leading to undesirable consequences, i.e. a poor validity of the model.

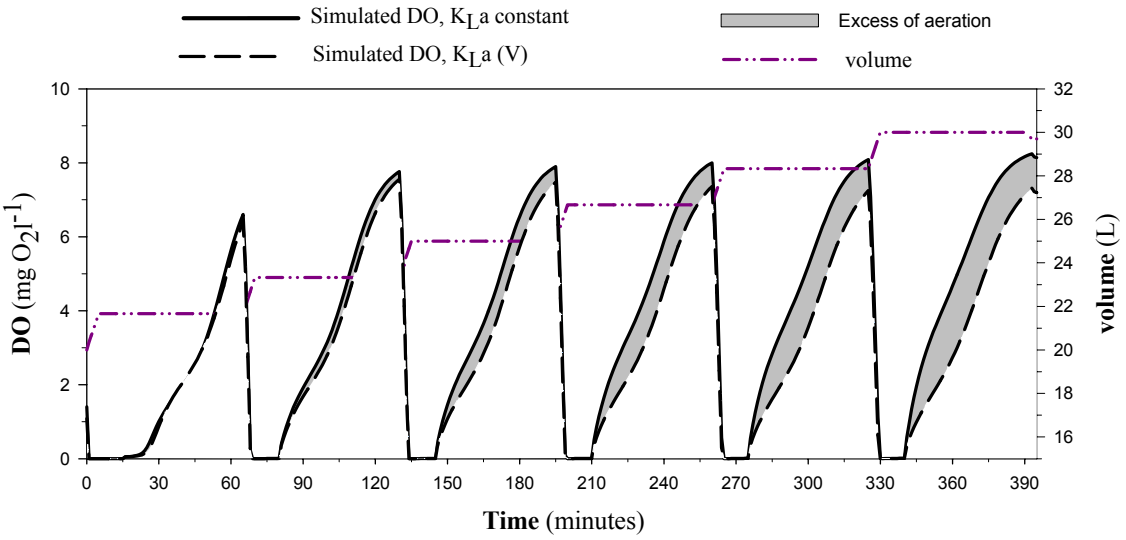


Figure 5-11. Influence of the reactor's volume on K_La.

The error of a fixed K_La assumption is observed to be proportional to the volume of the reactor (see grey colored area in Figure 5-11). Therefore, Equation 5-5 is proved to be necessary for the correct calibration.

STAGE V. *Evaluation*

The quality of the fit between the simulated values and the experimental data was evaluated by calculating the Average Relative Deviation (ARD).

$$ARD = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\left|X_{i,exp} - X_{i,sim}\right|}{X_{i,exp}}\right) \qquad \text{Equation 5-7}$$

where, $X_{i,\,exp}$ is the experimental value and $X_{i,\,sim}$ is the simulated value.

For calibrating the ammonia and oxidized nitrogen the ARD was 27% and 21% respectively. The ARD for the dissolved oxygen profile was calculated only during aerobic conditions obtaining a value of 11%. The ARD values for the validation profile were 14% for NO_x-N and 9% for dissolved oxygen. All these values are close to the values considered acceptable in Petersen *et al.* (2002). These results mean that the simulated and experimental values are close and hence, it is possible to use this model to define and test control strategies.

Therefore, using only historical data for calibrating an SBR has proved to be enough to accomplish the proposed objective. Thus, this calibration experience shows some strengths which can be considered for further calibration experiences:

- The step wise procedure for the whole calibration procedure is very useful.
- Defining the daily evolution period after the stable-state calibration and before the cycle calibration is necessary to obtain the initial conditions for the dynamic simulation properly, especially when the system is not under stable-state conditions. It is important to properly integrate the history of the system into the model calibration.
- Using the DO dynamics in the calibration process represents an advantage, because the oxygen profile is a good source of information on the rates of the process; not only for the aerobic parameters, but also for the decay and estimating the K_La.
- The ARD index can be useful for evaluating the success of the calibration by measuring the error between the experimental and simulated values.

For further calibration experiences and when the plant is running, some improvements in the methodology have been identified, which can make generalizing the final result and the extrapolation to other plants easier:

- Before the plant survey and data analysis it is necessary to define the experimental data collection.
- Regarding the process characterization (Stage III) several improvements can be applied:
    - The wastewater characterization should be accurately performed. An improvement could be achieved by experimentally determining the S_S fraction and also the biodegradable fraction of the total COD (BCOD).
    - The i_{XB} and i_{XP} fractions should be adjusted during the long-term calibration through the reactor TKN measurements.
    - Whenever possible, experimentally determining some parameters of the model could reduce the uncertainty for the assumed model parameters and could make the calibration procedure easier. For instance, expert-feeling gives indication that b_H and heterotrophic yield (Y_H) are key parameters for the calibration task, and their

experimental determination could help in both the stable-state and cycle calibration steps.

- When dealing with the calibration of the selected model (Stage IV) one point could help in improving the procedure:

    - The validation step, which is considered within the calibration Stage, could be improved in order to increase the reliability for model predictions. Apart from extrapolate the model for different operating conditions it is proposed to assess the validity of the model in the period of time between the measurement campaign used for calibration and the measurement campaign used for validation purposes. This also implies gathering more data during this period.

5.4. CONCLUSIONS

The use of only historical data has permitted to obtain a calibrated model for the SBR removing carbon and nitrogen, achieving the goals proposed at the beginning of the calibration procedure. From the whole experience the next conclusions are also remarkable:

1. The calibrated ASM1-based model obtained in this work provided a good description of the dynamics of carbon and nitrogen removal in an SBR reactor. Therefore it can be used for defining and testing control strategies.
2. A calibration procedure adapted from the BIOMATH protocol was successfully applied to the calibration with historical data, and only a few parameters were adjusted.
3. The majority of the parameters were calibrated using the DO profile ($k_{a,}$ b_H, K_{NH}, K_{OA}, K_La), which contains considerable information concerning the nitrification and decay processes.
4. The dependence of K_La on the volume of the reactor was clearly observed when the reactor volume changed due to the step-feed nature of the influent feeding. This volume effect was taken into account by using a linear function which was observed to work successfully.
5. In addition, the model was validated using a data set from the lab-scale SBR run with an operation strategy that is significantly different from the calibration period thereby increasing the confidence into the model.
6. The evaluation of the calibration procedure allowed detecting some strengths and weaknesses that can help with future calibration experiences.

6 Improving the SBR model calibration with a predefined experimental data collection

6. IMPROVING THE SBR MODEL CALIBRATION WITH A PREDEFINED EXPERIMENTAL DATA COLLECTION

6.1. MOTIVATION

The motivation of this Chapter is to calibrate an activated sludge model that can be further used for supporting a supervisory control system of the SBR. Hence, it is necessary to describe the SBR process performance accurately, describing properly the concentrations of the nitrogen and dissolved oxygen compounds.

To increase the reliability on the model, an accurate procedure is followed, considering the improvements detected in the previous calibration experience. This procedure may permit establishing a straightforward calibration protocol to be used for both new calibration experiences and recalibrations of the actual model.

6.2. THE SBR PILOT PLANT

The lab-scale SBR pilot plant described in Chapter 3 was used and synthetic wastewater was fed into it. The operating conditions, the cycle structure and the composition of the synthetic wastewater in this particular study are explained below.

6.2.1. Operating conditions and cycle definition

In this study 7L of wastewater per cycle were treated in the lab-scale SBR using a cycle of 8 hours divided into reaction (425 minutes), settling (40 minutes) and discharge (15 minutes). The step-feed strategy for nitrogen removal described in the introduction was applied with four filling events and alternating anoxic and aerobic conditions (see Figure 6-1). Feeding of the SBR was split into four parts (2L+2L+2L+1L) so that the last filling volume was half the size of the others to ensure low values of nitrogen concentration in the discharge due to the dilution effect.

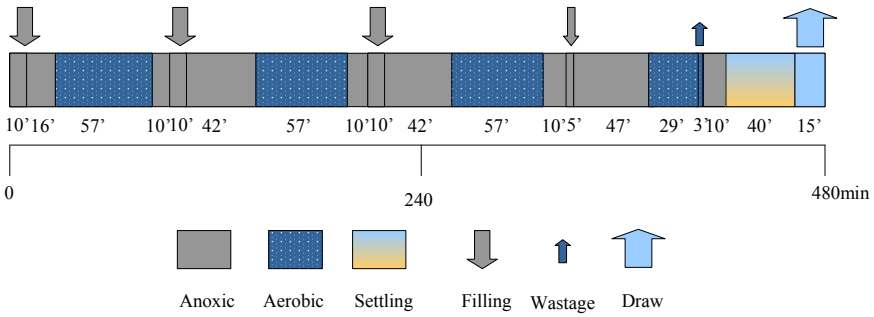


Figure 6-1. SBR cycle definition indicating anoxic, aerobic and filling phases.

After the aerobic phases and prior to filling there were ten-minute long anoxic phases which were useful for obtaining information about the decay rate (see Figure 5-9). During aerobic

phases a dissolved oxygen On-Off controller was implemented establishing a set-point at 2mgDO·L^{-1}. The operating conditions are summarized in Table 6-1.

Table 6-1. Operating conditions applied.

Description	Symbol	Units	Values
Influent flow	Q_I	$L \cdot d^{-1}$	21
Total cycle time	Tc	h	8
Volumetric exchange ratio	R_E	-	0.30
Minimum volume	V_{MIN}	L	16
Reaction time	t_R	h	7.08
Anoxic reaction time	%ANOXIC *	%	52
Aerobic reaction time	%AEROBIC *	%	48
Hydraulic Retention Time	HRT	d	1.1
Sludge Retention Time	SRT	d	15
Temperature	Temp	ºC	18.4

(* % Aerobic and Anoxic reaction time are calculated over the reaction time)

6.2.2. Synthetic wastewater

The composition of the synthetic wastewater used in this study was similar to the one used in the previous calibration experience. It is presented in Table 6-2 and consisted of a mixture of carbon source, ammonium source, alkalinity solution, microelements solution and phosphate buffer.

Table 6-2. Synthetic water composition.

Concentration	Formula	Name	Solution
0.27 mL·L^{-1}	CH_3CH_2OH	Ethanol (96%)	Carbon source
13.3 mL·L^{-1}	-	Leachate	
0.4 mL·L^{-1}	-	Milk	
0.56 g	-	Dehydrated Meat Extract (DME)	
183 mg·L^{-1}	NH_4Cl	Ammonium chloride	Ammonium source (~70 mg NH_4-N·L^{-1}, ~80 mgTKN-N·L^{-1})
280 mg·L^{-1}	$NaHCO_3$	Sodium bicarbonate	Alkalinity solution
0.19 mg·L^{-1}	$MnCl_2.4H_2O$	Manganese (II)chloride tetrahydrate	Microelements solution
0.0018 mg·L^{-1}	$ZnCl_2.2H_2O$	Zinc chloride dihydrate	
0.022 mg·L^{-1}	$CuCl_2.2H_2O$	Copper (II) chloride dihydrate	
5.6 mg·L^{-1}	$MgSO_4.7H_2O$	Magnesium sulphate heptahydrate	
0.88 mg·L^{-1}	$FeCl_3.6H_2O$	Iron (III) chloride hexahydrate	
1.3 mg·L^{-1}	$CaCl_2.2H_2O$	Calcium chloride dihydrate	
7.0 mg·L^{-1}	KH_2PO_4	Potassium dihydrogen phosphate	Phosphate buffer
18 mg·L^{-1}	K_2HPO_4.	Dipotassium hydrogen phosphate	
14 mg·L^{-1}	$Na_2HPO_4.7H_2O$	Disodium hydrogen phosphate heptahydrate	

Nevertheless, the carbon source was modified in this study to obtain synthetic wastewater with fractions that are closer to real wastewater. Typical fractions of S_S in domestic wastewater

treatment plans are between 10 and 40% (Roeleveld and Van Loosdrecht, 2001), and the influent S_S obtained in the previous study was close to 80%, which is far from the real wastewater values. Therefore, it was decided to increase the fraction of slowly biodegradable organic matter and decrease the fraction of readily biodegradable organic matter. In this case the carbon source consisted of ethanol, milk, dehydrated meat extract and leachate.

6.3. CALIBRATION OF THE SBR PILOT PLANT

6.3.1. Simulation software

The model calibration and validation were conducted using the GPS-X software (Hydromantis). The differential equations were integrated by means of a variable step-size fourth order Runge Kutta algorithm.

6.3.2. Calibration procedure

The general structure of the BIOMATH protocol was followed in this calibration study. Nevertheless, some modifications were applied such as the influent wastewater characterization which was conducted according to the STOWA protocol. The improvements detected in the calibration presented in Chapter 5 were also taken into account in this experience.

The calibration procedure scheme followed in this study is presented in Figure 6-2. The step-wise model calibration was divided into five stages: i) target definition and decisions about the information needed, ii) plant survey and data analysis, iii) model structure and process characterization, iv) calibration and validation and v) evaluation. Each stage was divided further to obtain eight steps which are explained and executed in detail in the next points.

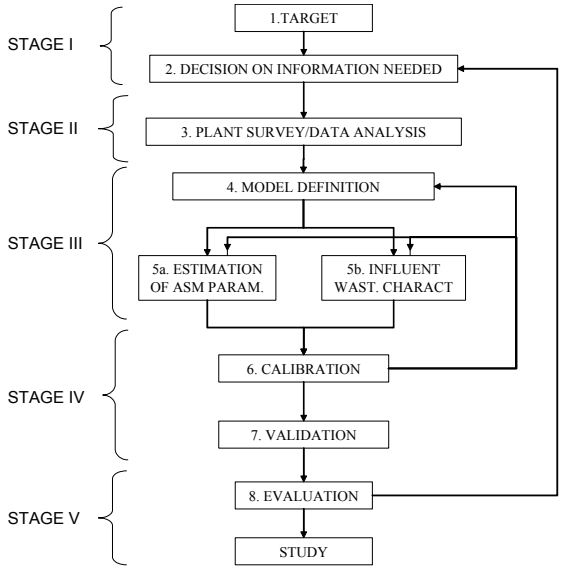


Figure 6-2. Calibration procedure.

The three first stages were used to gather data, get information about the process and construct the model. The simulations start in Stage IV, running the model over three periods (stable-state, daily evolution and cycle evolution), as in the methodology presented in Chapter 5 (see Figure 5-2). In this case study, the periodic variation in the influent composition, due to the degradation in the influent tank, was also taken into account during the stable-state period simulations.

6.3.3. Step-wise model calibration

In this point the step-wise model calibration of the lab-scale SBR plant is explained in detail following the eight steps of the calibration protocol: 1) Target definition, 2) Decision about the information needed, 3) Plant survey/Data analysis, 4) Model definition, 5) Process characterization (subdivided into 5a) parameter estimation and 5b) influent wastewater characterization), 6) Calibration, 7) Validation, and 8) Evaluation.

STAGE I

1. Target definition

In this case study the target of the calibration was to obtain a model basically focused on carbon and nitrogen removal that is able to describe the dynamic behaviour of the SBR. The model was expected to describe the ammonia, the oxidized nitrogen, the oxygen dynamics in the system, and the evolution of the solids concentration in the reactor.

2. Decision about the information needed

This step considers everything related to planning the calibration procedure. On the one hand, the logistic aspects such as the equipment and material used, timing and software are considered, and on the other hand, there is the planning of the information needed about the plant, and especially the decision about monitoring intensity.

Table 6-3 presents a list of the measurements to be conducted during the three periods considered in this study, together with the periodicity. The list is also divided into the measurements sampled from the influent wastewater, from the reactor during the operation, and the ones sampled from the discharged effluent. The data provided by the on-line sensors (DO, pH and ORP and Temp) located inside the reactor are also considered.

During the stable-state period, periodic analysis of the organic and nitrogen compounds evolution in the influent and effluent can be performed. Then, during the daily evolution period, intensive monitoring is required for approximately one week, which is useful for the influent wastewater characterization. Afterwards, it is necessary to perform a measurement campaign. In the case of SBRs this measurement campaign is based on the evolution of nitrogen compounds during one cycle, taking samples at short time intervals.

Table 6-3. Plan of the data required for the calibration.

Measurements		Stable-state	Daily evolution	Cycle evolution
- Influent				
COD (total, filtrated(0.1µm))		3 times/week	daily	1 sample (replicate)
Nitrogen (TKN, NH_4^+,NO_2^-, NO_3^-)				
BOD		1 time	-	-
TSS, VSS		2 times/week	2 times/week	
- Effluent				
COD (soluble)		2 times/week	4 times/week	
Nitrogen (NH_4^+, NO_2^-, NO_3)				
TSS, VSS		2 times/week	3 times/week	
- Reactor/wastage				
COD	**Total**	1 time/week		
	Soluble	1 time/week		
Nitrogen	**TKN**	1 time/week		
	NH_4^+, NO_2^-, NO_3	1 time/week		Every 5, 10 or 15 min.
TSS, VSS		2 times/week	2 times/week	1 sample
On-line (DO, pH, ORP, Temp)				Every 10 seconds

STAGE II

3. Plant Survey/Data analysis

The information was collected (if available) or generated. The plant survey was divided into i) complete process description, ii) the SBR's performance and iii) the measurement campaign. An analysis of the data in all these steps was performed.

3.a. Plant survey (Data collection/generation)

Design data and operating conditions were collected. Periodic analysis were conducted following the planning of Table 6-3 and two measurement campaigns were performed within the studied period. Moreover, activated sludge was taken from the reactor during calibration period to conduct batch experiments to obtain information about kinetic and stoichiometric parameters.

Process description

A complete description of the plant was done in terms of the physical characteristics and the operational data. This information consisted in working volume, type of aeration, volumetric exchange ratio, flow rates, SRT, HRT, and also the description of the phase scheduling of the SBR cycle. This information has been already presented in point 2 of this Chapter.

The SBR's performance

The performance of the plant was assessed using analytical measurements and data from on-line sensors. Analyzing the evolution of the COD and nitrogen concentrations in the influent and effluent permits us to know the state of the process at any operating time.

Figure 6-3 shows the evolution of the COD and nitrogen compounds in the influent and effluent, the evolution of total and VSS in the reactor and total suspended solids in the effluent and the temperature of the reactor.

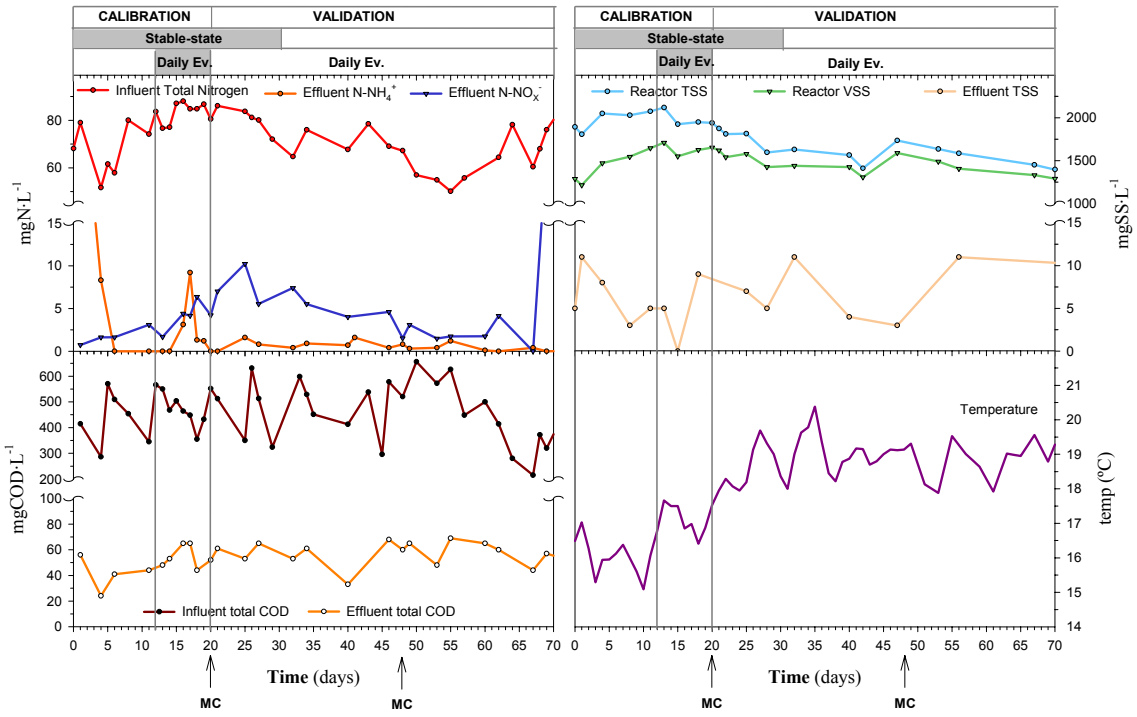


Figure 6-3. Evolution of the COD and nitrogen in the influent and effluent (left); Evolution of total and VSS in the reactor and total suspended solids in the effluent and the temperature of the reactor (right). MC: Measurement campaign.

Although synthetic wastewater was used, high variability was observed in the influent. This is related to the degradation of the synthetic wastewater in the influent tank, in spite of being kept at 4ºC and being prepared twice a week. A clear pattern can be observed for the influent COD in which the COD increases when the feed is prepared and then degraded in the influent tank during the following days.

The system's performance was stable during the entire period except on day 17 when the influent flow was accidentally increased and between days 64 to 70 when the influent COD was accidentally decreased. The effluent total solids concentration was very low (below 10mg·L^{-1}) which is an indication of good settling. The reactor's temperature increased during the period from values near 16ºC up to values of 19ºC.

Table 6-4 shows the scheduling for the calibration and validation periods. It should be noted that although the calibration is considered from day 0 to 20, data until day 30 was averaged for the stable-state period influent wastewater characterization. These periods are also located in the upper part of Figure 6-3.

Table 6-4. Scheduling for the calibration and validation periods.

Periods	Calibration (days)	Validation (days)
Long-term evolution	0 to 30	-
Daily evolution	11 to 20	20 to 70
Measurement Campaign (MC)	20	48

Measurement campaign for calibration

The measurement campaign was performed on day 20 of operation to observe the dynamics of the nitrogen compounds and the on-line variables (DO, pH and ORP) during one cycle. The explanation of the results obtained is divided into off-line and on-line measurements.

Off-line measurements

The evolution of ammonium, nitrite, nitrate and filtered COD during the measurement campaign are presented in Figure 6-4. The filling events take place during ten minutes under anoxic conditions. It can be seen that the ammonia concentration increases linearly due to both the addition of ammonia from the influent and hydrolysis of organic nitrogen also from the influent. In the aerobic phases the ammonium concentration decreases and nitrite and nitrate increase as a result of the aerobic growth of the autotrophs (nitrification). It can also be seen that there is a transient build-up of nitrite. Nevertheless, at the end of the aerobic phase the nitrite concentration is very low as it has been completely oxidized. During the anoxic phases denitrification takes place reducing nitrate and nitrite to nitrogen gas using the readily biodegradable substrate as carbon and the electron donor source, and nitrate as the electron acceptor.

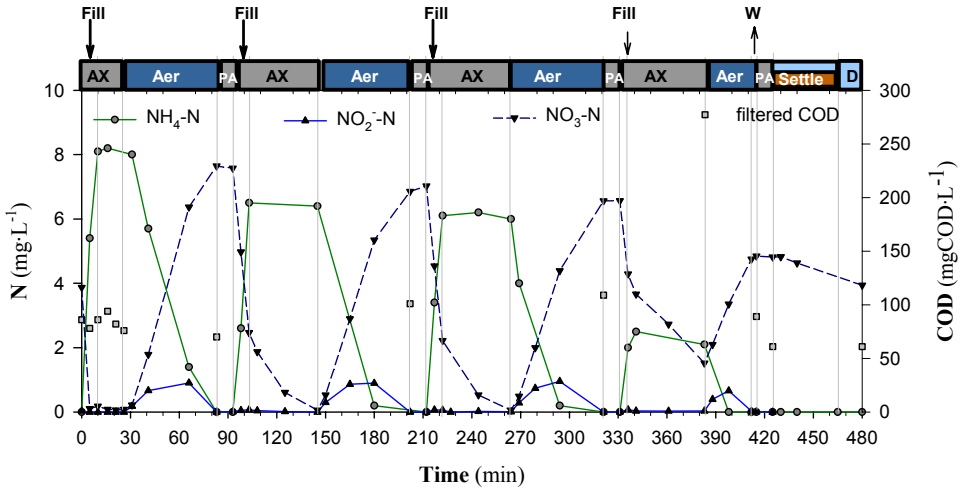


Figure 6-4. Measurement campaign for calibration (Off-line measurements).

The soluble COD was also measured mainly during the first filling and anoxic phase showing a slight increase during filling and decrease during denitrification due to the organic matter being consumed. During the settling and draw phases the COD value remained constant.

On-line measurements

The on-line measurements of pH, DO and ORP from the two-cycle operation are presented in Figure 6-5. During the first cycle operation (0 to 480 minutes), in which the samples for analytical measurements were taken (Figure 6-4), the DO On-Off controller was enabled. The cycle after the measurement campaign was conducted with the DO On-Off controller disabled.

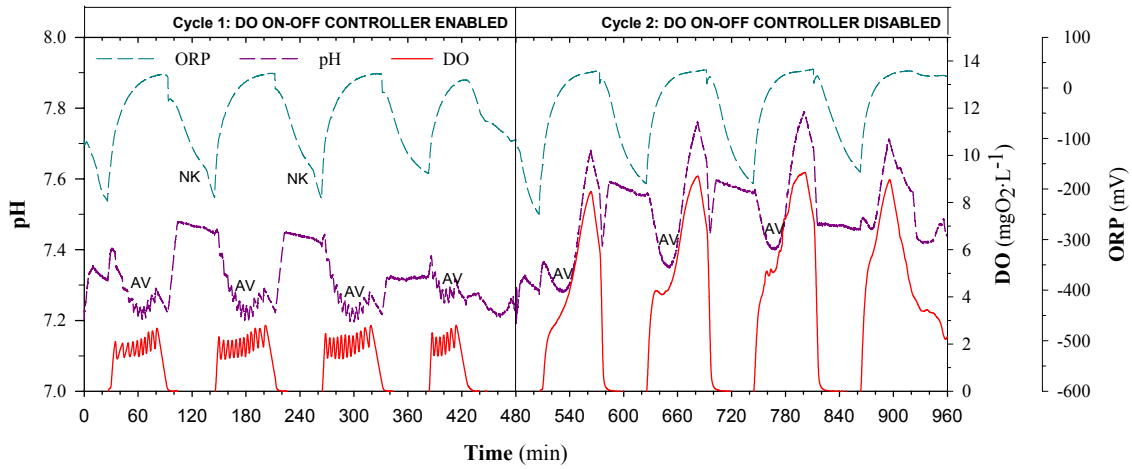


Figure 6-5. Measurement campaign for calibration: on-line measurements.

Interpreting the on-line measurements during the first cycle operation also contributes to understanding the system better, and even to checking the quality of the analytical measurements. Regarding the DO and focusing on aerobic phases, it can be seen that at the beginning of the aerobic phase DO concentration remains at very low values due to the consumption of readily biodegradable organic matter. When this substrate is finished, the DO concentration increases gradually because nitrification does not consume as much oxygen as organic matter removal. When all ammonia is finished a minimum in the pH profile (Ammonia Valley, AV in Figure 6-5) is observed because of the equilibrium between alkalinity consumption during the nitrification process (decreases pH) and stripping of CO_2 (increases pH).

Some information can be extracted from the ORP profile, especially for the anoxic phases. When all nitrate is consumed (end of denitrification) an inflexion point in the ORP profile appears (Nitrate Knee, NK in Figure 6-5) which is related to the electron acceptor changing from nitrates to sulfates or other components. This means that at this point all nitrate should be depleted, which is in accordance with the analytical measurements.

Measurement campaign for validation

Another measurement campaign was conducted on day 48 of operation which was used for the validation step. This monitoring was less intensive than the one used for calibration and the samples were only taken in the first 210 minutes of the cycle operation. Figure 6-6 presents the evolution of ammonium, nitrite and nitrate, and filtered COD of the validation measurement campaign.

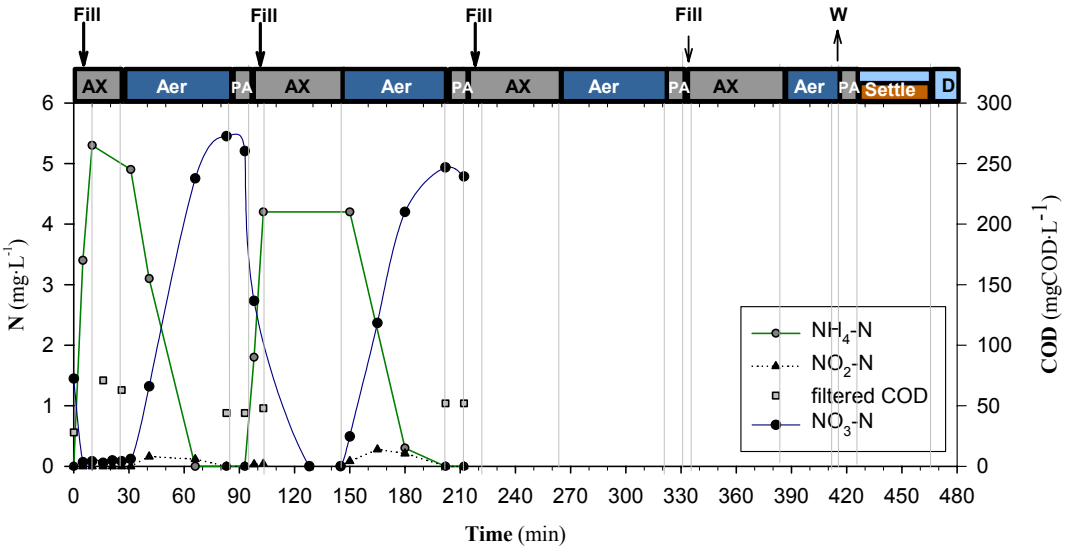


Figure 6-6. Measurement campaign for validation (Off-line data).

In Figure 6-7 the on-line measurements (ORP, pH and DO) for the measurement campaign cycle using the On-Off controller (Left) and also for the following cycle (Right) with the On-Off controller disabled are presented.

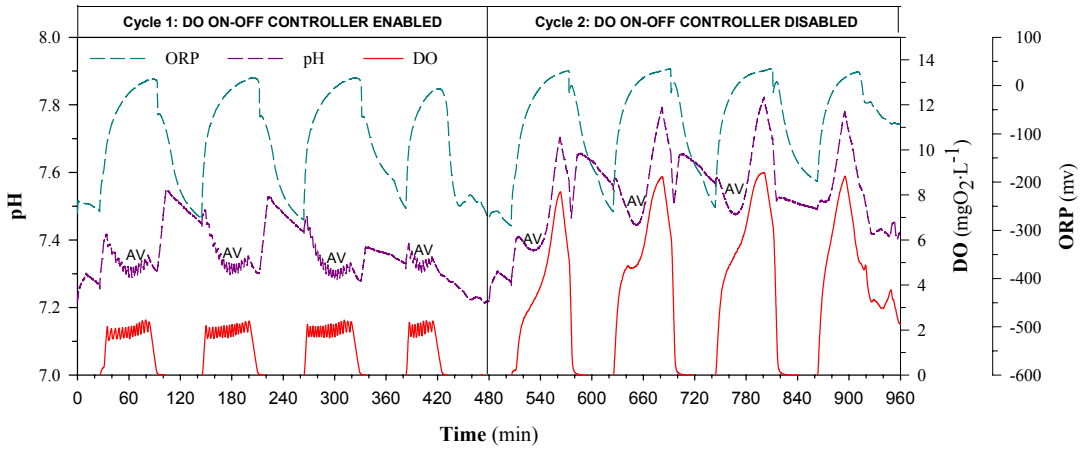


Figure 6-7. Measurement campaign for validation (On-line data).

As in the measurement campaign for calibration the DO On-Off controller was disabled during the following cycle of the measurement campaign in order to obtain more information about the process using the DO profile.

3.b. Data analysis

The objective of the data analysis is to verify the collected data by means of mass balances and identify possible outliers or errors. It is recommended to check the laboratory analysis and measurement accuracy using standards.

In this study, once the data about the plant was collected an analysis was performed. Most of the experimental measurements were reliable since standards were used and the measurement accuracy analysis was periodically checked.

For a reliable simulation, the SRT should be known with 95% accuracy (Meijer, 2004) because the SRT is highly sensitive in the simulated model. The experimental SRT was estimated frequently based on waste flow data (the wastage volume was measured often) and sludge concentration measurements. In this sense it could be assumed that the accuracy of the SRT estimation was only subject to the inaccuracies in the VSS measurement. Therefore, as we are dealing with a small pilot plant the total phosphorus mass balance was not necessary. In this case the SRT was calculated as presented in Table 1-1.

STAGE III. Model structure and process characterization

4. Model definition

Three sub-models were considered in the model structure: the mass transfer, settler and biokinetics.

4.a. Mass transfer

The key parameter to model the mass transfer is the oxygen transfer efficiency (K_La). Based on the experience acquired in the previous calibration it was decided to adjust the K_La value during the calibration procedure (step 6 of the calibration protocol) by trial and error. This could be done since the DO On-Off control was disabled in the cycle after the measurement campaign, so the DO dynamics could be observed.

4.b. Settler

The suitable settling model was selected by following the decision tree already presented in Figure 5-4. The first question is whether detailed settling characterization is needed or not. In this case, the total suspended solids in the effluent were maintained at low values as seen in Figure 6-3. The sedimentation phase in the SBR was oversized, permitting enough time the sludge to settle before starting drawing, although the mean value for the Diluted Sludge Volumetric Index (DSVI) was 210 $mL \cdot g^{-1}$. The floc was compact as presented in Figure 6-8.

Figure 6-8. Picture of a floc (Magnification: 400X).

The good performance of the settling was also assessed following the sludge blanket during the settling phase as presented in Figure 6-9. At 40 minutes (sedimentation time considered in the cycle) compression settling was occurring and the blanket was located at a height below 10L. The reactor was drawn from a level of 16L (minimum volume) and therefore the sludge layer was 6L below the minimum volume, so that the total suspended solids in the effluent could be considered to be the non-settleable fraction (f_{ns}). Therefore, it was concluded that the settling did not influence the plant's performance and the point settler model was selected as the best option, in view of adequate model complexity.

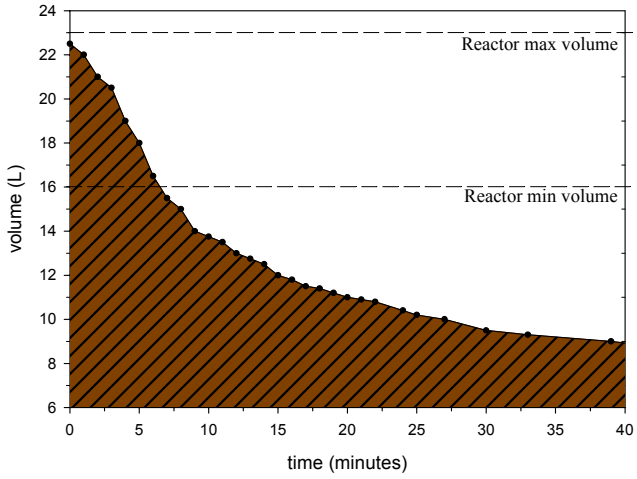


Figure 6-9. Sludge blanket during the settling phase.

If biological reactions in the settler are detected and they influence the process, a reactive settler model can be applied to allow biological reactions take place. In this case, looking at the monitoring campaign (see Figure 6-5) during the settling phase one can see that there was no change in the ammonium concentration, and variation in the oxidized nitrogen was minimal. Hence, the reaction could be considered negligible.

4.c. Selecting the biological model

In this step the activated sludge model to be used for the calibration was selected. The later wastewater characterization and parameter estimation are conditioned by this selection.

As stated in the previous calibration experience, the choice of model depends on the biological activity observed in the reactor and the processes and variables to be considered. A decision tree for selecting the model to be used has already been presented in Figure 5-5.

In this case, the same reasoning used in point 5.3.3 when selecting the biological model, was applied here. Hence, the model used in this calibration was the ASM1 because it can describe the processes of carbon and nitrogen removal properly and it is simpler than ASM3.

The decision tree already presented in Figure 5-5 represents the simplified selection of the suitable model. Sometimes it is necessary to make some modifications or extensions to the selected model (e.g. consider two-step nitrification/denitrification). In this case a modification was implemented: both heterotrophic aerobic and anoxic growth rates were dependent on ammonium concentration, to take into account the limitation of ammonium as substrate, as presented in the Stage IV of the point 5.3.3.

The effect of temperature on the kinetics was also contemplated in the model implementation using the Arrhenius equation (Metcalf and Eddy, 2003). The default values of ASM1 for the correction factors were applied.

5. Process characterization

In this calibration study, since the calibration was conducted when the pilot plant was running, it was possible to determine some of the parameters of the model (presented in 5a), and also to perform a complete influent wastewater characterization (presented in 5b).

5.a. Estimation of ASM parameters.

To make the calibration easier it is important to determine experimentally some of the parameters of the activated sludge model. Therefore, some parameters can be fixed and the calibration goes through the rest of the parameters. The literature shows that respirometry assays are commonly used for determining these parameters (Vanrolleghem *et al.*, 1999). In this study the heterotrophic yield (Y_H) and the heterotrophic decay rate (b_H) were experimentally determined mainly for their importance in the long-term behavior of the system. In Petersen *et al.* (2003) these parameters were considered relevant for the calibration process. Moreover, it was considered that it is not necessary to determine more parameters since for SBR technology the dynamics of the nitrification and denitrification processes can be observed when performing a measurement campaign during one operation cycle.

Heterotrophic yield (Y_H)

The ratio of the amount of biomass produced to the amount of substrate consumed (mg biomass/mg substrate) is defined as the biomass yield, and is typically defined in relation to the electron donor used (Metcalf and Eddy, 2003). In the case of heterotrophic microorganisms, their yield (Y_H) is the amount of heterotrophic biomass produced to the amount of biodegradable organic matter (S) consumed.

As presented in Figure 6-10, from a unit of substrate consumed the Y_H fraction goes to biomass growth and the rest ($1-Y_H$) is used for respiration. Thus, the yield coefficient can also be related to the DO consumption of the heterotrophic organisms under particular conditions and this consumed DO can be "easily" measured using a respirometer.

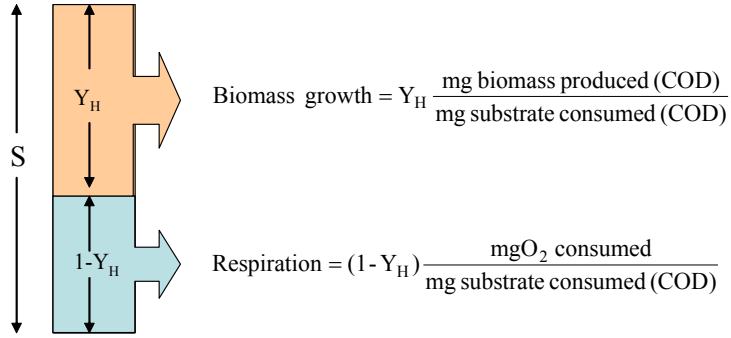


Figure 6-10. Description of the substrate transformation for the biomass growth and the biomass respiration.

The respirometer is an instrument that permits measuring the Oxygen Uptake Rate (OUR) as the decrease in the DO concentration due to the biomass activity. The integration over time of the OUR measurements during an experiment represents the DO consumed. Thus, the heterotrophic yield coefficient can be calculated with Equation 6-1.

$$(1-Y_H) = \frac{mgO_2 consumed}{mgS consumed} = \frac{\int OUR \cdot dt}{S} \text{ --->} \int OUR\ dt = (1-Y_H)S \qquad \text{Equation 6-1}$$

Equation 6-1 describes that adding substrate to the sludge represents oxygen consumption. The slope of the function corresponds to the factor ($1-Y_H$). In these respirometry assays the quantity of DO consumed is measured for each quantity of substrate added to a sludge sample. Repeating this experiment varying the amount of substrate added provides different values of consumed oxygen, and therefore different values of the consumed DO/substrate relation. The graphical representation of the pairs of values obtained in the different additions has a linear adjustment, and the slope is ($1-Y_H$).

Hence, respirometry was the methodology chosen to determine the Y_H. The closed sequential respirometer presented in Chapter 3.1 was used and the method described in Gutierrez (2003), which was adapted from Dircks *et al.* (1999), was followed.

The experiment consisted in inoculating the respirometer with sludge from the SBR achieving a concentration of 1000mgVSS·L^{-1}. Then an inhibitor of the autotrophic activity, allylthiourea (ATU), was added to obtain only the response of the heterotrophic organisms. The big reactor of the respirometer was continuously aerated until endogenous conditions were achieved. Then, increasing volumes of influent wastewater with known COD were added. The DO consumed was calculated by computing the integral of the OUR profile.

Table 6-5 presents the volume of influent added with the supplied COD concentration, the degraded COD and the consumed DO for the different additions during the respirometry assay.

Table 6-5. Characteristics of the respirometric assay.

Nº Addition	Volume of influent added (L)	Reactor Volume (L)	Supplied COD (mg COD)	Degraded COD (mg COD·L^{-1})	Consumed DO (mg·L^{-1})
1	0.025	4.025	407.5	101.2	26.0
2	0.050	4.075	815.0	200.0	56.0
3	0.100	4.175	1630.0	390.4	128.8
4	0.100	4.275	1630.0	381.3	119.0
5	0.250	4.525	4075.0	900.6	299.0
6	0.005	4.530	81.5	18.0	4.3
7	0.010	4.540	163.0	35.9	8.3
8	0.050	4.590	815.0	177.6	49.4

The consumed DO was calculated with the software PAR developed in Gutierrez (2003). An example of calculating the respirogram area for the fifth addition is presented in Figure 6-11.

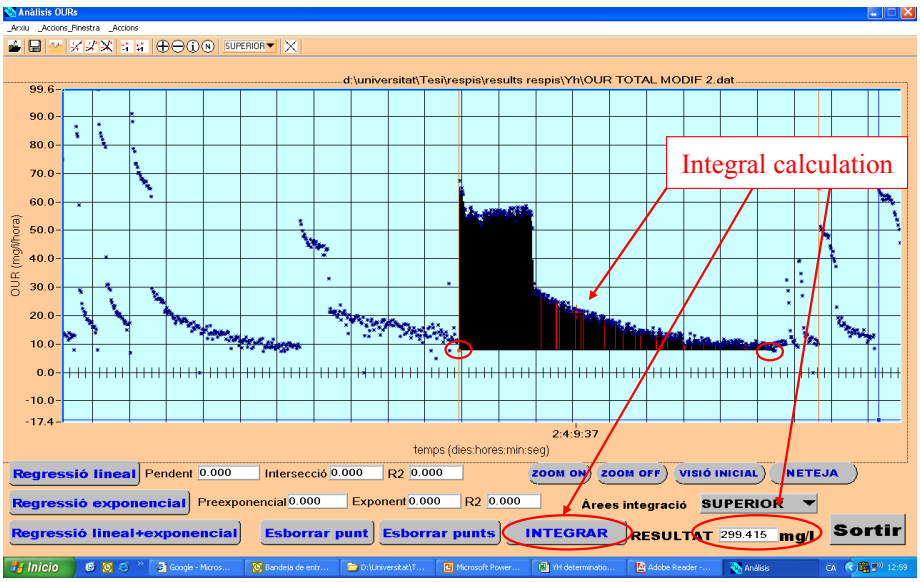


Figure 6-11. Fifth addition area calculation with the PAR software.

Representing the values of consumed oxygen versus the COD supplied, a linear equation is found in which the slope is equal to the factor 1-Y_H (see Figure 6-12).

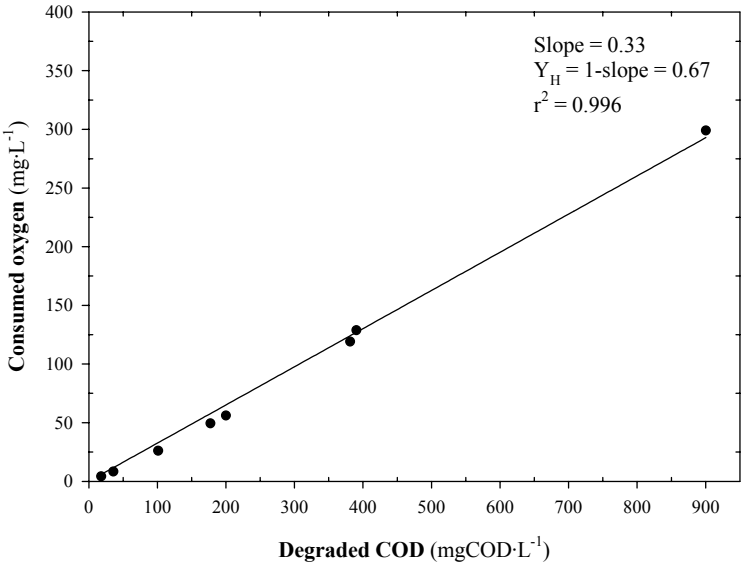


Figure 6-12. Consumed oxygen versus degraded COD in the respirometry assay.

A value of **0.67** was found for the Y_H, which is in accordance with the literature, e.g. the default value proposed in ASM1 is 0.67. The results of the assay are summarized in Table 6-6.

Table 6-6. Results of the Y_H respirometric assay.

Slope	R^2	Y_H value	Std. error	Nº points	Range of substrate concentrations (mg COD·L^{-1})
0.33	0.996	0.67	0.0058	8	81.5 – 4075

Heterotrophic decay rate (b_H)

The heterotrophic decay rate (b_H) is very important for predicting sludge production and oxygen requirements (Henze *et al.*, 2000). The most commonly used method is that defined in Ekama *et al.* (1986). It consists in taking sludge from the reactor and putting it into a aerated and mixed batch reactor in which the OUR can be measured several times over a period of several days (between 10 and 15 days). The slope of a plot of the natural logarithm of the OUR versus time is the traditional decay coefficient k_d. Then, this decay rate can be transformed into the model decay rate (b_H) based on the death regeneration concept via Equation 6-2, in which the heterotrophic yield (Y_H) and the fraction of biomass leading to particulate products (f_p) can be assumed to be known.

$$b_H = \frac{k_d}{1 - Y_H(1 - f_p)} \qquad \text{Equation 6-2}$$

The heterotrophic decay rate was determined following the method described in Ekama *et al.* (1986). The fermenter presented in point 3.1.2 was used. The reactor was insulated in order to avoid superficial oxygen transfer. A simple Data Acquisition and Control system was also installed in order to control the aeration and temperature of the reactor and monitor the DO and temperature. The reactor was fed with 4L of mixed liquor from the SBR and the system was maintained at oxygen saturation level. Several times per day, the aeration was switched off in order to measure the decrease in the oxygen concentration which represents the OUR.

The process for calculating the traditional decay coefficient (k_d) is presented in Figure 6-13. First of all the mass balances for the biomass and oxygen for the decay process are performed. From these mass balances the expression of the OUR versus time is obtained, and after a linearization the slope of the equation represents the traditional decay coefficient k_d.

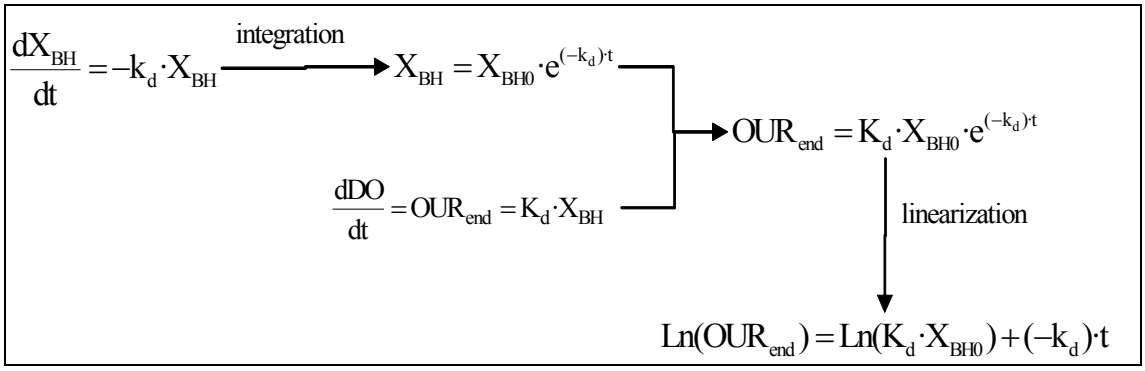


Figure 6-13. Mathematical background for determining b_H.

The evolution of the OUR and the OUR logarithm during the eleven days of operation is presented in Figure 6-14. The k_d obtained was 0.1842d^{-1}, and since the experiment was conducted at 24ºC, a correction for the temperature had to be applied. A value of 1.12 for the temperature correction factor was used (Henze *et al.*, 2000), and the k_d obtained at 20ºC was 0.1173 d^{-1}.

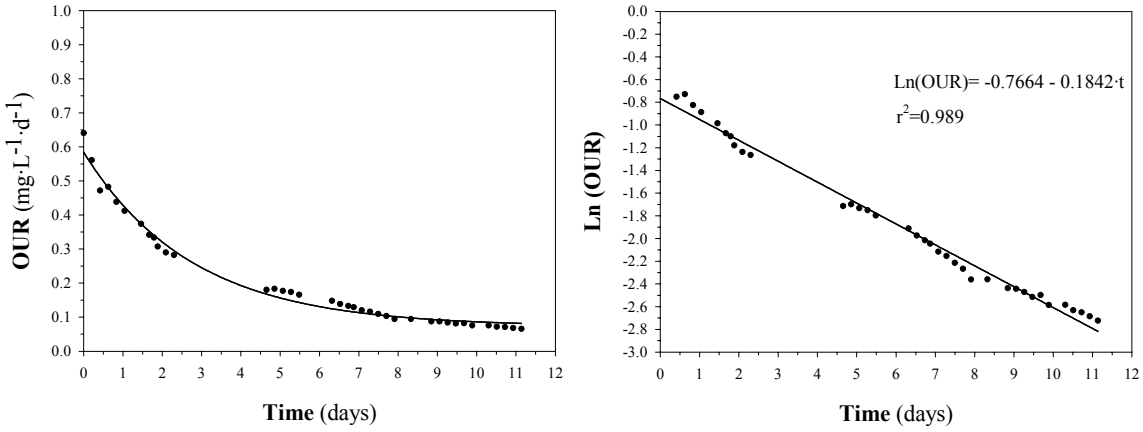


Figure 6-14. Results of the heterotrophic decay rate assay, with the evolution of the OUR (Left) and the OUR logarithm (Right) over time.

Finally, the decay rate obtained was transformed to the death and regeneration concept as described in Equation 6-2 using a value of 0.67 $gCOD \cdot gCOD^{-1}$ for the Y_H and a value of 0.08 for the f_P. The final value for b_H at 20ºC was **$0.30 d^{-1}$**. This value is lower than $0.62 d^{-1}$, which is the proposed value in the ASM1. Nevertheless, it is within the range between 0.05 and 1.6 reported in Hulsbeek *et al.* (2002). In SBR systems the rates can be different from those in continuous systems. Alternating anoxic and aerobic conditions and the feast/famine phenomena could be related to the differences in the parameters' values. The value of b_H obtained experimentally is similar to the one obtained in the calibration conducted in Chapter 5 (0.25), determined by trial and error during the calibration procedure.

Table 6-7. Summary of the results from determining the decay rate.

K_d (d^{-1})	Std. error	b_H (d^{-1})	R^2	Nº points	Assay duration (d)
0.18	0.0033	0.30	0.989	36	12

5.b. Influent wastewater characterization

The influent wastewater characterization was based on the STOWA protocol. This methodology is based on physical-chemical and BOD measurements, and was used since reproducibility and consistency was preferred over the biological aspects.

The data used in this step has already been presented in point 3.1. Within the evolution of the influent composition a clear weekly pattern was observed and this was taken into account during the whole procedure.

The influent fractionation was conducted separately for the three different simulation periods (stable-state, daily and cycle). During the stable-state simulations the weekly pattern observed was considered by averaging the values of each day of the week, using the thirty first experimental days (see Table 6-2). A weekly composition was obtained, and was repeated five times so that a thirty day influent file was obtained. Figure 6-15 presents the evolution of the influent COD_T and 0.1 μm filtered COD ($COD_{0.1\mu m}$) obtained over fourty days, in which the weekly pattern can be clearly observed.

It can be seen in Figure 6-15 that the COD_T begins with values of 545 $mgCOD \cdot L^{-1}$ and then drops to values of 502. On the third day it decreases sharply to values of 377 $mgCOD \cdot L^{-1}$, which represents a degradation of 31% of the total COD. This phenomenon is mainly related to biological degradation in the influent tank. This influences the denitrification process, which was not complete when the COD/TKN ratio was low. The starting value of the $COD_{0.1\mu m}$ was 313 $mgCOD \cdot L^{-1}$ then it decreased to 304 $mgCOD \cdot L^{-1}$ on the second day, and finally on the third day it dropped down to a value of 207 $mgCOD \cdot L^{-1}$, which represents a reduction of 45%.

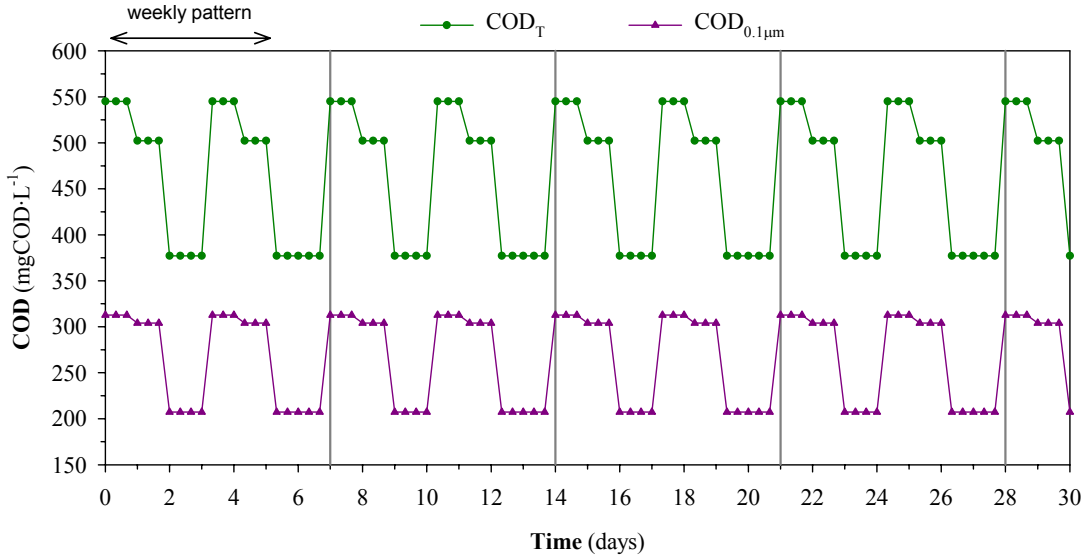


Figure 6-15. Influent composition pattern used for characterizing the organic fractions during the stable-state period.

The evolution of the nitrogen compounds is presented in Figure 6-16. The nitrogen fractions degrade less than the organic compounds. For instance the TKN_T decreases 3% on the third day, and the ammonia 6%. The ammonium fraction was the highest (between 80 and 85% of the total nitrogen, depending on the day).

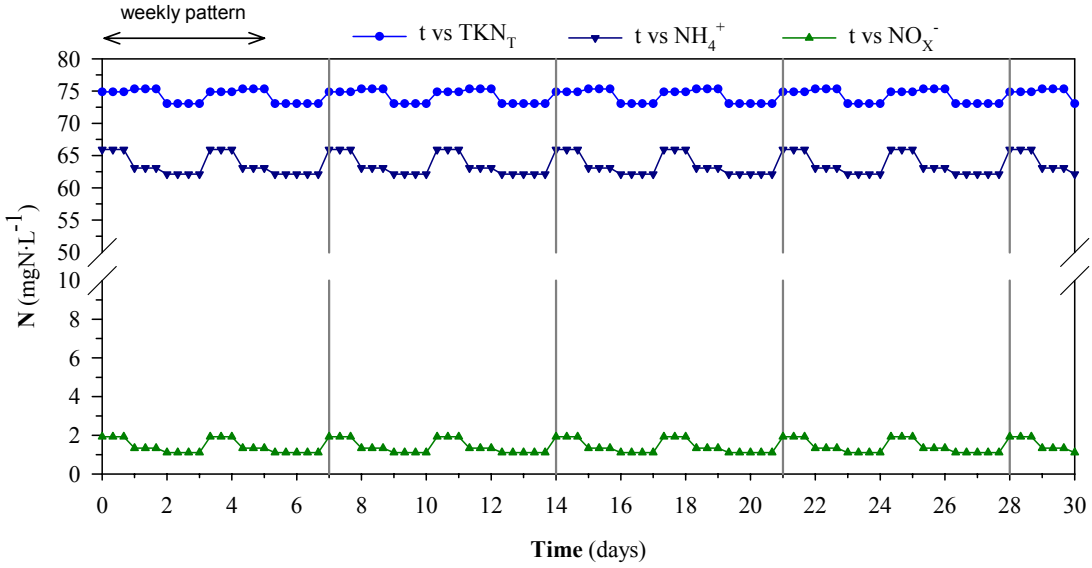


Figure 6-16. Influent composition pattern used for characterizing the nitrogen fractions during the stable-state period.

Moreover, the degradation effect on the influent wastewater was studied conducting a BOD analysis to determine the influent biodegradable fraction of the total COD. Figure 6-17

represents the experimental values obtained from samples taken from the influent tank on three consecutive days: the first day the feed was prepared, the next day, in which some degradation occurred, and the third day, in which as explained before a degradation of 31% in the COD_T was achieved.

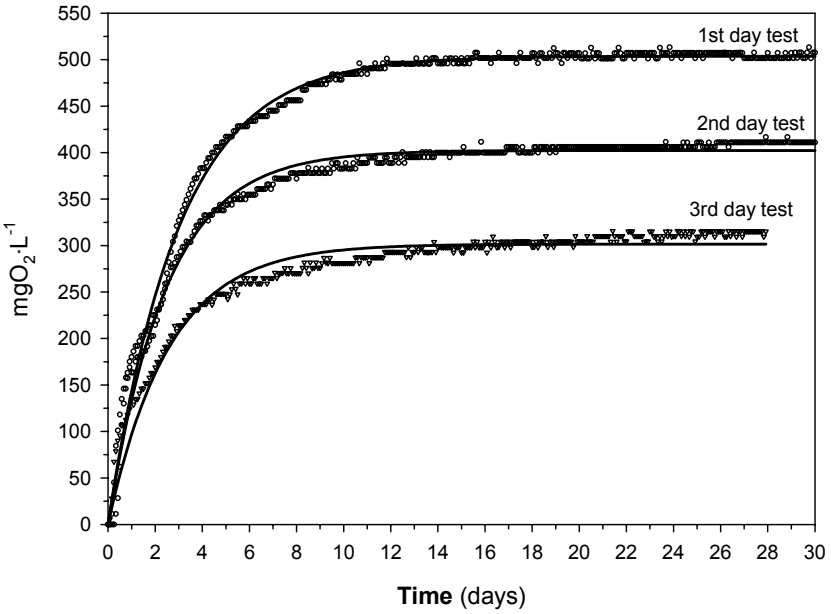


Figure 6-17. BOD results for three samples taken during consecutive days.

The values of the BOD test were fitted to Equation 6-3 to obtain the value of the ultimate BOD (BOD_U) and the reaction constant (k). This value was corrected using Equation 6-5 to estimate the biodegradable COD (BCOD). The results of the fit are presented in Table 6-8.

Table 6-8. Fit of the BCOD curves.

	BOD_U ($mgO_2 \cdot L^{-1}$)	k (d^{-1})	BCOD ($mgO_2 \cdot L^{-1}$)	BCOD/CODtotal (%)
1st day test	503	0.33	558.89	90
2nd day test	402	0.40	446.67	89
3rd day test	301	0.38	334.44	85

Hence, the biodegradable fraction also decreased due to the influent wastewater degrading from 90% on the first day to 89% on the second day, and 85% on the third day. These percentages can be taken into account during the influent wastewater characterization. These results are in agreement with the synthetic wastewater composition, presented in Table 6-2, which basically contains biodegradable substrate as carbon source (ethanol, milk and DME).

During the daily and the cycle evolution period, the influent wastewater characterization was done day by day with the data obtained in the intensive monitoring, as well as by applying the biodegradable percentages obtained from the BOD test.

Procedure for the influent wastewater fractionation

The influent wastewater characterization was divided into the organic matter fractionation and the nitrogen fractionation. These were performed following the procedures described in Figure 6-18 and Figure 6-19, which were based on the standard Dutch STOWA guidelines (Roeleveld and Van Loosdrecht, 2002).

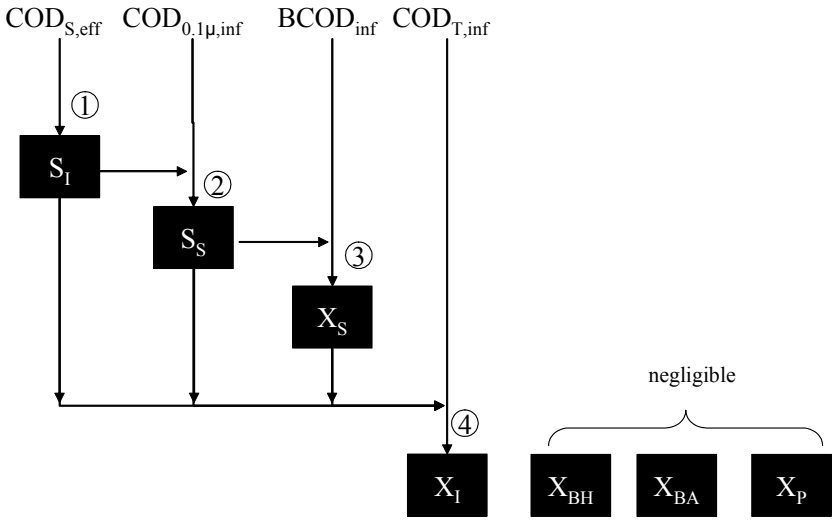


Figure 6-18. Organic matter fractionation.

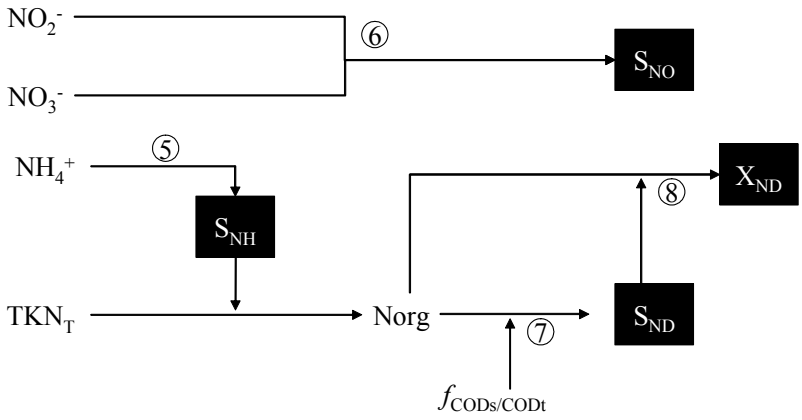


Figure 6-19. Nitrogen fractionation.

The equations used for the influent characterization are presented in Table 6-9 and a more detailed explanation that deals with each fraction separately is also presented.

Table 6-9. Equations used for the organic matter and nitrogen fractionation.

Definition (compounds)	Symbol	Units	Equation
Inert soluble organic	S_I	g COD·m^{-3}	$S_I=COD_{S,eff}$ (1)
Readily biodegradable organic	S_S	g COD·m^{-3}	$S_S=COD_{0.1\mu m,inf}-S_I$ (2)
Slowly biodegradable organic	X_S	g COD·m^{-3}	$X_S=BCOD_{inf}-S_S$ (3)
Inert particulate organic	X_I	g COD·m^{-3}	$X_I= COD_{t,inf} - X_S - S_S - S_I$ (4)
Ammonium	S_{NH}	g N·m^{-3}	$S_{NH}=NH_4^+$ (5)
Oxidized nitrogen	S_{NO}	g N·m^{-3}	$S_{NO}=NO_2^-+NO_3^-$ (6)
Soluble organic nitrogen	S_{ND}	g N·m^{-3}	$S_{ND}=(COD_{f,inf}/COD_{t,inf})\cdot(TKN_T-NH_4^+)$ (7)
Particulate organic nitrogen	X_{ND}	g N·m^{-3}	$X_{ND}=(TKN_T-NH_4^+)-S_{ND}$ (8)

1) Determining influent soluble inert COD (S_I)

The S_I is assumed to be the filtrated COD in the effluent ($COD_{S,eff}$). This means that all the biodegradable substrate of the influent is depleted in the reactor and only the inert fraction remains in the effluent.

2) Determining readily biodegradable COD (S_S)

The S_S is determined by means of the 0.1µm filtered samples. According to Roeleveld and Van Loosdrecht (2002), similar results can be obtained either using flocculated COD or 0.1µm filtered COD. The difference in COD after 0.1 µm filtration or flocculation is rather small with approximately 1% difference. Differences would only be significant in industrial wastewaters that may have a large number of soluble compounds with a wide range of biodegradation rates (Melcer *et al.*, 2003).

3) Determining slowly biodegradable COD (X_S)

The X_S is determined by subtracting the S_S from the total biodegradable substrate ($BCOD_{inf}$). The $BCOD_{inf}$ is calculated from the BOD tests, after adjusting the experimental BOD curve to Equation 6-3, to obtain the ultimate BOD (BOD_U) and the k values.

$$BOD(t) = BOD_U \cdot (1 - e^{-k \cdot t}) \qquad \text{Equation 6-3}$$

During the BOD measurement there is an interaction of biomass growth and decay. For a long-term BOD measurement this results in converting a part of the biodegradable substrate into an inert fraction. Therefore, the BCOD is finally obtained after applying a correction factor (f_P=0.08) as shown in Equation 6-4.

$$BCOD_{inf} = \frac{1}{1 - f_p} \cdot BOD_u \qquad \text{Equation 6-4}$$

4) Determining inert particulate COD (X_I)

Once the biodegradable and the inert soluble fractions are determined the X_I is obtained after applying the COD mass balance.

$$X_I = COD_{T,inf} - X_S - S_S - S_I \qquad \text{Equation 6-5}$$

4) Determining S_{NH}

The S_{NH} is obtained directly from the ammonium measurement.

5) Determining S_{NO}

The S_{NO} is obtained directly from the sum of the nitrite and nitrate measurements.

6) Determining S_{ND}

The difference between TKN and ammonium is the organic nitrogen, which is divided into soluble organic nitrogen and particulate organic nitrogen. The division into soluble and particulate is done assuming the same percentage of soluble/particulate obtained in the COD fractionation.

7) Determining X_{ND}

The X_{ND} is obtained directly from the S_{ND} and the total organic nitrogen.

Results of the fractionation

The average contribution of the organic components to the total COD, and the results of the influent ASM1 based fractionation for organic matter and nitrogen are presented in Table 6-10 and Table 6-11. The results for the stable-state period, together with the daily evolution and the cycle evolution periods are shown. Notice that the X_I estimated was very low, with a fraction no higher than 4%. This is because the components of the synthetic wastewater were mainly soluble and biodegradable.

Table 6-10. Influent ASM1 based fractionation for organic compounds.

Analytical data	Stable-state period						Daily evolution period											
	1st mean		2nd mean		3rd mean		day 11		day 12		day 13		day 14		day 15		day 16	
	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)
$COD_{T, inf}$	545.1	100	502.3	100	377.1	100	345.0	100.0	566.0	100.0	550.0	100.0	468.0	100.0	504.0	100.0	464.0	100.0
$COD_{0.1\mu m, inf}$	312.6	57.3	304	60.5	207.2	55	227.1	65.8	330.6	58.4	320.2	58.2	207.2	44.3	312.3	62.0	294.9	63.6
$COD_{S, effl}$	51.3	9.4	51.3	10.2	51.3	13.6	44.0	12.8	48.0	8.5	48.0	8.7	53.0	11.3	65.0	12.9	44.0	9.5
$BCOD_{inf}$	490.6	90	447	89	320.6	85	293.3	85.0	509.4	90.0	489.5	89.0	397.8	85.0	428.4	85.0	417.6	90.0
State variables																		
S_S	261.3	47.9	252.7	50.3	155.9	41.3	183.1	53.1	282.6	49.9	272.2	49.5	154.2	33.0	247.3	49.1	250.9	54.1
S_I	51.3	9.4	51.3	10.2	51.3	13.6	44.0	12.8	48.0	8.5	48.0	8.7	53.0	11.3	65.0	12.9	44.0	9.5
X_S	229.3	42.1	194.3	38.7	164.7	43.7	110.2	31.9	226.8	40.1	217.3	39.5	243.6	52.0	181.1	35.9	166.7	35.9
X_I	3.2	0.6	3.9	0.8	5.3	1.39	7.8	2.2	8.6	1.5	12.5	2.3	17.2	3.7	10.6	2.1	2.4	0.5

Analytical data	Daily evolution period						Cycle evolution	
	day 17		day 18		day 19		day 20	
	Conc.	(%)	Conc.	(%)	Conc.	(%)	Conc.	(%)
$COD_{T, inf}$	448.0	100.0	432.0	100.0	545.1	100.0	512.0	100.0
$COD_{0.1\mu m, inf}$	252.3	56.3	298.4	69.1	312.6	57.4	255.8	50.0
$COD_{S, effl}$	44.0	9.8	52.0	12.0	51.3	9.4	61.0	11.9
$BCOD_{inf}$	398.7	89.0	367.2	85.0	490.6	90.0	435.2	85.0
State variables								
S_S	208.3	46.5	246.4	57.0	261.3	47.9	194.8	38.0
S_I	44.0	9.8	52.0	12.0	51.3	9.4	61.0	11.9
X_S	190.4	42.5	120.8	28.0	229.3	42.1	240.4	47.0
X_I	5.3	1.2	12.8	3.0	3.2	0.6	15.8	3.1

Table 6-11. Influent ASM1 based fractionation for nitrogen compounds.

	Stable-state period						Daily evolution period											
Analytical data	**1st mean**		**2nd mean**		**3rd mean**		**day 11**		**day 12**		**day 13**		**day 14**		**day 15**		**day 16**	
	Conc.	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**
NH_4^+	65.9	85.8	63.1	82.3	62.1	83.8	65.0	87.6	65.6	78.4	64.0	83.5	63.2	82.0	76.9	88	76.9	88.4
TKN_T	74.9	97.5	75.3	98.3	73.0	98.5	73.8	99.5	81.7	97.7	74.9	97.7	76.2	98.8	87	100	87.0	100.0
NO_X^-	1.9	2.5	1.3	1.7	1.1	1.5	0.4	0.5	2.0	2.3	1.8	2.3	0.9	1.2	0	0	0.0	0.0
State variables																		
S_{NH}	65.93	85.8	82.3	82.3	62.13	83.8	65	87.6	65.6	78.4	64	83.5	63.2	82.0	76.9	88	76.9	88.4
S_{ND}	5.90	7.7	11.1	11.1	6.88	9.3	6.66	9.0	10.81	12.9	7.29	9.5	6.62	8.6	7.38	8.5	7.38	8.5
X_{ND}	3.05	4.0	4.9	4.9	4.02	5.4	2.14	2.9	5.29	6.3	3.61	4.7	6.38	8.3	2.72	3.1	2.72	3.1
S_{NO}	1.9	2.5	1.3	1.7	1.1	1.5	0.4	0.5	2.0	2.3	1.8	2.3	0.9	1.2	0	0	0.0	0.0

	Daily evolution period						Cycle evolution	
Analytical data	**day 17**		**day 18**		**day 19**		**day 20**	
	Conc.	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**	**Conc.**	**(%)**
NH_4^+	73.6	85.7	66.7	76.9	66.7	76.9	67.9	78.8
TKN_T	84.8	98.8	13.18	15.2	13.18	15.2	81.2	94.3
NO_X^-	1.1	1.2	3.42	3.9	3.42	3.9	4.9	5.7
State variables								
S_{NH}	73.6	85.7	66.7	76.9	66.7	76.9	67.9	78.8
S_{ND}	7.25	8.4	83.3	96.0	83.3	96.0	7.64	8.9
X_{ND}	3.95	4.6	3.5	4.0	3.5	4.0	5.66	6.6
S_{NO}	1.1	1.2	3.42	3.9	3.42	3.9	4.9	5.7

STAGE IV. Calibration and validation

6. Calibration of the biokinetic model

For the calibration of the biokinetic model first a stable-state and then a cycle evolution calibration were performed. The simulation procedure was similar than the one presented in Figure 5-2.

First a simulation of thirty days was performed with averaged composition and flows but taking into account the periodic variability of the influent (first, second and third days). During this thirty day period the stable-state calibration was performed and the long-term behavior parameters were adjusted. Then a ten day simulation was run (daily evolution period) applying the dynamics of the influent composition and flow. Finally, the cycle in which the measurement campaign was conducted was simulated (cycle evolution period), and the parameters related to the dynamic behavior could be adjusted. Changing any of these parameters implied running the whole simulation procedure (stable-state + daily evolution + cycle evolution).

The default values of the ASM1 parameters were taken as a starting point for the simulations and then a procedure for the calibration of the biokinetic model was applied. This consisted in a step-wise methodology, which clearly differentiated between the stable-state calibration and the cycle evolution calibration. It was based on expert knowledge and consisted in four iteration steps that first considered the sludge production and then the dynamics of the NH_4-N, DO and NO_X-N profiles. Figure 6-20 shows the scheme of the methodology used for calibration. The explanation is divided into the stable-state and the cycle evolution calibration.

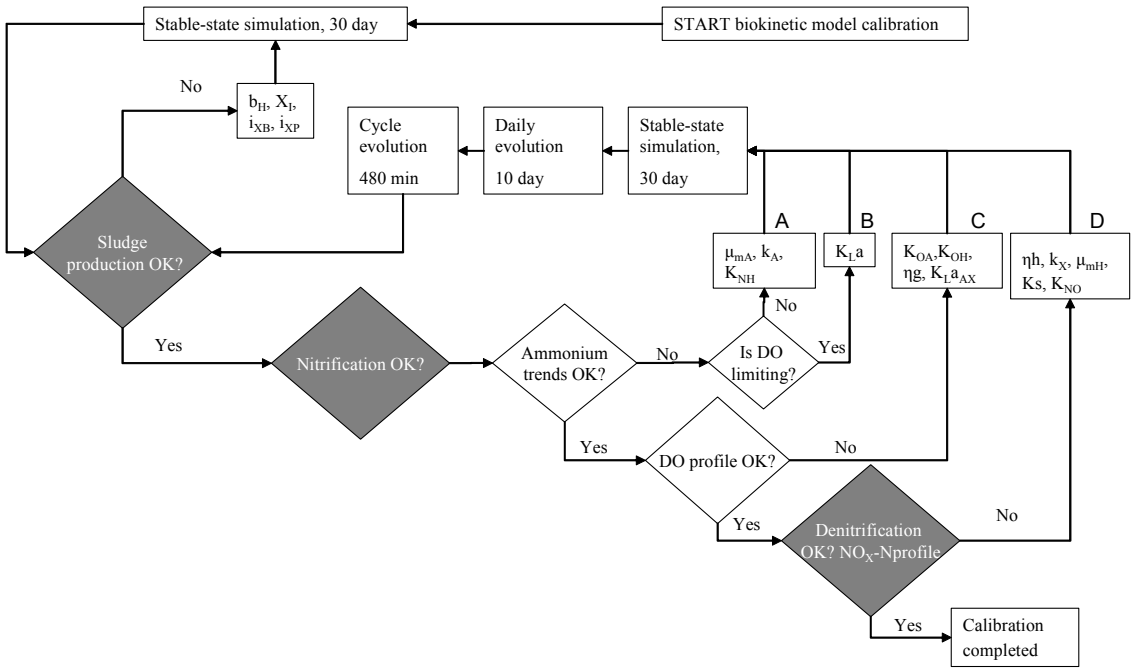


Figure 6-20. Step-wise procedure for the model calibration.

6.a. Stable-state calibration

The aim of the steady state calibration is to adjust the modeled sludge production by fitting the parameters responsible for long-term behavior. Furthermore, it is necessary to fit the solids concentration to the effluent by adjusting the settling parameters. This procedure was applied in Nowak *et al.* (1999) and Petersen *et al.* (2002).

In this case, fitting the sludge production implied combining the experimental batch experiment for b_H and the influent wastewater characterization for determining the inert organic fraction (X_I). The experimental value of the heterotrophic decay rate determined in a batch test was $0.30 d^{-1}$. For X_I a value between 3.2 and 5.3 $mgCOD \cdot L^{-1}$, depending on the day, was obtained. Combining both parameters led to a good fit of the MLVSS concentration in the reactor and thus no further calibration of the X_I/X_S fraction was needed.

For the biomass characterization the nitrogen content of the biomass could be estimated. The simulated total nitrogen of the reactor should equal the experimental TKN of the reactor. Here, the mass of nitrogen per mass of COD in the biomass (i_{XB}) and the mass of nitrogen per mass of COD in products from the biomass (i_{XP}) could be adjusted to fit the experimental and simulated values of total nitrogen inside the reactor. Using the trial and error method the i_{XB} and i_{XP} fractions were found to be 0.06 and 0.05 respectively, which fitted the TKN mean value in the reactor of 140 $mgN \cdot L^{-1}$.

6.b. Cycle evolution calibration

The aim of the cycle evolution calibration is to adjust the nitrification and denitrification processes with the help of experimental data obtained in the measurement campaign and step by step adjustment of the critical parameters involved in the processes. Although each calibration study is case-particular, in this protocol a proposal of the parameters to be tuned is presented and discussed.

In Figure 6-20, the procedure begins with nitrification fitting the experimental ammonium trends. As dissolved oxygen is a limiting parameter for nitrification, first of all one has to make sure that the simulated oxygen level coincides with the experimental level. For this purpose the dissolved oxygen profile is used, and the K_La value tuned. Afterwards it is recommended to adjust the maximum specific growth rate of the autotrophic biomass (μ_{mA}), the ammonium half saturation coefficient for autotrophic biomass (K_{NH}) and the ammonification rate (k_A). Then the maximum slope of the ammonium profile can be adjusted (using μ_{mA}) and also the final trend of the ammonium profile (with K_{NH}). The k_A is normally increased from the default value, considering that the ammonification process is very fast. In this sense this process has been removed in ASM3 since the conversion of soluble organic substrate into ammonium is very fast.

Following the procedure presented in Figure 6-20, the next step is to adjust the DO profile. In Figure 6-21 a detailed procedure for the DO profile adjustment is presented. First of all, the rise in DO at the beginning of the aerobic phase gives information about the organic substrate depletion. When all the readily available biodegradable substrate has been consumed then the oxygen profile increases following a trend which depends on the consumption of the S_S coming from the hydrolysis and also on the nitrification process. The parameters K_{OH} and η_g can be adjusted. Nevertheless, hydrolysis parameters are not tuned here since they have much more influence on the denitrification process. If nitrification is complete then a bending point appears in the oxygen profile and the localization of this bending point can be adjusted by tuning K_{OA}. If after the aerobic phase there is an anoxic phase with no filling, then a decrease in the oxygen profile is observed which can be adjusted with the K_La in the anoxic phases. This anoxic K_La represents a small fraction of oxygen that is transferred through the surface of the liquid phase. If a major modification for the anoxic K_La is needed one should consider reviewing the experiment for the b_H determination.

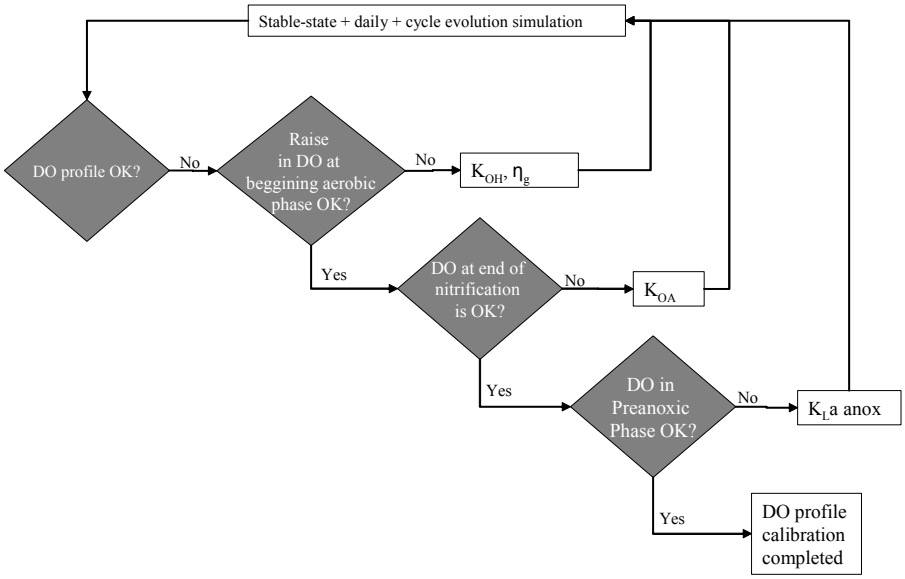


Figure 6-21. Procedure for the DO profile adjustment.

Finally, the denitrification process is adjusted basically by fitting the NO_X-N profile (see Figure 6-20). The main limitation for denitrification is the availability of S_S. Therefore, it is important to first adjust the hydrolysis parameters η_H, K_X (or k_H) and then adjust the parameters related to the heterotrophic anoxic growth such as μ_{mH}, K_S and K_{NO}, taking into account the NO_x-N profile trend.

The procedure followed in this case-study for the cycle evolution calibration is now presented taking into consideration the basic rules explained above. First of all, it should be noted that the simulations started with the default ASM1 values.

A) The first step was to obtain enough nitrifying activity to produce the NO_x-N necessary for the denitrification process. First, the ammonification process was accelerated increasing k_A from 0.08 to 0.1 $L\cdot(mgCOD\cdot d)^{-1}$.

B) In the nitrification process the available dissolved oxygen is a limiting variable. It is necessary to adjust the oxygen supply by means of the K_La value. The oxygen profile adjustment permitted the K_La value ($350d^{-1}$) to be calibrated.

C) K_{NH} was decreased from 1 to 0.4 mg NH_3-$N\cdot L^{-1}$ to lower the effect of ammonia as substrate limitation.

D) The next step was to adjust the NO_X-N profile. The main limitation in the denitrification process is the availability of readily biodegradable substrate. Once the wastewater characterization was performed the extra S_S needed to complete the denitrification process might be originated from the hydrolysis process of both the slowly biodegradable substrate coming from the influent wastewater and coming from the death and regeneration process. In this case the hydrolysis was dependent on the electron acceptor but was not lowered under anoxic conditions. The correction factor for hydrolysis under hydrolysis was η_H=1. Therefore, hydrolysis occurred quickly during the beginning of the anoxic phase (when S_S is needed for denitrification).

Figure 6-22 shows the evolution of the simulated and experimental ammonia and oxidized nitrogen during the cycle of the measurement campaign. The simulated values were obtained after conducting the dynamic calibration presented above. As can be seen, the simulated profile matches the experimental values.

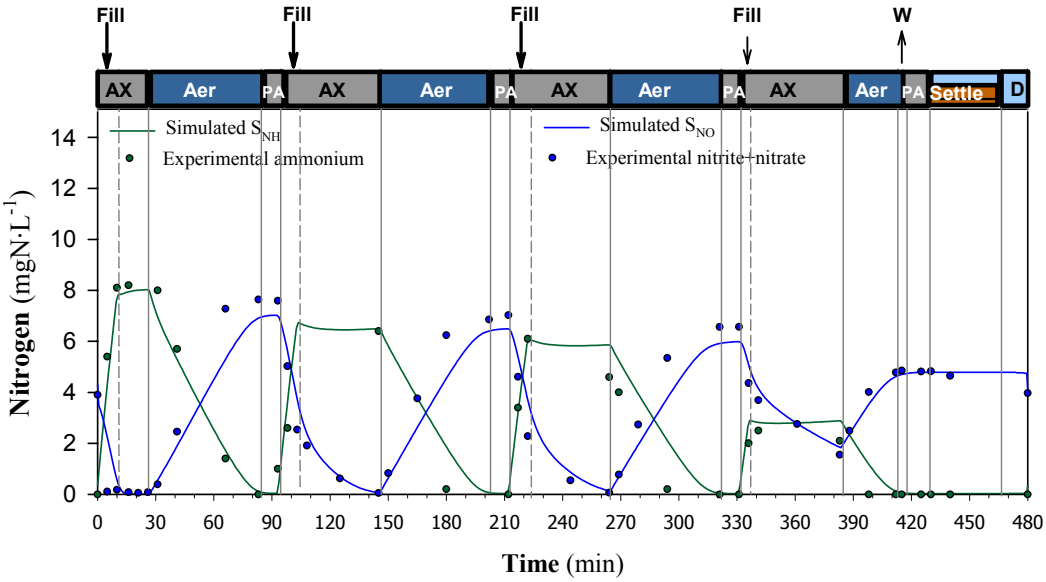


Figure 6-22. Simulated vs. experimental values for the nitrogen components during the cycle evolution period.

In Figure 6-23 the evolution of simulated and experimental DO concentration is presented. The first cycle on the left corresponds to the measurement campaign cycle working with an On-Off

controller and on the right the following cycle with the On-Off controller disabled. Thus, it can be seen that the dynamics of the simulated dissolved oxygen follow the experimental values closely. The last phases of the cycles correspond to the settling and therefore DO data are not reliable there.

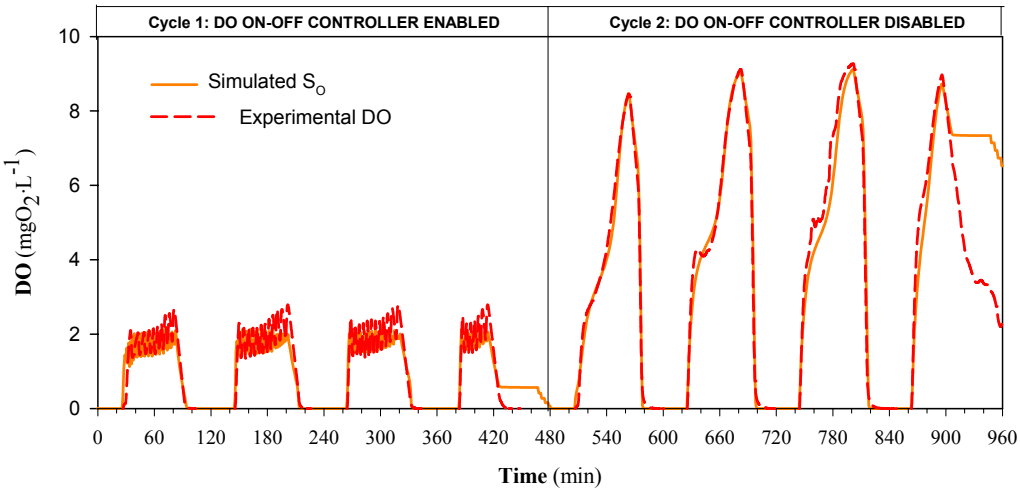


Figure 6-23. Simulated vs. experimental DO values for the cycle evolution period.

The values obtained in this calibration procedure are presented in Table 6-12. For the parameters that were not mentioned the ASM1 default value was used. It is worth comparing the calibrated values in this study with the ASM1 default values, and also with the values obtained in Chapter 5 with similar characteristics.

Table 6-12. ASM1 values obtained after stable-state and cycle evolution calibration.

Parameter	Symbol	Unit	default (20ºC)	This study	Previous study
Ammonification rate	k_a	$L \cdot (mgCOD \cdot d)^{-1}$	0.08	0.1	0.1
Correction factor for hydrolysis under anoxic conditions	η_H	-	0.4	1	-
Hydrolysis rate	k_H		3	-	2
Heterotrophic decay coefficient	b_H	d^{-1}	0.62	0.3	0.25
Autotrophic maximum growth rate	μ_A	d^{-1}	0.80	-	0.95
Ammonium substrate saturation constant for nitrifiers	K_{NH}	mg NH_3-N·L^{-1}	1.0	0.4	1.3
Oxygen substrate saturation constant for nitrifiers	K_{OA}	mg $O_2 \cdot L^{-1}$	0.4	-	0.25
g N(g COD)$^{-1}$ in biomass	i_{XB}	mg N·mg COD^{-1}	0.086	0.06	0.06
g N(g COD)$^{-1}$ in endogenous mass	i_{XP}	mg N·mg COD^{-1}	0.06	0.05	0.05
Oxygen mass transfer coefficient (1st aerobic phase)	K_La	d^{-1}	-	350	266

First of all, fewer parameters were changed during this calibration compared to the experience presented in Chapter 5 (6 compared to 8 parameters). Similar values were found regarding the ammonification rate, the decay and the nitrogen fractions of the biomass. In this study, the hydrolysis was adjusted with the correction factor for hydrolysis under anoxic conditions (η_H) whereas in the previous experience it was done with the hydrolysis rate (k_H).

7. Dynamic validation

The validation process consists in using the calibrated model with a set of data that is different from that used for calibration, to check whether the experimental and simulated values still fit well or not.

In this case, taking the values of the calibration as the initial conditions, the model was run from day 20 until day 70 (see Table 6-4) applying all the operating changes and taking into account the influent variability. Thus, the model inputs for each day were: influent composition, influent flow, wastage flow, effluent flow and reactor temperature. No changes in the kinetic or stoichiometric parameters or the K_La value were applied during this validation.

The results obtained in the validation using the measurement campaign of day 48, are presented in Figure 6-24 showing a good fit between the simulated and experimental values for the nitrogen compounds.

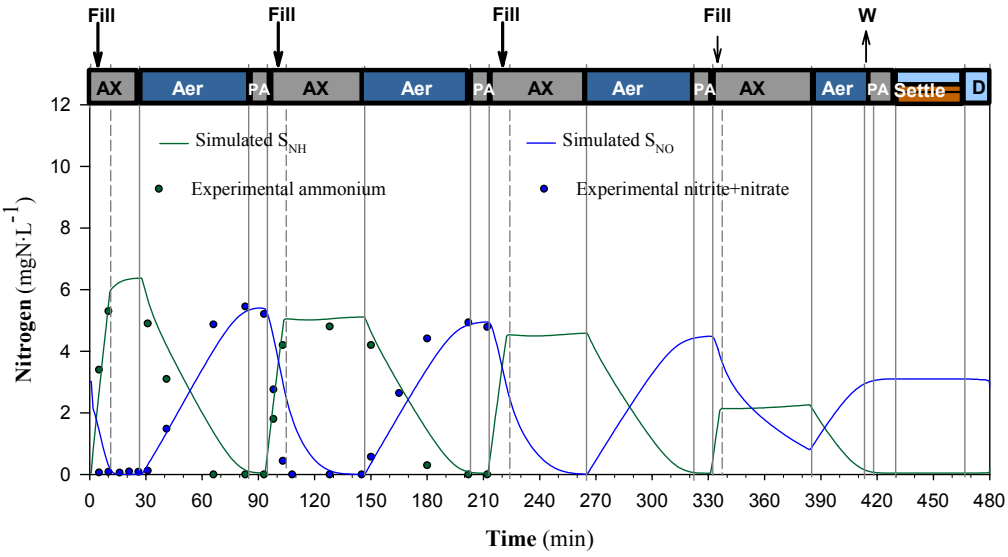


Figure 6-24. Validation during the second measurement campaign (Nitrogen compounds).

In Figure 6-25 the fit between the experimental and simulated DO concentration in the reactor is presented. In general, it shows a good fit. Nevertheless, for the first aerobic phase in the cycle in which the DO On-Off controller was disabled the trends were less well described. This could be related to a transient phenomenon. In Vanrolleghem *et al.* (2004) different causes for this

situation are analyzed: dynamics in the dissolved oxygen electrode, mixing characteristics, physicochemical phenomena (diffusion of substrate into activated sludge flocs) and finally a modeling error. In this case, the more probable causes would be the dynamics in the dissolved oxygen electrode and the modeling error.

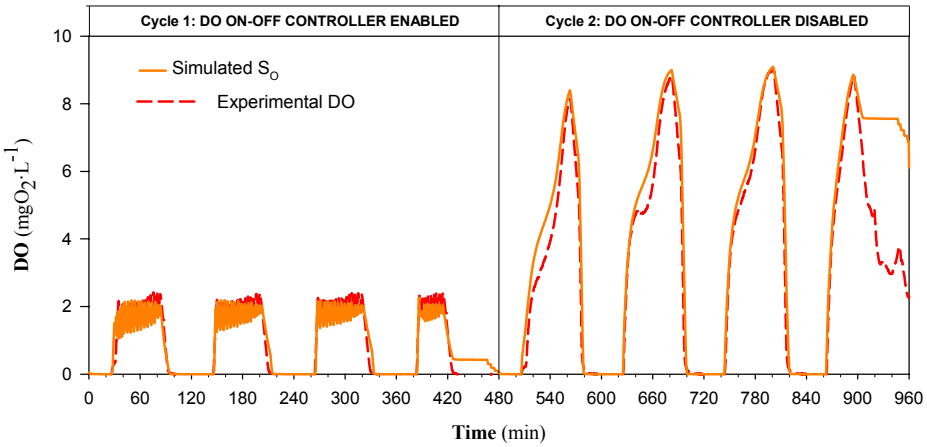


Figure 6-25. Validation during the 2nd measurement campaign (DO).

Finally, to make sure that the model is able to describe the behavior of the pilot plant, a simulation was performed during the whole study period. Hence, a validation was applied after preparing a dynamic influent file with the influent characterization for each day. The comparison between the simulated and experimental values is presented in Figure 6-26. The VSS evolution is presented in the upper part and the ammonia and oxidized nitrogen in the lower part.

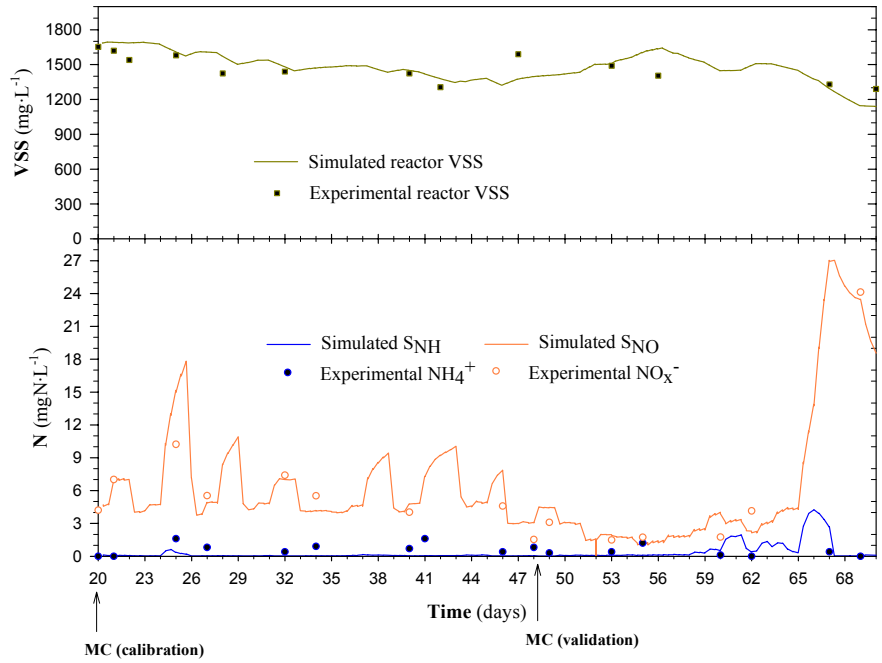


Figure 6-26. Results of the dynamic validation.

It can be seen that the dynamics in the solids concentration and in the nitrogen components are properly described over fifty days. The dynamics of the process can be described mainly due to the influent wastewater variability. During the last days of operation the effluent oxidized nitrogen increased due to a decrease in the organic load, which limited the denitrification process. This was properly described with the calibrated model.

STAGE V

8. Evaluation of the results.

Finally, when the entire process was completed it was necessary to evaluate whether the results of the calibration were in accordance with the objective of the calibration or not. If the objectives are not accomplished then the procedure should go back to step 2 of the calibration in which the decision about the information needed is taken.

In this case the objectives of the calibration were accomplished since the calibrated model was able to describe the SBR performance over seventy days, with varying influent and operating conditions that were applied to the model.

The quality of the fit between simulated values and experimental data was evaluated by calculating the Average Relative Deviation (ARD). For the calibration of the ammonia and oxidized nitrogen the ARD was 15% and 19% respectively. Thus, the trends of the ammonia and oxidized nitrogen were well predicted. For the DO profile the ARD calculated only during the aerobic phases was 8%. During the validation profiles the ARD was 14% for ammonium, 16% for oxidized nitrogen and 16% for the DO profile.

From the ARD results calibration can be considered accurate enough to obtain a good fit between the experimental and simulated values. This calibrated model is ready to be used for control purposes, and even for on-line simulation of the plant's behavior. Nevertheless, from a practical point of view, it is known that changes in the operating conditions may lead to changes in the microbial community of the system (Yuan and Blackall, 2002; Sin *et al.*, 2005b). This may in turn shift the behaviour of the system beyond the validity domain of the model. The underlying reason of this loss of validity is attributed to the inability of the used models to account for changes in the microbial community under quite different operational conditions (Sin *et al.*, 2005b).

Therefore, in order to adapt the model adjustment to microbial community changes, a periodic recalibration of the model must be considered. The procedure presented in this chapter can be the base to perform this recalibration successfully.

It has to be pointed that the methodology followed is based on the BIOMATH protocol also considering the improvements detected in the calibration presented in Chapter 5. These improvements are below explained:

- An accurate influent wastewater characterization combined with the estimation of the b_H and Y_H allowed to decrease the uncertainty in the influent wastewater characterization.
- The correct planning of the analytical measurements permit to gather all the necessary data, minimizing assumptions necessary when having lack of data.
- The validation during a long period fitting experimental and simulated values of the daily effluent values of the SBR.

Therefore, the methodology applied in this Chapter increases the reliability on the model and reduces the effort needed during the calibration step of Stage IV. However, the ARD values of this calibration study are similar to the ones obtained in the calibration presented in Chapter 5. Hence, the ARD values do not reflect the improvements of this calibration. In order to evaluate the real improvement further research would be needed by applying model falsification under different operating conditions. Alternatively, practical identifiability could be studied to check whether the available data is informative enough to identify the model parameters and give them a unique an accurate value (De Pauw, 2005).

6.4. CONCLUSIONS

The results obtained were in agreement with the main goal of the calibration, obtaining a model for the SBR able to describe the dynamics of the nitrogen compounds. Hence, it can be used as a support tool of a supervisory control system of the SBR. Thus, the calibration procedure was improved by taking into account the experience acquired in the previous calibration. More specific conclusions are:

1. The calibration procedure based on the BIOMATH protocol was successfully applied for the model calibration of the SBR.
2. An experimental data collection was defined during the first stage of the calibration what permitted to easily conduct the calibration.
3. An accurate influent wastewater characterization was conducted determining the S_S fraction and performing a BOD analysis, apart from the routine plant measurements.
4. The kinetic and stoichiometric parameters (b_H and Y_H) were obtained experimentally using respirometric assays and were successfully applied to the calibration procedure, making the stable-state and cycle evolution calibrations easier.

5. During the stable-state calibration the experimental determination of b_H, Y_H and the complete influent wastewater characterization permitted the reactor VSS to be predicted well. No further calibration of the X_I/X_S fraction was needed, what indicates decreasing uncertainty in influent wastewater characterization.
6. The N content of the biomass was adjusted with the experimental reactor TKN values.
7. During the cycle evolution calibration only a few parameters were adjusted (k_a, η_H, K_{NH}, K_La).
8. Adjusting the K_La using the DO profile proved to be a good methodology that saves the effort of its experimental determination.
9. Long-term validation was possible, so that a proper description of the process behavior was obtained by applying only the influent wastewater characterization and the operating conditions without modifying any kinetic or stoichiometric parameter.

SECTION 2

DEVELOPING A REAL-TIME CONTROL SYSTEM

General frame of section 2

Controlling the activated sludge process improves the functioning of the wastewater treatment plants by increasing the efficiency, optimizing the process and even increasing the reliability of the system. Moreover, the flexibility and the high automation degree of the SBR technology favour the implementation of control strategies.

The aim of this section is to develop a real-time control system to achieve the optimal operation of the carbon and nitrogen removing SBR. Different levels of control have been defined:

- The lower level control that is in charge of establishing and mantaining the operating conditions.
- The medium level of control is established by optimizing the length of the reaction phases, both the aerobic and the anoxic.
- The higher level is the supervision of the process and the consequent adaptation of the whole cycle structure.

This section is divided into four Chapters (7, 8, 9 and 10). In Chapter 7, knowledge is extracted from historical SBR studies, identifying patterns and possible options for detecting the nitrification and denitrification endpoints. In Chapter 8, a real-time control strategy is defined and this is evaluated by means of the calibrated model. In Chapter 9 the evaluated strategy is applied to a semi-industrial pilot plant treating real wastewater. Finally, in Chapter 10 a design proposal of a supervisory control system is presented.

Publications

Major part of this section 2 has been published in conference proceedings or peer review international journals. These publications are listed below with the complete reference:

- Part of Chapter 7 was presented in the ICA 2005 conference as oral presentation and it has been published in the journal Water Science and Tehcnology:
    - Puig S., Corominas Ll., Traore A., Colomer J., Balaguer M.D. and Colprim J. (2006). An on-line optimization of a SBR cycle for carbon and nitrogen removal based on on-line pH and OUR: the dissolved oxygen control role. *Wat. Sci. Tech.*, **53** (4-5), 171-178.

- The main part of Chapter 8 was presented in the ICA 2005 conference as oral presentation and it has been published in the journal Water Science and Technology.:

- Corominas Ll., Traore A., Sin G., Puig S., Balaguer M., Colprim J., and Vanrolleghem P.A. (2006). Model-based evaluation of an on-line control strategy for SBR's based on OUR and ORP measurements. *Wat. Sci. Tech.*, **53** (4-5), 161-169.

- The main part of Chapter 9 has been published in the journal Industrial & Engineering Chemistry Research:
  - Puig S., Corominas Ll., Vives M.T., Colomer J., Balaguer M.D. and Colprim, J., (2005). Development and Implementation of a Real-Time Control System for Nitrogen Removal Using OUR and ORP as End Points *Ind. Eng. Chem. Res*., **44**, 3367-3373.

- The main part of Chapter 10 has been accepted as oral presentation in the Small Water and Wastewater systems conference:
  - Corominas Ll., Puig S., Balaguer M.D., and Colprim J.(2006). A supervisory control system to manage and optimize a SBR performance for nutrient removal. In: *7th IWA Specialised Conference on Small Water and Wastewater Systems*. Mexico City, Mexico, March 7-10, 2006 (CD-Room).

7 Identifying control options for the nitrogen-removing SBR

7. IDENTIFYING CONTROL OPTIONS FOR THE NITROGEN-REMOVING SBR

7.1. MOTIVATION

The activated sludge process has to be conducted under controlled operating conditions to permit the bacteria responsible for organic matter and nitrogen removal to carry out their activity properly. The environmental parameters influence the process and therefore they have to be maintained at desired levels. Within this context, the development of instrumentation (e.g. on-line sensors) is decisive for the application of control and automation.

In the case of SBR systems, the use of on-line sensors can serve not only for monitoring, but also for understanding the processes occurring in the reactor better. The evolution of their signal can be used to assess the process performance and even to implement control strategies. This can be achieved by identifying possible patterns in these signals that are related to the end of the reactions. In this Chapter the patterns described in the literature are identified in several historical case studies to obtain a conceptual background for generating different ideas for controller. Special attention is given to the control of the dissolved oxygen (DO) during the aerobic phases since it can influence other variables and hence, to higher levels of control.

7.2. MATERIALS AND METHODS

The methodology consisted in extracting knowledge from historical SBR case-studies (Vives, 2004 and Puig, 2004) and new experiences, identifying patterns and also the possible control options. Data from a lab-scale pilot plant and from a semi-industrial pilot plant were analyzed.

Lab-scale pilot plant

The lab-scale pilot plant SBR located at the Laboratory of Chemical and Environmental Engineering (see point 3.1.1) worked at a fixed cycle of 8 hours alternating anoxic and aerobic phases. Two studies were performed in this pilot plant (Case 1 and Case 2), applying different operating conditions (number of filling events, M; maximum volume, V_T; volumetric exchange ratio, R_E; the type of DO control) and working with synthetic wastewater. Table 7-1 summarizes the main operating conditions of these studies.

An important variable for controlling the process is the OUR, which can be calculated from the DO data when using a DO set-point control. In Case 2, an On-Off DO controller was implemented by using an On-Off valve, and thus the OUR was calculated (in this case off-line) obtaining discrete values, as presented in Table 7-1.

Table 7-1. Operating conditions for the two case-studies in the lab-scale pilot plant.

	Case 1	Case 2
Wastewater	Synthetic	Synthetic
M	2	4
V_T (L)	30	23
R_E	0.42	0.30
DO control	No	On-Off
OUR calculation	No	Discrete values (Off-line)

Semi-industrial Pilot Plant

This plant has already been described in point 3.1.1. The main advantage is that it can be set up at a WWTP and treat fresh wastewater from sewer system that arrives at the facility. Two case studies were conducted locating this plant at two different WWTPs (Case 3 and Case 4) following an eight hour cycle alternating six anoxic-aerobic reaction phases, operating at 20 days SRT. The main operating conditions are presented in Table 7-2.

Table 7-2. Operating conditions for the two case-studies in the semi-industrial pilot plant.

	Case 3	Case 4
Wastewater	Real	Real
M	6	6
V_T (L)	683	716
R_E	0.30	0.33
DO control	On-Off	Fuzzy
OUR calculation	Discrete values (On-line)	Continuous values (On-line)

In Case 3 the DO was controlled using an On-Off valve and in Case 4 a variable frequency engine, coupled with the blower, was installed together with an air flow meter. The OUR was calculated on-line, obtaining discrete values with the On-Off controller and continuous values with the Fuzzy controller (see Table 7-2). Thus, the calculation is different when using an On-Off controller than when using a continuous DO controller.

Calculating OUR using an On-Off DO controller

The mass balance for oxygen in a well-mixed region of the SBR is presented in Equation 7-1, though it must be taken into account that no influent or effluent flow occurs in an SBR during the reaction phase:

$$\frac{dSo}{dt} = K_L a^{(T)} \cdot (So_{sat}^{(T)} - So) - OUR \qquad \text{Equation 7-1}$$

where:

So=DO concentration in the reactor, $mg \cdot L^{-1}$; $So_{sat}^{(T)}$=saturation DO concentration, $mg \cdot L^{-1}$; $K_L a^{(T)}$=oxygen mass transfer coefficient, h^{-1}; T=temperature, ºC.

Nevertheless, during air off periods, the mass balance can be reduced to Equation 7-2:

$$\frac{dSo}{dt} = -OUR \qquad \text{Equation 7-2}$$

This OUR calculation does not account for the surface aeration. Nevertheless, for controlling purposes the evolution in the OUR measurements is the key point and not the absolute values themselves. Thus, the effect of the surface aeration is considered small and constant during the operation, and therefore not affecting the trends of the signal.

Hence, to obtain the oxygen consumption only the DO derivative has to be determined during air off periods. This can be done by measuring the decrease in DO as a function of time due to biological activity, which is equivalent to approximating the differential terms with a finite difference term. The dynamic of the sensor must be taken into account and therefore the first measurements (50 seconds) after deactivating the aeration system are not used. Next, DO values are acquired until the airflow is switched-On again, and finally the linear regression can be obtained.

Calculating OUR using a continuous DO controller

The calculation of OUR is presented in Equation 7-3, which has been obtained directly from Equation 7-1. It depends on the oxygen mass transfer coefficient (K_La), the dissolved oxygen concentration (So), the dissolved oxygen saturation concentration (So_{sat}) and the derivative of the oxygen concentration (dS_O/dt):

$$OUR = K_L a^{(T)} \cdot (So_{sat}^{(T)} - S_O) - \frac{dS_O}{dt} \qquad \text{Equation 7-3}$$

The different terms of Equation 7-3 can be calculated as follows:

A) $K_La^{(T)}$ calculation: K_La depends on the airflow rate, the partial pressure of oxygen, the dissolved oxygen saturation concentration, the volume, the type of diffusers and the temperature. $K_La^{(T)}$ is calculated using Equation 7-4.

➢ $$K_L a^{(T)} = \frac{\alpha \cdot Q_{air} \cdot \eta \cdot y_{O_2} \cdot 1333.3}{V \cdot So_{sat}} \cdot \theta^{(T-20)} \Rightarrow d^{-1} \qquad \text{Equation 7-4}$$

where,

Q_{air} : Air flow rate ($m^3 \cdot d^{-1}$).

y_{O_2} : Fraction of oxygen in air = 21%.

V : aeration volume (m^3) .

So_{sat} : Dissolved oxygen saturation concentration ($g \cdot m^{-3}$).

and the correction factors are,

1333.3 = g $O_2 \cdot m^{-3}$ unit conversion.

θ : Temperature correction factor.

α : Factor to correct the parameters of the device which are normally determined for a range of operating conditions using tap water. Values of α vary with the type of aeration device, the basin geometry, the degree of mixing and the wastewater characteristics. The values for diffused aeration equipment are in the range of 0.4 to 0.8 (Metcalf & Eddy, 2003).

$$\alpha = \frac{K_L a(\text{wastewater})}{K_L a(\text{tap water})} \qquad \text{Equation 7-5}$$

η : Is the Standard Oxygen Transfer Efficiency and it is a factor that accounts for the efficiency of oxygen transfer. It depends on many factors such as the type, size and shape of the diffuser, the air flow rate, depth of submersion, tank geometry and wastewater characteristics.

B) $So_{sat}^{(T)}$ calculation: This depends on the temperature and the atmospheric pressure. Equation 7-6 has been obtained from adjusting a third order polynomial to the Henry's constant values at different temperatures obtained from Foust *et al.* (1960).

➢ $$So_{sat}^{(T)} = P_{atm} \cdot \left[14.515 - 0.3286T + 4.173 \cdot 10^{-3} T^2 - 1.815 \cdot 10^{-5} T^3\right] \Rightarrow mg \cdot L^{-1} \qquad \text{Equation 7-6}$$

where,

P_{atm}=Atmospheric pressure (atm).

T= Temperature (ºC).

C) Derivative of oxygen concentration: The derivative is approximated to small increments calculating the difference in the DO concentration at each time interval of the monitoring software.

➢ $$\frac{dSo}{dt} = \frac{\Delta So}{\Delta t} = \frac{S_{O(t)} - S_{O(t-1)}}{\Delta t} \Rightarrow mgO_2 \cdot L^{-1} \cdot d^{-1} \qquad \text{Equation 7-7}$$

7.3. RESULTS

In the SBR technology, the variables pH, ORP, DO and OUR (which can be easily measured or calculated) can give valuable information about the state of the process. In the case of carbon and nitrogen removal processes, these variables can show patterns which indicate the end of the nitrification and denitrification reactions (see point 1.3.4.2).

As one of the objectives of the chapter is to study the effect of DO control on the identification and detection of the endpoints, the four different historical cases defined in point 7.2 are discussed separately in the next points.

The analysis of each case is performed based on the evolution of the on-line variables (pH, ORP, DO and OUR) during one cycle of the SBR under stable state conditions. In Cases 1 and 2 the on-line measurements were complemented with the off-line analysis of ammonium and oxidized nitrogen. Cases 2, 3 and 4 are focused on the aerobic phase and specifically on the OUR profiles. For each case, the type of aeration control is described and then a discussion on the identified endpoints and the possibilities of detecting them is presented.

7.3.1. Case 1: Lab-scale without DO control

In the first study a two step feed strategy was implemented in the lab-scale pilot plant (Figure 7-1), treating 10L of synthetic wastewater per cycle. The volumetric exchange ratio was 0.42 and the mean influent COD and TKN concentrations were 650 mgCOD·L^{-1} and 80 mgN-TKN·L^{-1} respectively.

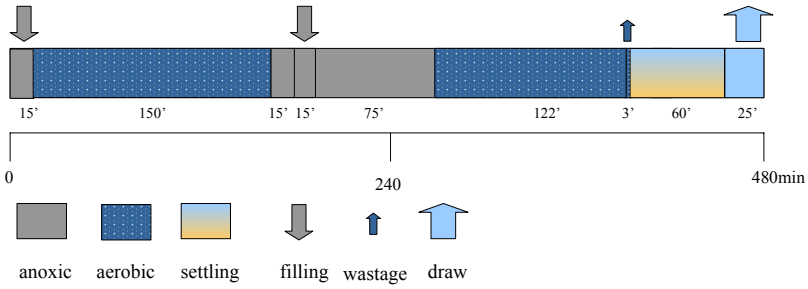


Figure 7-1. Cycle configuration for Case 1.

Figure 7-2 presents the results of a measurement campaign of an eight hour cycle conducted when the system was under stable conditions. The evolution of the off-line analysis (NH_4-N, NO_2-N and NO_3-N) is presented in Figure 7-2-A, and the on-line measurements (pH, ORP and DO) in Figure 7-2-B.

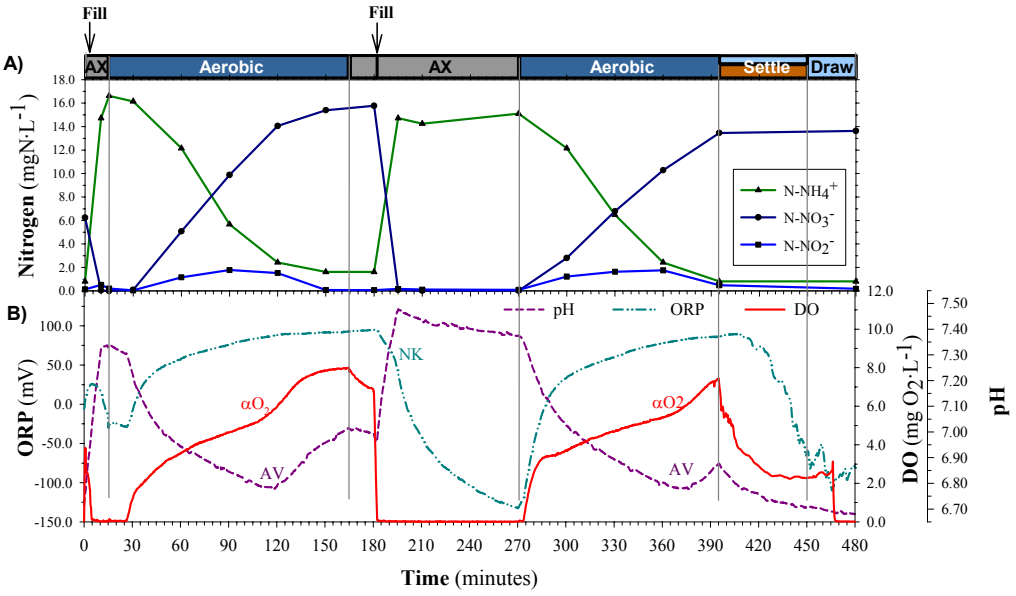


Figure 7-2. Measurement campaign for Case 1.

Aerobic phase

No DO control was used. From the DO profile it can be seen that there is an excess in the aeration supply, which affects both the process (there are high oxygen concentrations at the beginning of the anoxic phase) and the cost of the treatment (excess of aeration energy).

Identified endpoints

The measurement campaign reveales that complete nitrification and denitrification occur during aerobic and anoxic conditions respectively. In aerobic phases, once ammonium is below 2 $mg \cdot L^{-1}$ and stable (Figure 7-2-A), a minimum in the pH, the so-called Ammonia Valley (AV), and a flexion point in the DO profile (αO_2) can be observed (see Figure 7-2-B, at minutes 110 and 370).

During anoxic phases, when all nitrate has been consumed (end of denitrification) a bending point in the ORP profile appears at minute 190 which is called Nitrate Knee (NK, in Figure 7-2-B).

Endpoint detection

In the measurement campaign presented in Figure 7-2 it can be observed that the cycle could be optimized, mainly during the aerobic phases. The first aerobic phase could be shortened by 60 minutes and the second anoxic phase by 80 minutes.

Therefore, an optimization of the aerobic phase could be performed by detecting the AV and the αO_2. This implies detecting on-line a minimum in the pH and an inflexion point in the oxygen profile. The length of the anoxic phase can be adjusted by detecting the NK, an inflexion point in the ORP profile.

7.3.2. Case 2: Lab-scale with On-Off DO control

In a second study the lab-scale SBR was designed to treat 7L of influent synthetic wastewater per cycle, determining a volumetric exchange ratio of 0.3 and applying an eight hour cycle using a step feed strategy (Figure 7-3).

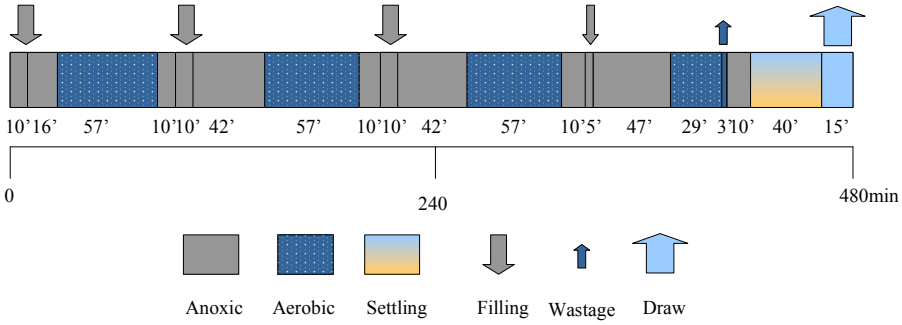


Figure 7-3. Cycle configuration for Case 2.

Feeding the SBR was split into four parts (2L+2L+2L+1L). The last filling was half the size of the others to ensure low nitrogen concentration values in the discharge due to the dilution effect. After the aerobic phases, there were Pre-Anoxic phases (PA) of 10 minutes to get information used for modeling purposes (see Chapter 6). The mean influent COD and TKN concentrations were 545 mgCOD·L^{-1} and 75 mgN-TKN·L^{-1}.

Figure 7-4 presents the results of a measurement campaign during an eight hour cycle of the pilot plant SBR under stable conditions. The evolution of nitrogen compounds is presented in Figure 7-4-A, and the on-line measured profiles (pH, ORP, DO and OUR) are shown in Figure 7-4-B.

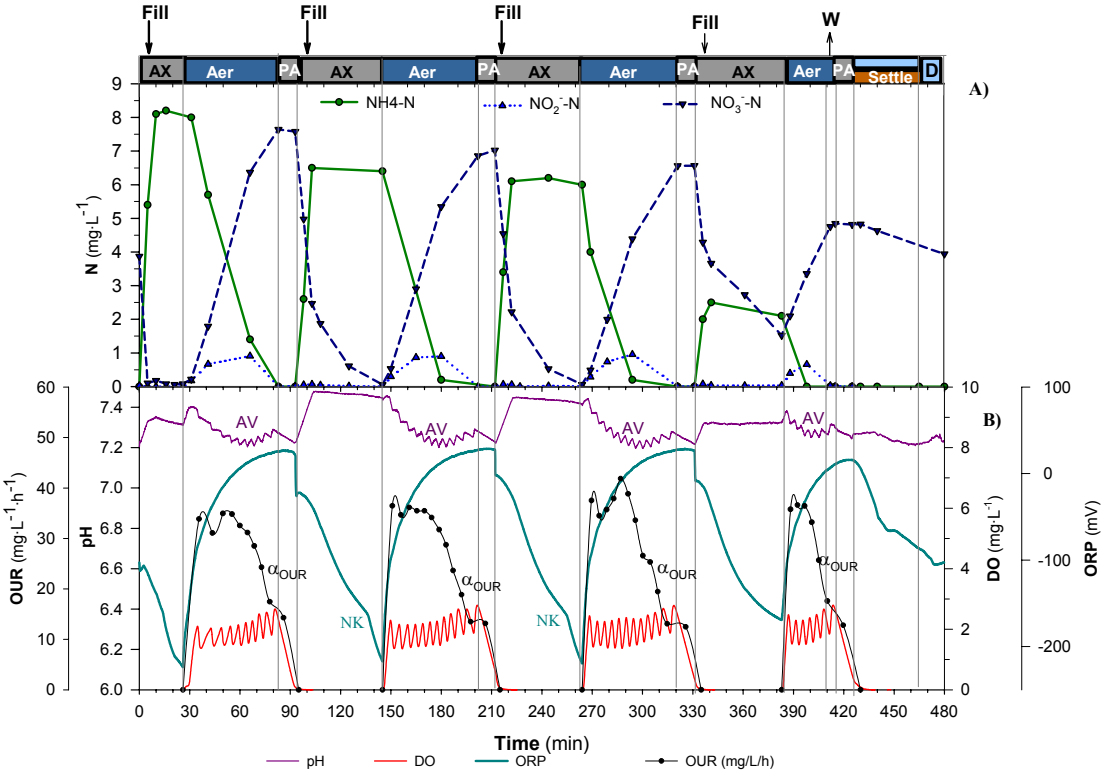


Figure 7-4. Measurement campaign for Case 2.

Aerobic phase

In this case an On-Off controller for the DO was implemented establishing a set-point value of 2mgDO·L^{-1} (see Figure 7-4-B). Implementing a DO controller can represent an advantage in terms of saving energy. Moreover, it can lead to improving the denitrification capacity since the remaining DO at the end of the aerobic phase can be reduced (with low DO set-points), and the complete anoxic conditions are achieved more quickly. It can be seen in Figure 7-4-B that the DO needs 10 minutes (the PA phase) to go from 2mg·L^{-1} to 0 mg·L^{-1}. Thus, finishing the aerobic phases with low DO concentration means that during the feeding (at the beginning of the anoxic phase) the major part of the readily organic matter is depleted anoxically, and its aerobic consumption is minimized.

In addition, implementing the DO controller permits calculating the OUR and its evolution can also give information about the state of the process.

Identified endpoints

In the aerobic phases, the AV appears when ammonium concentrations below 1 $mg \cdot L^{-1}$ are reached (see Figure 7-4-B, at minutes 60, 180, 300 and 400). The fluctuations in the pH signal are caused by the airflow being switched On and Off, which is directly related to the CO_2 stripping.

The discrete values of OUR are also presented in the Figure 7-4-B. These values are obtained by calculating the slope in the DO each time the airflow is switched Off (see point 7.2). It can be seen that ammonia depletion coincides with a sharp decrease in the OUR values. This decrease is called α_{OUR} and is related to the nitrifiers' reduced activity due to the depletion of their substrate (NH_4^+).

During anoxic phases, the NK (in the ORP profile, at minutes 10, 135 and 250) indicates the end of the denitrification process.

Endpoint detection

The cycle during aerobic phases can be optimized by detecting the AV. However, the pH signal fluctuates due to the On-Off aeration control, which makes detecting the minimum complicated. Hence, the α_{OUR} can be used for detecting the endpoint of ammonia depletion. This implies detecting the sharp decrease in the OUR profile.

The length of the anoxic phase can be adjusted by detecting the NK, the inflexion point in the ORP profile.

7.3.3. Case 3: Semi-industrial scale with On-Off DO control

This case implies a scale-up of the process, from lab-scale (23L maximum volume) to semi-industrial scale (683L of maximum volume), and uses real wastewater instead of synthetic.

The semi-industrial SBR was located at the Cassà-WWTP treating real wastewater with average concentrations of 532±220 mg COD $\cdot L^{-1}$ and 53.6±25.0 mg N $\cdot L^{-1}$. The SBR treated 200L per cycle, with a volumetric exchange ratio of 0.3 and worked at a fixed cycle of eight hours to remove organic matter and nitrogen (Figure 7-5).

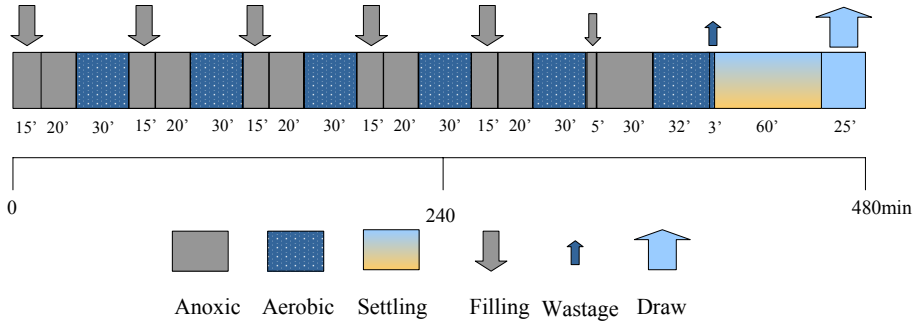


Figure 7-5. Cycle configuration for Case 3.

Once the system was stable an analysis of the on-line variables was performed using the data from an eight hour cycle of the SBR when nitrification/denitrification was completed. Figure 7-6 shows profiles of pH, DO and OUR, and the identified bending points.

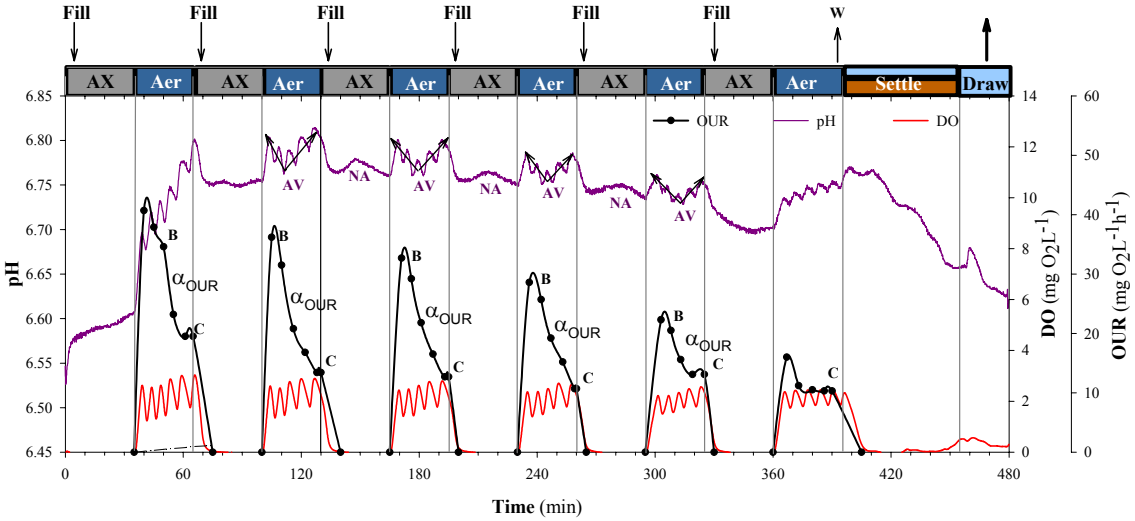


Figure 7-6. pH, DO and OUR profiles during the 8 hour cycle length used in the Pilot Plant SBR.

Aerobic phase

In this case an On-Off DO controller was used with a set-point value of 2mg·L^{-1}, as in Case 2. As stated before, implementing this controller results in a reduction in the aeration energy used and an improvement in the denitrification capacity of the system.

Identified endpoints

In the aerobic phases, the AV appears at minutes 115, 180, 245 and 315 as presented in Figure 7-6. Nevertheless, the AV cannot be easily observed because of the stripping effect of the On-Off aeration control causing fluctuations in the pH profile as in Case 2. At the same time, the calculated OUR data plotted in Figure 7-6 shows a sudden decrease in the OUR from point B to C (α_{OUR}) caused by the end of ammonia depletion. Then, the calculated OUR data stays in a flat pattern until the end of the aerobic phase (Figure 7-6, point C). Such a stable minimum OUR value (OUR_V), clearly observed during the last aerobic phase, indicates that the system is under endogenous conditions and at least 95% of the organic material in the waste has been treated (Watts and Garber, 1995).

During anoxic phases, the appearance of the Nitrate Apex (NA, in the pH profile at minutes 150, 215 and 280) indicates the end of the denitrification process. Nevertheless, NA may not be observed in all the conditions since within the charges equilibrium many factors interact (e.g. charge of the carbon source, alkalinity, other species...) that can modify the pH trend.

Endpoint detection

As in Case 2 the α_{OUR} can be used for detecting the nitrification endpoint. The pH signal could also be used but care should be taken with the fluctuations which make it difficult to detect the minimum. Another possibility which is more conservative is to make sure that the system is under endogenous conditions before changing from aerobic to anoxic conditions. This is achieved by detecting the OUR_V, the stabilization of the OUR.

The length of the anoxic phase can be adjusted by detecting the NA in the pH profile. Although an ORP profile is not presented in this case, these sensors can also give useful information as explained in Cases 1 and 2.

7.3.4. Case 4: Semi-industrial scale with Fuzzy DO control

The semi-industrial SBR was located at the Celrà-WWTP. It worked at a fixed cycle treating 233L per cycle of real wastewater with an average composition of 494 mg COD $\cdot L^{-1}$ and 49.9 mg N $\cdot L^{-1}$. The volumetric exchange ratio established was 0.33, and the cycle used was the same as that presented in Case 3 (see Figure 7-5).

The evolution of pH, DO and OUR during one cycle of SBR operation under stable conditions is presented in Figure 7-7.

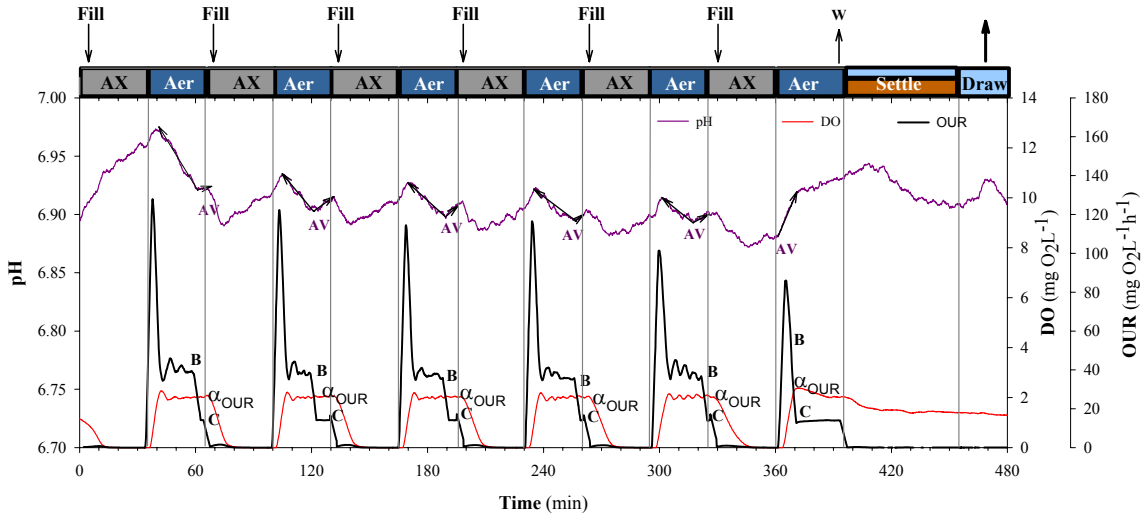


Figure 7-7. pH, DO and OUR profiles during one cycle using Fuzzy DO control.

Aerobic phase

A continuous DO controller was implemented. It was based on a Fuzzy logic strategy and was implemented after installing a variable frequency engine coupled with an air flow meter. The developed Fuzzy DO controller, a Mamdani FIS (Mamdani, 1975), was based on the error between the DO measured and the DO set-point, and the cycle phase number running. The output was the air quantity injected into the reactor via the voltage supplied to the engine. This structure (only two inputs and one output) allows a simple representation of the various Fuzzy rules, and integrates and interprets human knowledge easily. A complete description of the Fuzzy DO controller can be found in Traoré *et al.* (2005). Figure 7-7 shows that the pH and DO fluctuations observed in the previous On-Off control strategy (Figure 7-6-DO profile) were considerably reduced due to the continuous adjustment of the air flow injection. Measured DO values were always between 1.9 and 2.1 $mgO_2 \cdot L^{-1}$.

One of the advantages of using a continuous DO controller was the possibility of obtaining a continuous OUR profile with more available OUR values. Thus, the OUR was calculated with Equation 7-3, applying the following correction factors: θ=1.024, α =0.8 and η=0.07.

Identified endpoints

During aerobic phases the AV appears in the pH profile at minutes 60, 120, 190 and 320 (Figure 7-7). This bending point appears at the same time as another bending point related to OUR evolution, i.e. the α_{OUR} (decrease between point B and C, Figure 7-7). Moreover, all aerobic phases reach a final OUR constant value (OUR_V; point C, Figure 7-7). This final, nearly flat OUR value can be used to identify when the endogenous conditions are reached and that organic matter, ammonia and nitrite have been completely oxidized.

The sharp increase in the OUR profile observed at the beginning of aerobic phases could be related to high activity of the microorganisms. Nevertheless, the magnitude of the values is quite high, which are related to the non-linear calculation of the OUR.

Endpoint detection

The AV (minimum in the pH) and the α_{OUR} (sharp decrease in the OUR) can be used for detecting the endpoint of ammonium depletion. Moreover, the OUR_V (stabilization of OUR) can be used as an indicator of the depletion of organic matter, ammonium and nitrite.

7.4. DISCUSSION

The analysis of the historical data shows that pH, ORP, DO and OUR are potential variables to be used for control purposes since they can be used to detect the endpoints of nitrification and denitrification. It may be possible to optimize the aerobic and anoxic stages using the identified endpoints in the control variables to adapt the cycle length to the influent characteristics without

affecting the effluent quality. The control variable and identifying the endpoints depends on the type of phase: aerobic or anoxic. In the aerobic phase the type of DO control is crucial.

From the analysis of the four cases it can be concluded that it is feasible to implement a control strategy for the SBR, both at a lower level controlling the DO, and at a second level that determines the end of the reaction phases.

The lower level of control for the aerobic phases controls DO at a value defined by expert knowledge and based on the objectives of the treatment. When dealing with organic matter and nitrogen removal a level between 1 and 2 $mg \cdot L^{-1}$ is recommended. There are two possibilities for controlling the DO as seen in the historical examples: A discrete controller (On-Off) and continuous controller (Fuzzy).

The On-Off controller is characterized by a huge fluctuation in the DO profile around the set-point and permits discrete OUR values to be calculated, from which meaningful information can be extracted. The continuous controller is characterized by a tiny overtaking around the set-point and allows a continuous OUR profile to be obtained, which increases the possibilities of control. Fuzzy control is now being applied for DO control, instead of the traditional PID (Proportional, Integral and Derivative), since it is able to overcome naturally occurring process changes (Turmel *et al.*, 1998; Traoré *et al.*, 2005).

The second level of control would permit adjusting the length of the reaction phases based on identifying and detecting the endpoints. Table 7-3 presents a summary of the knowledge acquired, describing the possible control variables and the bending point identification for the reaction phases, taking into account the type of DO control used.

Table 7-3. Identifying the control variables for the aerobic and anoxic phases.

Phase	DO control used or not	Type of DO control	Control Variable	Identification	Bending point
Aerobic	No DO control	-	DO pH	**αO_2** **Ammonia Valley**	Inflexion point Minimum
	DO control	On/Off	Discrete OUR	**α_{OUR}** **OUR_v** Ammonia Valley	Decrease Stabilization Minimum
		Continuous	Continuous OUR Continuous OUR pH	**α_{OUR}** **OUR_v** Ammonia Valley	Decrease Stabilization Minimum
Anoxic	-	-	ORP	**Nitrate Knee**	Inflexion point
	-	-	pH	Nitrate Apex	Maximum

***** The identification options marked in bold are the more appropriate options

It has been shown that when no DO control is used the αO_2 in the oxygen profile can be detected and the pH signal has no fluctuations, which makes detecting the AV easier. When applying a discrete DO controller the pH has high fluctuations, which makes it not so reliable. However, the OUR can be calculated and this also provides good information about the process (mainly the OUR permits detecting the end of nitrification, α_{OUR}). The possibility of using a continuous DO controller gives the advantage of obtaining a continuous OUR profile and a pH profile with fewer fluctuations compared to the On-Off controller. Hence, it is possible to establish a control strategy based on both variables, the pH and the OUR, so it is possible to detect not only the end of nitrification (AV, α_{OUR}) but also the carbon, ammonia and nitrite depletion (OUR_V).

NK is a robust parameter for the anoxic phases and therefore it can be used as the endpoint for the anoxic phases. Another possibility is the NA in the pH signal but this is dependent on the influent wastewater characteristics and is not always detected.

Finally, implementing the strategies would require dynamically detecting the minimum, maximum or flexion points, using filtering methods, derivatives and episode representation (Rubio *et al.*, 2004). Nevertheless, a simpler alternative could be based on using fixed set-points for the controlled variables.

7.5. CONCLUSIONS

The analysis of historical data permitted detecting several control points that are related to the end of the biological reactions. For the aerobic phase these points were the AV, the αO_2, the α_{OUR} and the OUR_V. Regarding the anoxic phases, the NK and the NA were identified. More specific conclusions are:

1. Implementing a DO controller permitted the OUR to be calculated. When using an On-Off controller the OUR values were obtained discretely and using a continuous DO controller, the OUR was obtained continuously.
2. The type of DO controller affected the possible control variables for the aerobic phase:
   > Without DO control, the suitable control points were the AV and the αO_2.
   > Using an On-Off DO control, the suitable control points were the α_{OUR} and the OUR_V. In this case the detection of the AV was conditioned by the fluctuations in the pH signal.
   > Using a Fuzzy DO control, the best control options were α_{OUR} and the OUR_V. However, in this case the AV could be also used because the use of a continuous controller overcame the problem of fluctuations in the pH signal.
3. For the anoxic phase the NK was the suitable control variable.

8

Model-based optimization of an SBR

8. MODEL-BASED OPTIMIZATION OF AN SBR

8.1. MOTIVATION

The SBRs normally operate below their capabilities working at a fixed cycle configuration with fixed lengths for the reaction phases. However, the nature of the SBR, able to deal with a flexible operation, together with a high degree of automation favours implementing control strategies which increase the benefits of SBR operation. Hence, the SBR performance, the energy requirements, the treatment capacity and the process efficiency can be optimized.

The previous Chapter presents the potential variables to be used to control the reaction phases. In this Chapter, these variables are used to define a medium level of control to adjust on-line the length of the aerobic and anoxic phases of the cycle. First of all, a control strategy is developed and implemented in a simulating platform including the calibrated model. Then, a simulation procedure is applied for evaluating the effectiveness of the control strategy using process indices.

8.2. MATERIALS AND METHODS

Pilot plant model

The model used in this study was the one obtained in Chapter 5, using WEST software for the calibration and following a stepwise procedure based on the BIOMATH protocol. The evaluation of the calibration process showed that it was possible to use this model to define and test control strategies. The final state of the simulation conducted for the validation of the model was taken as the initial conditions to start the model-based evaluation. The same operation for Period 2 described in point 5.2.1 was applied.

Software

The software used in this model-based evaluation was GPS-X and Matlab. Thus, the layout was configured according to the operating conditions of the validation profile (see Chapter 5) and then the parameter values and the initial conditions were transferred from WEST to GPS-X. Moreover, Matlab was linked to GPS-X and was used to code the control strategy.

Simulation procedure

Simulations were run for seven days with varying influent composition data and constant influent flow as presented in Table 8-1.These measurements were obtained from Period 2 of operation presented in point 5.2.1.

Table 8-1. Influent composition and flow for each simulated day.

Measurement	Day						
	1	2	3	4	5	6	7
COD_T ($mg \cdot L^{-1}$)	670.3	503.9	645.67	682.5	729.9	639.9	789.6
NH_4^+ ($mg \cdot L^{-1}$)	78.4	66	79.21	78.6	74.4	79.9	79.2
Influent Flow ($L \cdot d^{-1}$)	30						

The time interval was set at 10 seconds, which was the time established for action for the experimental pilot plant DO On-Off controller. A first-order delay of 30 seconds in the DO variable was considered during the simulations to account for the delay observed in the DO probe of the Pilot Plant.

Evaluation indices

Three indices were used to evaluate the process performance: The Effluent Quality (EQ), the Aeration Energy (AE) and the treated volume (V_t). These indices were calculated using data from the seven days of simulation (t=7).

- The EQ index presented in Equation 8-1 was adapted from Copp (2001) and was calculated using the average effluent Total Suspended Solids concentration (TSS), total COD, Total Nitrogen (TN), BOD_5 and wastewater flow (Qe).

$$EQ = \frac{1}{1000 \cdot t \cdot Vt} \int_{t_0}^{t} [2 \cdot TSS(t) + COD(t) + 20 \cdot TN(t) + 2 \cdot BOD_5(t)] \cdot Qe(t) \cdot dt \quad (Kg \cdot d^{-1} \cdot L^{-1}) \qquad \text{Equation 8-1}$$

  The EQ index was also expressed as a function of the V_t since the length of the phases was different in each cycle, which influenced the amount of water treated.

- The AE index presented in Equation 8-2 was calculated by integrating the energy required per time interval (calculated with Equation 8-3) and dividing by the total time and the volume of treated wastewater.

$$AE = \frac{24}{t \cdot V_t} \int_{t_0}^{t} (energy) \cdot dt \quad (KW \cdot h \cdot d^{-1} \cdot L^{-1}) \qquad \text{Equation 8-2}$$

$$energy = \frac{\frac{Q_{air} \cdot \rho_{H_2O} \cdot g \cdot H}{86.4 \cdot 10^6}}{\eta_{pump}} \ (KW) \qquad \text{Equation 8-3}$$

where AE is the Aeration Energy Required ($kW \cdot h \cdot d^{-1} \cdot L^{-1}$), energy is the aeration energy for each time interval (kW), Q_{air} is the air flow rate ($m^3 \cdot d^{-1}$) which is calculated from the K_La using

Equation 7-4, ρ_{H2O} is the density of water ($Kg \cdot m^{-3}$), g is the gravity ($m \cdot s^{-2}$), H is the hydraulic head (m) and η_{pump} the pump efficiency (unitless).

For calculating the accumulated energy, the variable "cumulative blower energy required (Kw·h)" given directly by GPS-X (Hydromantis, 2003) was used.

- The V_t index was calculated by integrating the volume of treated wastewater during the seven days of simulation as presented in Equation 8-4.

$$V_t = \int_{t_0}^{t} Q_I(t) \cdot dt \ (L) \qquad \text{Equation 8-4}$$

where Q_I is the influent flow rate.

8.3. RESULTS

8.3.1. Background

Defining the on-line control strategies correctly is very important for successfully optimizing the SBR performance. As presented in Chapter 7, optimal reaction phase length can be based on detecting the endpoints of the nitrification and denitrification processes. The expert knowledge already presented in Table 7-3 gives indication of the possible control variables that can be used to establish an open loop control. Based on expert knowledge and with the help of a calibrated model, different control strategies can be proposed and evaluated before they are implemented in a pilot plant or full-scale system.

The possibilities for optimizing the functioning of the lab-scale pilot plant under the proposed operating conditions can be assessed after simulating an eight hour cycle, and analyzing the profiles obtained of the nitrogen compounds together with the OUR evolution. Figure 8-1 shows the simulation of one cycle using an On-Off DO controller during the aerobic phases. The state variables ammonia (S_{NH}) and the sum of nitrites and nitrates (S_{NO}) are shown in Figure 8-1-A, the evolution of OUR in Figure 8-1-B and the derivative of OUR is presented in Figure 8-1-C.

It can be seen in Figure 8-1-A that the cycle can be optimized (see grey zones) when the ammonium is completely depleted about 20 minutes before finishing the phase. Nevertheless, the anoxic phases cannot be improved much since the nitrate concentration achieves low values just at the end of the phase.

In this study more effort is put into the aerobic phase, and specifically into the OUR variable. At the beginning of the aerobic phases, a fast increase in the OUR is observed (Figure 8-1-B) because the rates of heterotrophic and autotrophic growth are high. As soon as the ammonia is

depleted (Figure 8-1-A, circles), a drop in the OUR profile can be observed (α_{OUR}). After that, the OUR profile remains constant (OUR_V) which indicates that the system is under endogenous conditions.

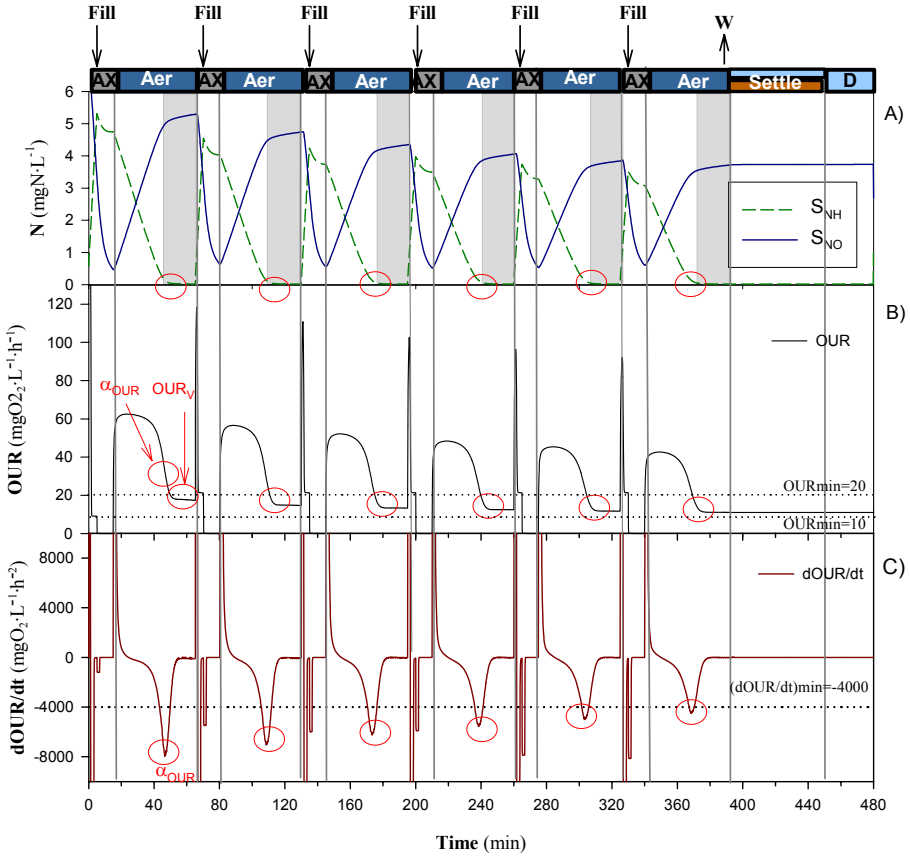


Figure 8-1. A) Evolution of S_{NH} and S_{NO} , B) OUR and C) OUR derivative, during a simulated eight hour cycle.

In Figure 8-1-C the derivative of the OUR is presented. At the beginning of the aerobic phase the derivative is positive and very high due to the sharp increase in the OUR values. When the OUR starts to decrease the derivative goes to negative values, reaching a minimum. The minimum in the derivative coincides with the complete depletion of ammonia (α_{OUR}).

By observing Figure 8-1 one can see that different possibilities of aerobic phase control can be applied using the OUR, its derivative or a combination of both signals. Moreover, the methodology for on-line control could be based on fixing a threshold value or using mathematical tools to detect the bending points in the signals (minimum in the derivative of OUR or inflexion point in OUR). In this case, taking into account the principle of "keeping it easy" and considering that the control strategy will be applied later in a plant, a strategy based on establishing a threshold value for the OUR signal is selected. This threshold value is a minimum value of OUR (OUR_{min}) which is the value obtained when the system is under

endogenous conditions (OUR_V). From Figure 8-1-B it can be seen that the OUR_{min} value for this particular case could be established between 10 and 20 $mgO_2 \cdot L^{-1} \cdot h^{-1}$.

In the specific case presented in Figure 8-1 the anoxic phases cannot be optimized since the oxidized nitrogen is not completely consumed. Nevertheless, changes in the influent wastewater composition or flow rate can lead to conditions in which denitrification finishes before the end of the anoxic phase. Hence, to make sure that even the length of the anoxic phases is optimized when necessary, a strategy for these phases can also be designed.

As stated in Chapter 7 the end of anoxic phases can be determined by detecting the NK (in the ORP profile) or NA (in the pH profile). Nevertheless, the model used in this experience does not include pH or ORP descriptions, and therefore the strategy might be simplified to establishing a minimum value in the oxidized nitrogen (S_{NOmin}). As soon as the oxidized nitrogen concentration (S_{NO}) reaches the S_{NOmin} value the system can change to the next phase.

8.3.2. Defining the control strategy

The objective of the control strategy is to adjust the length of the aerobic and anoxic reaction phases when the endpoints of the nitrification and denitrification processes are detected. The background showed that using a threshold OUR_{min} value during aerobic phases and a threshold S_{NOmin} value for the anoxic phases is appropriate for achieving this aim.

Moreover, some security factors are applied in the strategy to account for uncertainties related to the process:

- A minimum time (t_{min}) for the phases is defined for two reasons: First, to avoid false minimum OUR points at the beginning of the phases, and second to avoid aerobic phase ending prematurely caused by the transient response of the activated sludge from the sequence of intracellular reactions involved in substrate degradation by activated sludge (Vanrolleghem *et al.*, 2004).
- A maximum phase time (t_{max}) is also defined in order to keep working with the predetermined cycle definition.
- A waiting time (t_{wait}) is applied at the end of the algorithm to avoid detecting errors due to possibly incorrect measurements.

Figure 8-2 shows a scheme of the reaction phase length indicating the security factors explained above. It is important to note that the t_{wait} begins when the end of the phase is detected, and thus it can be located from the end of t_{min} until the end of the reaction phase.

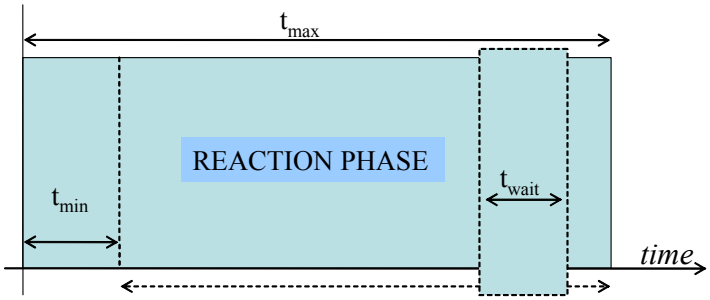


Figure 8-2. Security factors for the reaction phases.

The scheme of the on-line control strategy is presented in Figure 8-3 as a dynamic diagram with the control variables and the security factors.

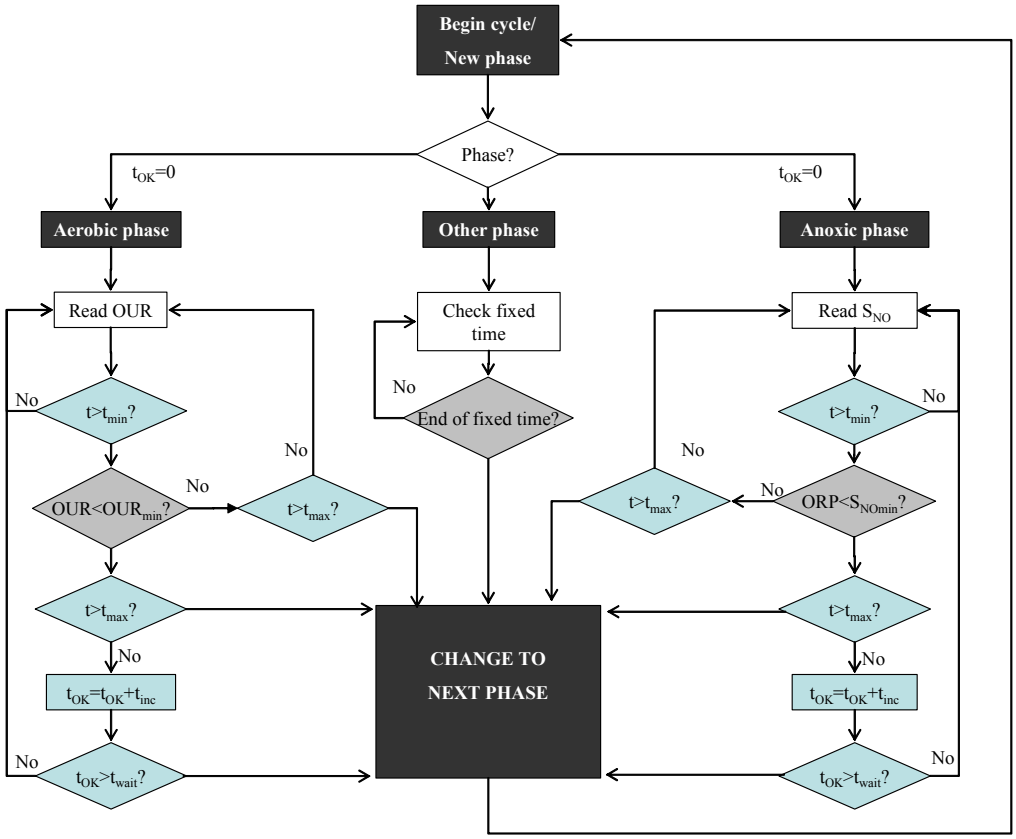


Figure 8-3. Scheme of the on-line control strategy.

The functioning of the control algorithm starts by detecting whether the phase is aerobic, anoxic or other (i.e. filling, settling, wastage or draw). In the aerobic phases a minimum time is waited. Then, OUR values are read from the monitoring module every sampling time (10 seconds) and compared with the OUR_{min} value. When the OUR value is lower than the OUR_{min}, a wait time (t_{wait}) is applied, and then the system changes to the next phase. The functioning of the device also guarantees the process performances by adopting a maximum time length (t_{max}). When the phase is anoxic, the control system works similarly to the aerobic one, comparing in this case S_{NO} values with S_{NOmin}. The minimum, the maximum and the wait time are also required. When the phase is neither aerobic nor anoxic, a fixed time is applied and checked for the phase.

This strategy was implemented in Matlab which was linked to GPS-X. The layout of the plant and the model were configured in GPS-X using the manual mode of the SBR object. The platform Matlab permitted i) a recipe for the work plan to be created, and ii) the recipe to be executed and the cycle and phase time scheduling to be controlled based on the coded control strategy.

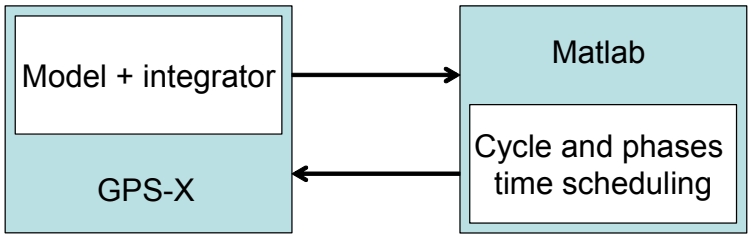


Figure 8-4. Link between GPS-X and Matlab.

A file with extension mtl. was created to link GPS-X and Matlab in which the Matlab inputs and outputs were specified. The variables used in this connection are presented in Table 8-2.

Table 8-2. Inputs and outputs of the Matlab-GPS-X connection.

Matlab inputs (from GPS-X)	Matlab outputs (to GPS-X)
Time	Mixing or not (1 or 0)
Dissolved oxygen	Influent flow
OUR	Effluent flow
Derivative of OUR	Wastage flow
Sum of nitrite and nitrate	K_La

Therefore, the time of the simulation was given by GPS-X at each time interval since it was in charge of performing the integrations. Moreover, DO concentration, the OUR, its derivative, and the sum of nitrite and nitrate were also transferred from GPS-X to Matlab. Then, the control algorithm coded in Matlab, evaluated these inputs and gave an output able to run the timing and the operating conditions of the cycle.

8.3.3. Model-based evaluation of different control strategies

Once the strategy was successfully implemented in Matlab and properly connected to GPS-X, different operating alternatives for comparing the SBR performance were defined:

i) No control strategy without an On-Off DO controller: This is the reference case.

ii) No control strategy with an On-Off DO controller: Controlling the DO at a certain low level means that there is not an excess of DO in the system and the anoxic reaction time is increased, improving the denitrification process with a reduction in the nitrite and nitrate concentration in the effluent.

iii) Three different control strategies based on a minimum OUR and a minimum S_{NO}: Success in implementing the control strategy depends on the threshold values chosen for the aerobic and anoxic phases. For the OUR_{min} a value of 10 $mgO_2 \cdot L^{-1} \cdot h^{-1}$ was tested, which is more conservative and means that only the last phases of the cycle are adjusted. The other chosen value was 20 $mgO_2 \cdot L^{-1} \cdot h^{-1}$ which permits the OUR_{min} to be achieved in all of the aerobic phases. For the S_{NOmin}, values of 0.2 and 0.5 $mgN \cdot L^{-1}$ where tested, being the last one less restrictive.

Having defined the possible strategies, the next step was to test them using the calibrated model following the simulation procedure described in point 8.2. The results of the EQ, the AE and the Vt for the different strategies are presented in Table 8-3.

Table 8-3. Results of the performance indexes used to evaluate the control strategies.

On-line Control strategy			DO control	EQ ($Kg \cdot d^{-1} \cdot L^{-1}$)	AE ($KW \cdot h \cdot d^{-1} \cdot L^{-1}$)	Vt (L)
Nº	OUR_{min} ($mgO_2 \cdot L^{-1} \cdot h^{-1}$)	$S_{NO,min}$ ($mgN \cdot L^{-1}$)				
1	-	-	No	0.0298	0.1916	210
2	-	-	On-Off	0.0188 (37%)	0.1397 (27%)	210
3	10	0.2	On-Off	0.0184 (38%)	0.1377 (28%)	226 (7.5%)
4	20	0.2	On-Off	0.0180 (39%)	0.1249 (35%)	279 (33%)
5	20	0.5	On-Off	0.0179 (40%)	0.1251 (35%)	284 (35%)

The percentages refer to case Nº1.

For the reference case (Nº 1, Table 8-3) in which no DO control or strategies were applied the EQ index obtained was 0.0298 $Kg \cdot d^{-1} \cdot L^{-1}$ and the AE index 0.1916 $KW \cdot h \cdot d^{-1} \cdot L^{-1}$, with a total volume of 210L of wastewater treated in the seven days of operation.

When an On-Off DO controller was used (Nº2, Table 8-3), the EQ decreased from 0.0298 $Kg \cdot d^{-1} \cdot L^{-1}$ to 0.0188 $Kg \cdot d^{-1} \cdot L^{-1}$, which represents a 37% reduction. This decrease was mainly related to a decrease in the effluent nitrogen concentration, with a high weight (20) in the EQ calculation (see Equation 8-1). The cost savings related to the aeration energy used represented a 27% reduction (from 0.1916 to 0.13975 $kw \cdot h \cdot d^{-1} \cdot L^{-1}$) compared to the reference system with no control strategy (Nº 1, Table 8-3).

The control strategy was implemented for Cases 3 to 5 presented in Table 8-3. In Case 3 an OUR_{min} of 10 $mgO_2 \cdot L^{-1} \cdot h^{-1}$ and a S_{NOmin} of 0.2 $mgN \cdot L^{-1}$ were applied. Although the EQ and AE indices obtained were similar to those in Case 2, the volume of treated wastewater increased 7.5% compared to the reference case (Nº1, Table 8-3). In Case 4 the OUR_{min} value was

increased to 20 $mgO_2 \cdot L^{-1} \cdot h^{-1}$ which resulted in a major improvement in the capacity of the plant with an increase in the treated volume of up to 33%.

Finally, by combining an OUR_{min} of 20 $mgO_2 \cdot L^{-1} \cdot h^{-1}$ and a S_{NOmin} value of 0.5 $mgN \cdot L^{-1}$ (Case 5) it was possible to obtain a reduction of 35% in the aeration energy used (Nº 5, Table 8-3), compared to the uncontrolled conditions (Nº 1, Table 8-3). In addition, the capacity of the plant was increased, which means that the treated wastewater volume could be increased up to 35% or that the required volume of the reactor could be reduced. This improvement with respect to Case 4 presented in Table 8-3 is not significant since the anoxic phase could not be much optimized.

The improvements resulting from applying the on-line control strategy were achieved without affecting the quality of the effluent. This was shown by the EQ index, which was near the values obtained with the simple On-Off DO control (Nº 2, Table 1).

Figure 8-5 shows the evolution of the simulated nitrogen compounds and OUR profile obtained with the on-line control strategy and a DO On-Off controller (Nº 5, Table 1).

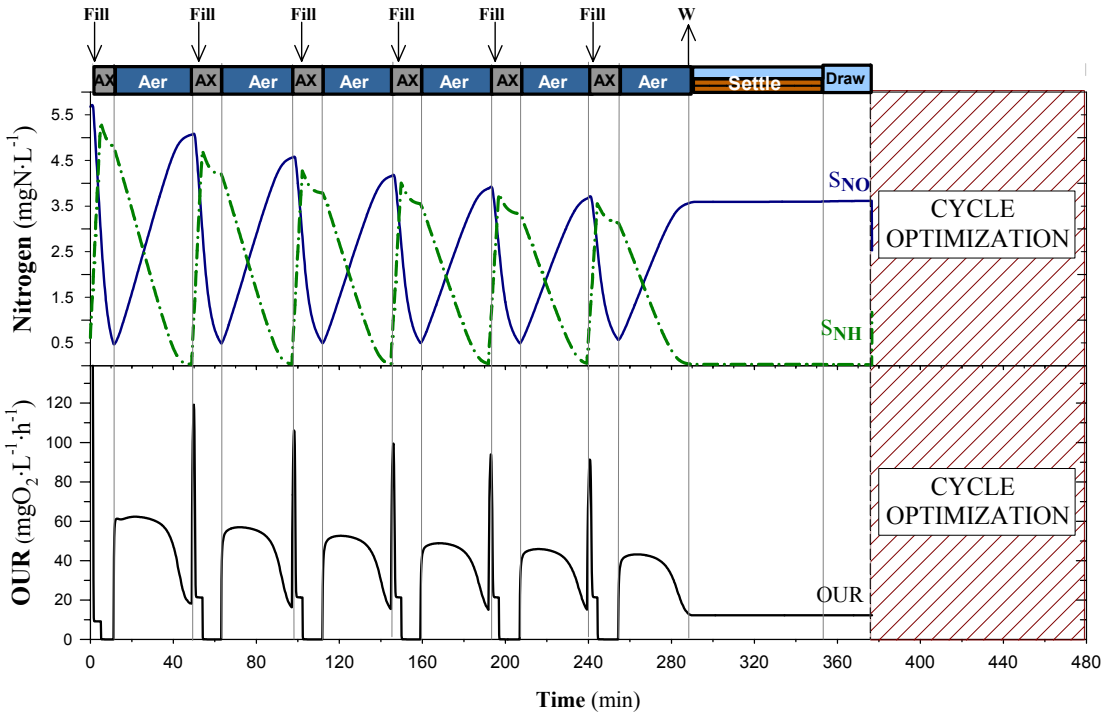


Figure 8-5. Simulated data profile applying an on-line control strategy and On-Off DO controller.

It can be seen that the total cycle length of the SBR was reduced by 21% with respect to the proposed fixed cycle, with considerable cycle optimization.

8.4. DISCUSSION

These promising results, achieving with the control strategy up to 35% reduction of energy and increase the treatment capacity, are dependent on the cycle design. Normally plants are designed under the worst operating conditions and normally this results in over sizing the plant. Therefore, the obtained percentages are strictly relative to the reference performance of the SBR and they can not be interpreted as absolute improvement of the control strategy. However, it has been demonstrated that implementing this control strategy permits adjusting the cycle at real-time depending on the influent wastewater.

The control strategy based on fixing a threshold has been proved to be effective and since its concept is easy it could be implemented directly into a plant. Nevertheless, further work could be done to improve this control strategy, using more sophisticated methods (e.g. Episode representation) in order to detect the bending points on-line, making the control strategy more independent. Moreover, double-checking conditions could be applied in the control algorithm in order not to depend on only one variable but on the various possibilities identified at the beginning of the chapter.

However, care should be taken when interpreting these promising results, since the new operation and control may change the system to such an extent that the model may no longer hold. This could mean that for long-term studies the model would have to be recalibrated or even the structure of the model modified (Sin *et al.*, 2005b).

8.5. CONCLUSIONS

In this study, a model-based approach has proved to be useful for designing and evaluating control strategies to optimize the reaction phases. Furthermore, the use of process indexes has proved to be a useful tool to select the best control strategies. The specific conclusions are:

1. The indices EQ, AE and V_t were used as evaluation criteria for the proposed control strategies.
2. Different control strategies based on the on-line calculated OUR and the ORP values were evaluated.
3. The results of the simulations suggested that implementing a DO controller improved the denitrification process leading to a reduction in the nitrite and nitrate concentration in the effluent.
4. The use of a DO controller represented a 37% reduction in the EQ. This decrease was mainly related to an improvement in the denitrification capacity. The cost savings

related to the aeration energy used represented a 27% reduction. However, no improvement in the capacity of the plant was observed.

5. When implementing the on-line control strategy, no remarkable improvements respect the EQ and AE indices were achieved, comparing to the strategy using only a DO controller. However, the index V_t indicate that the capacity of the plant considerably increased.
6. The on-line control strategy using OUR and S_{NO} appeared to be useful for adjusting the cycle length of the reaction phases in the SBR technology, reducing the required aeration energy up to 35% and increasing the plant capacity up to 35%.

9 Implementing the control strategy in an SBR plant

9. IMPLEMENTING THE CONTROL STRATEGY IN AN SBR PLANT

9.1. MOTIVATION

In the previous chapter a control strategy based on the OUR and ORP was defined and tested using a simulation platform. Hence, the next step is to implement this control strategy in the SBR pilot-plant treating real wastewater.

This Chapter begins with the background of the control strategy showing the possibilities of optimizing the plant working at a fixed cycle configuration. The strategy defined in Chapter 8 is used but applying the values of the control parameters determined from the analysis of historical on-line profiles. Finally, this strategy is implemented for a long period, which permits the plant performance to be compared before and after the on-line control strategy is applied.

9.2. MATERIALS AND METHODS

The semi-industrial pilot plant presented in point 3.1.1 was used for implementing the control strategy. The advantage of using this plant is the possibility of testing the strategy by using real wastewater.

The semi-industrial pilot plant SBR treated 600L of real wastewater per day from the Cassà-WWTP. The cycle characteristics for achieving complete nitrification and denitrification were defined using the procedure presented in the introduction (point 1.2.3.) obtained through previous lab-scale studies (Vives, 2004). Figure 9-1 presents the fixed cycle used during the experimental period before applying the control strategy. An eight hour cycle with six feeding steps was implemented, introducing the wastewater in the anoxic phases, and alternating the anoxic and aerobic phases in order to improve carbon and nitrogen removal (Vives, 2004; Puig *et al.*, 2004). The cycle was divided into a reaction phase (395 minutes; 46.2% under aerobic conditions), settling (60 minutes) and draw (25 minutes).

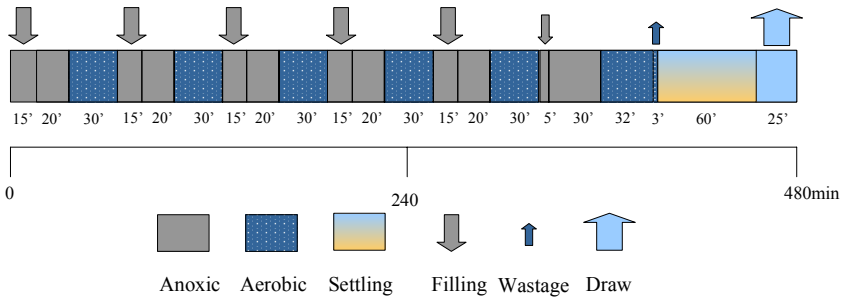


Figure 9-1. Operating periods of the semi-industrial SBR applying the step-feed strategy.

The semi-industrial SBR was DO-controlled at 2.0 mg $DO \cdot L^{-1}$ set-point by an air On-Off strategy in order to achieve complete nitrification and avoid high DO concentration at the start of the anoxic phase. The wastage in the SBR was performed under mixing and aeration conditions in the last aerobic phase in order to control the SRT of the system (20 days), assuming equal concentration of solids in the wastage and reactor.

9.3. RESULTS

9.3.1. Background of the control strategy

The semi-industrial SBR ran for 200 days at a fixed cycle. The results obtained (Puig *et al.*, 2004) demonstrated that these conditions may be useful in treating real wastewater (532 ± 220 mg $COD \cdot L^{-1}$ and 53.6 ± 25.0 mg $N \cdot L^{-1}$ on average), keeping effluent levels (54 ± 25 mg $COD \cdot L^{-1}$ and 4.7 ± 5.6 mg $N \cdot L^{-1}$ on average) lower than those of the European Directive 91/217/CEE (125 mg $COD \cdot L^{-1}$ and 15 mg $N \cdot L^{-1}$).

The potentials for optimization can be obtained from Figure 9-2, which shows the pH, ORP, OD and OUR profiles of a typical eight-hour cycle of the semi-industrial SBR under stable conditions. The grey zones represent the possible optimized time.

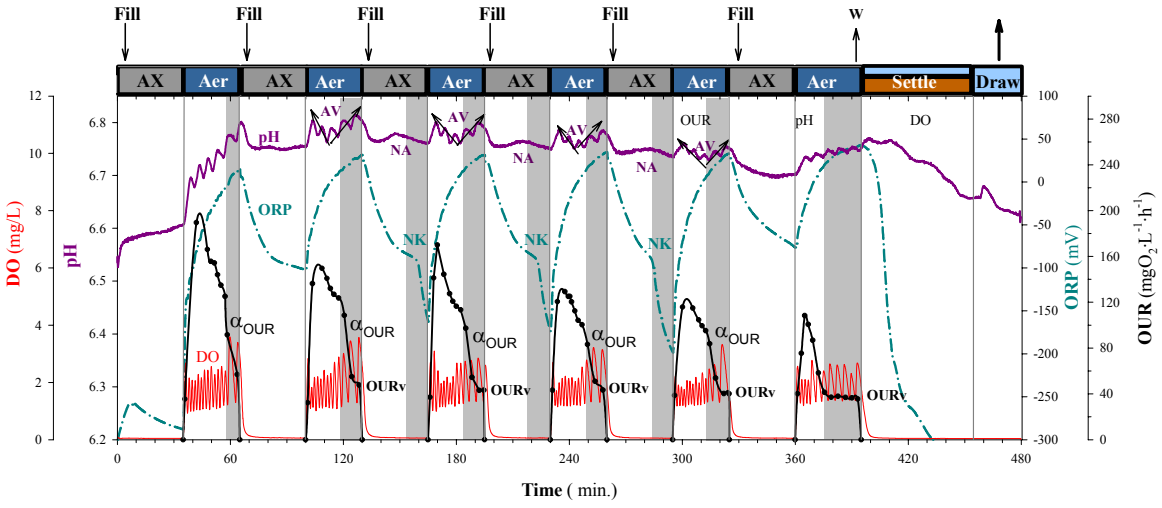


Figure 9-2. pH, ORP and DO profiles during an eigh hour cycle in the SBR.

In the aerobic phases, the Ammonia Valley can be observed (Figure 9-2-AV, at minutes 120, 185, 250 and 315) but the signal fluctuates due to the stripping effect of the On-Off aeration control. However, the OUR profile permits us to identify the α_{OUR} which determines the end of ammonia (see Figure 9-2, at minutes 55, 120, 185, 250, 315 and 375) and the OUR_V which determines when endogenous conditions are achieved (see Figure 9-2, at minutes 125, 190, 255, 320 and 380).

During anoxic phases, the appearance of Nitrate Knee (in the ORP profile, point NK) and Nitrate Apex (in the pH profile, point NA) at minutes 150, 215 and 285, indicate the end of the denitrification process.

Hence, it may be possible to optimize the aerobic and anoxic stages using these endpoints to adapt the cycle length to the influent wastewater characteristics without affecting the effluent quality. Based on both the monitoring and control systems and the background knowledge acquired, a module for controlling the alternation of aerobic and anoxic phases could be developed that detects the endpoints.

The AV in the pH profile in the aerobic phases was not considered for two reasons: i) the fluctuations in the signal, which could make it difficult to detect the ammonia valley, and ii) the AV was not detected in the first and sixth aerobic phases. Therefore, the OUR profile and more specifically the bending point OUR_V was used as it is more conservative than the α_{OUR}. The NK was considered a robust parameter, and therefore it was used as the bending point for the anoxic phases.

9.3.2. Defining the control strategy

The control system acts on the aerobic and anoxic phases of the SBR cycle according to the scheme already presented in Figure 8-3 using OUR and ORP measurements for controlling the aerobic and anoxic phases respectively. Before the implementation of this strategy the controller parameters for the specific case study have to be determined. In this experimental application they were established from the analysis of historical data making sure that the selected threshold values would be the suitable for the actual operating conditions. These values should be periodically checked because changes in the influent wastewater or in the process performance could affect in the population dynamics. This is a conservative decision to improve the performance of the plant but maintaining the risks at the minimum.

The historical analysis of OUR and ORP data is now presented. Figure 9-3 shows the evolution over time of on-line OUR values in the fifth and sixth aerobic phases and ORP measurements in the anoxic fifth and sixth phases, of different stable operating cycles. An increasing trend for OUR values can be seen at the beginning of the aerobic phase (Figure 9-3-Left), which is caused by the changing conditions (from the anoxic phase to the aerobic phase). This transient response of the activated sludge is most likely from the sequence of intracellular reactions involved in substrate degradation by the activated sludge (Vanrolleghem *et al.*, 2004).

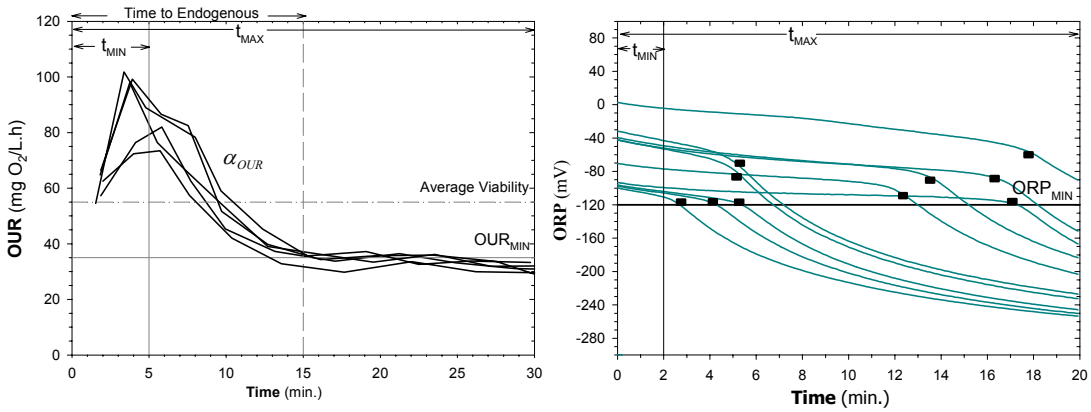


Figure 9-3. Analysis of previous OUR (Left) and ORP (Right) data corresponding to aerobic and anoxic phases of different cycles.

For this reason, the control system waits for a minimum time, t_{min}, of 5 min. After t_{min}, the OUR profile decreases slowly until α_{OUR}. After that, a minimum OUR value, OUR_V, near 35 mg of $O_2 \cdot L^{-1} \cdot h^{-1}$ was achieved for most cases; therefore, this was the end-point reference. At this point, which was referred to as the "time to endogenous" by Watts and Garber (1995), the system was assumed to be under endogenous conditions when at least 95% of the organic material in the waste was treated. This rate is also proportional to the biomass activity. Many factors, such as the following, have an impact on the biomass activity and thus activated sludge plant treatment: total load, biomass viability, and influent treatability or inhibition due to toxicity or temperature (Watts and Garber, 1995; Spanjers *et al.*, 1998). After the minimum OUR was achieved, a stabilization time, t_{wait}, of 2 min in the control strategy was applied to ensure that the system was under endogenous conditions. Furthermore, the device also guaranteed the process performance by adopting a maximum time length (t_{max}) of 30 min for the aerobic phase, equal to the time established in the fixed cycle.

In the anoxic phase, the parameter used to control the phase duration was the ORP. To determine a relationship between the end of the anoxic phase and the ORP, data from different profiles corresponding to anoxic phases were analyzed (Figure 9-3-Right). The NK endpoint occurs depending on the characteristics of the influent wastewater and on the performance of the SBR. The mean ORP value where the NK took place was -94mV with a standard deviation of 26.4. When the ORP values from different profiles obtained in the SBR are compared, the NK always takes place above an ORP value of -120 mV. Following a conservative criteria this value is the chosen threshold for ORP_{min}. The ORP minimum value has also been used by other authors (Tomlins *et al.*, 2002; Battistoni *et al.*, 2003). As in the aerobic phase, t_{min} and t_{wait} (2 and 5 min respectively) were also applied. The values used for the parameters obtained through the historical analysis are presented in Table 9-1.

Table 9-1. Parameter values for the control strategy.

Phase	OURmin ($mgO_2 \cdot L^{-1} \cdot h^{-1}$)	ORPmin (mV)	t_{min} (min)	t_{wait} (min)	t_{max} (min)
Aerobic	35	-	2	5	30
Anoxic	-	-120	2	5	35

Implementing the control strategy required developing software able to handle monitoring and controlling the process, following the defined strategy. This control program was developed using LabWindows® and was based on three synchronized modules which communicate with each other: the signal acquisition and monitoring device, the on-line OUR measurement module and the control system module. The control system module was responsible for detecting the aerobic and anoxic phase endpoints using minimum OUR (OUR_{min}) and ORP values (ORP_{min}), applying the security factors.

The control strategy scheme already presented in Chapter 8 (see Figure 8-3), was implemented in the control program. However in this case ORP can be used directly instead of using the effluent NO_X^- concentration used with the model-based approach. Special attention was given to the security factors since the responsibility is higher when treating real wastewater. Therefore, the controller works as follows: first, the control system detects whether the phase is aerobic, anoxic or other (i.e. filling, settling, wastage or extraction). If the phase is anoxic or aerobic, after the t_{min} it starts to check the measured values with the fixed minimum values to find the endpoint. When the measured value is lower than the minimum, the t_{wait} for stabilization is added. The function of the device also guarantees the process performance by adopting the t_{max} for each phase. If the minimum value is not achieved before the t_{max}, the control system changes to the next phase.

9.3.3. Pilot plant evaluation of the control strategy

After developing the control system, the next step was to test it. For this reason, the control system was used in the semi-industrial SBR for three months treating real urban wastewater. Figure 9-4 shows ORP (A) and OUR (B) profiles of a typical cycle from the Pilot Plant SBR with the developed control system.

In comparison with the 480 minutes taken by the fixed cycle, the cycle length with the control system applied was around 390 minutes. The anoxic periods were reduced by around 56%, a percentage that is relative to the reference conditions. The largest reductions always took place during the firsts steps due to the rapid decrease of the ORP profile, Figure 9-4-A, because the nitrate concentration in the reactor was the same as the effluent of the previous cycle. At the end of each anoxic phase, the NK was clearly observed. After the NK appeared, the control system detected that the ORP values were lower than the ORP_{min} and it changed to the aerobic phase.

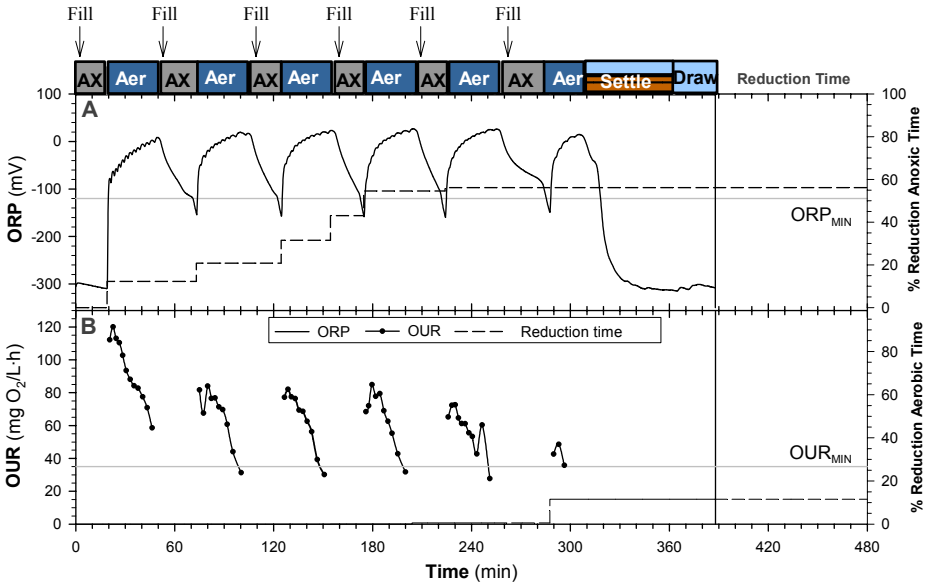


Figure 9-4. ORP(a) and OUR(b) profiles of an optimized cycle using the control system.

Figure 9-4-B also shows the evolution of the OUR profile in the aerobic phases of the cycle. In this phase, the reduction time was around 12%. The largest reduction always occurred in the last phase, when the substrate was depleted and OUR values reached the aerobic endpoint value (OUR_V).

In spite of the high cycle length reduction which depends on the cycle used and the influent characteristics, the aim of the control system was to adapt the cycle length to the influent conditions. If high effluent quality is achieved, this demonstrates that the control system was operating correctly. Figure 9-5 shows the evolution of the organic matter, both the influent and effluent, during the two experimental periods: operation with the fixed cycle and with the control system (after day 220).

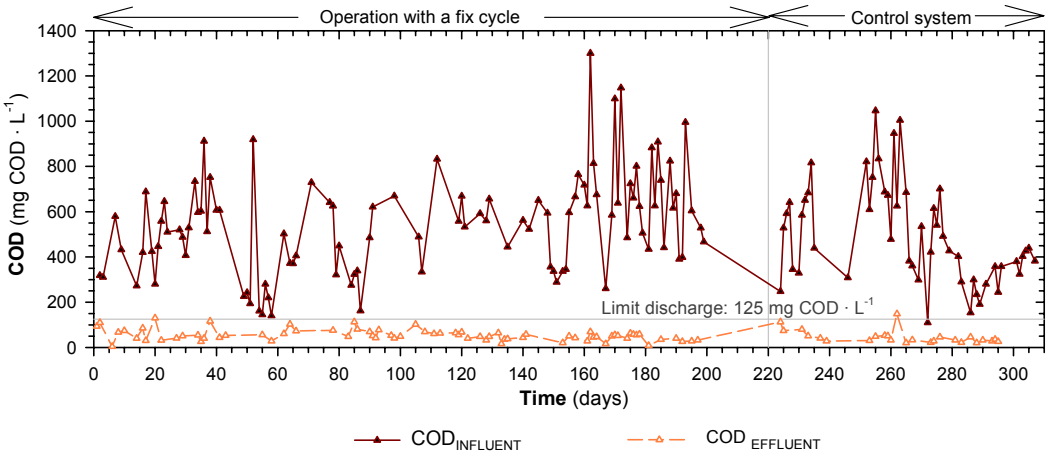


Figure 9-5. Evolution of the influent and effluent COD during the SBR operation.

In spite of the variability in the organic matter (black-triangles) influent (527±220 mg COD $\cdot L^{-1}$, on average), the organic matter effluent, 57 mg$\cdot L^{-1}$ COD on average, was always lower than the standard requirements. There were no major differences between the two periods in the effluent profile.

Figure 9-6 presents the total nitrogen evolution, influent and effluent, during the experimental period.

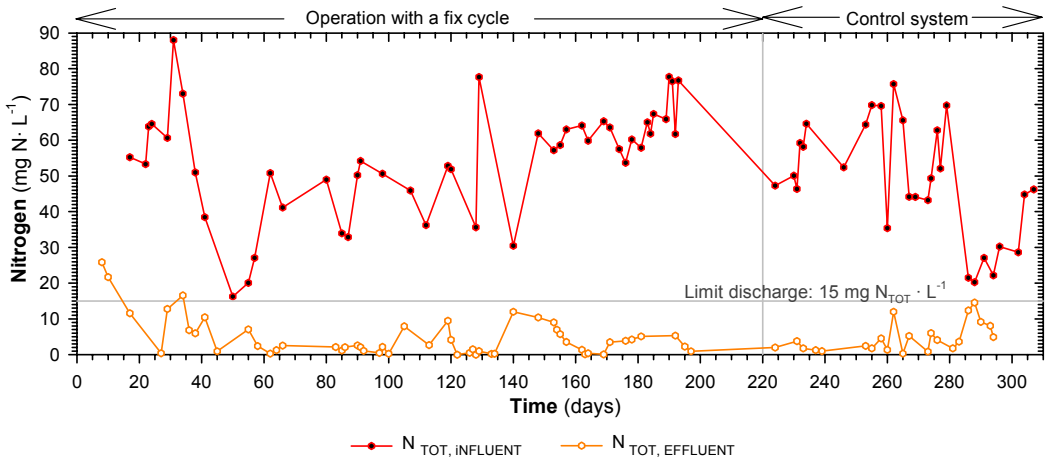


Figure 9-6. Evolution of the influent (black-dotted) and effluent (white-dotted) for nitrogen removal during the Pilot Plant SBR operation at the *Cassà-WWTP*.

Similarly to the organic matter, the high nitrogen influent concentration variability (51.1±17.1 mg N $\cdot L^{-1}$, on average), did not affect the effluent quality, 4.7 mg $N_{TOT}\cdot L^{-1}$. On days 260 and 290 the SBR pilot plant had some faults/incidents which resulted in the DO control system malfunctioning (i.e. air flow to the reactor was kept active for a whole cycle resulting in high nitrification and low denitrification) and a change in the settling properties of the sludge (i.e. some colloidal organic matter was observed in the effluent) because of strong variation in influent wastewater quality (i.e. influent COD and nitrogen decreased greatly because of a continuous rainy period). Nevertheless, after these incidents, the SBR performance rapidly recovered its normal efficiency without extra actions having to be applied.

9.4. DISCUSSION

These results have shown the advantages and the possibilities of using a control system to optimize the plant. In this case, the main reduction occurred during the anoxic phases because the strategy for aerobic phases was too conservative, and only the last aerobic phase was shortened when the OUR value indicated complete organic matter and ammonium removal (OURv). A better approach would consist in a different strategy finishing the aerobic phases when nitrification is complete for all the aeration phases (detection of α_{OUR}), except for the last one in which all the organic matter should be depleted (detection of OURv). A detailed description of this strategy is presented in Puig *et al.* (2005).

With the on-line control strategy less responsibility and more flexibility is given to the designer, and less conservative designs can be made. Additionally, the increase in the capacity of the plant saves costs for the influent buffer tanks which can be smaller.

Using the SBR control strategies based on probe measurements (pH, ORP, DO) or calculated from DO (OUR) implies a low investment in the on-line measurement equipment and can lead to important improvements in treatment capacity, and even for saving energy. Thus, it is economically reasonable to implement this strategy especially with SBRs treating wastewater from small communities or developing countries. However, there is the possibility of using on-line analyzers (e.g. of NH_4^+ or NO_x^-) which have also been successfully implemented to control SBR performance (Wiese *et al.*, 2004). Nevertheless, they require higher levels of maintenance and the investment in equipment for this is high (compared to the probes), which makes this technology more appropriate for plants treating wastewater from bigger communities.

Moreover, these kinds of strategies could be integrated into a more complex system that is able to deal with the other phases, such as settling and wastage. Wiese *et al.* (2004) presents a control for the settle and draw phases and also for the volumetric exchange ratio based on sludge level probes and suspended solids probes, which also permits calculating and adjusting the sludge retention time.

One step further consists in developing a control system able to manage the duration and definition of the whole cycle structure. Artificial intelligence and model-based tools can be used for this purpose taking advantage of the knowledge acquired.

9.5. CONCLUSIONS

A real-time control system has been implemented in the semi-industrial pilot plant that permits optimizing the length of the aerobic and anoxic phases based on the OUR and the ORP.

1. The DO monitoring during the aerobic phases of the SBR, using an air On-Off DO control strategy, permitted the on-line OUR to be calculated. The evolution of the OUR during the aerobic phases provides meaningful information about the state of the process.

2. From the analysis of previous on-line patterns minimum values of OUR and ORP were identified for the aerobic and anoxic phases respectively, to detect the end of the phases. A threshold value was established for these parameters that indicated the end of nitrification and denitrification processes.

3. This control system was implemented for real-time controlling an SBR treating urban wastewater. The results showed that it worked satisfactory for more than three months, optimizing the functioning of the plant. The length of the anoxic phases was reduced by around 56% and the aerobic phases were reduced by around 12%, considering these percentages relative to the reference conditions.

10

A supervisory control system to manage and optimize SBR performance for nitrogen removal

10. A SUPERVISORY CONTROL SYSTEM TO MANAGE AND OPTIMIZE SBR PERFORMANCE FOR NITROGEN REMOVAL: A FIRST APPROACH.

10.1. MOTIVATION.

The SBR's flexibility is due to the possibility of adjusting the cycle time, the duration of each phase and the mixing/aeration pattern during each cycle to achieve nitrogen removal. Normally the SBR operates with a fixed cycle configuration and the plant manager is in charge of supervising the process and manually adapting the cycle. Taking advantage of the easiness of automation of SBRs, a control system to on-line adjust the length of the aerobic and anoxic phases has been presented in Chapters 8 and 9. Nevertheless, a higher level of control is necessary when the system faces abnormal situations (e.g. significant changes in wastewater quality or quantity, environmental shifts, equipment faults…).

The objective of this Chapter is to ensure that the SBR is able to adapt the operating conditions to the wastewater variability without needing to be supervised continually by the plant manager. For this reason a supervisory control system is proposed which will be able to i) manage and control the evolution of the reaction phases of the SBR cycle, and ii) identify the process status and adapt the cycle definition by means of a supervisory module that uses artificial intelligence tools. Therefore, in this Chapter the structure of the control system for the SBR is presented including the lower and medium level of control already presented in Chapters 8 and 9. These levels have already been developed and implemented. In this Chapter, especial attention is given to the higher level of control which implies the supervision of the process. This is under development dealing with the different system units in parallel.

10.2. MATERIALS AND METHODS

10.2.1. SBR Pilot Plant

The different scale pilot plants presented in point 3.1.1 are used to obtain valuable information to develop the supervisory system. Moreover, the different modules can be implemented and validated in the SBR plants once they are developed.

10.2.2. Data Acquisition and Control system (DAC)

Controlling the operation of the SBR regarding the length and sequence of phases and the On-Off switch of the peristaltic pumps, mixing units and air supply is conducted using a DAC system. It consists in a computer, interface cards, meters, transmitters and solid-state relays. The set-up presented for the pilot plants in point 3.1.1. is suitable to obtain a robust DAC.

10.2.3. Programming environment

All the software of the supervisory control system is developed in LabVIEW®. This is a graphical development environment for creating flexible and scalable measurements and control applications. It permits module-based programming which makes it possible to adapt and include new modules within the system.

10.2.4. Mechanistic pilot plant model for biological processes

The mechanistic model describes the activated sludge process in the SBR. To obtain this model it is necessary to follow a calibration procedure so that the simulated values fit the experimental ones, as described in Chapters 5 and 6. The ASM1-based model obtained in Chapter 6 calibrated and validated over a 2-month period can be used for this purpose. The step-wise procedure followed in Chapter 6 showed to be accurate enough describing not only the trends but also the absolute values of the variables (e.g. S_{NH}, S_{NO}, VSS) during the measurement campaigns. Also, the evolution of the nitrogen effluent concentration during one month described accurately the reality. Nevertheless, a recalibration of the model might be conducted to make it ready for use, following the same procedure combining physical-chemical and biological analysis. This mechanistic pilot plant model is implemented in the simulator software GPS-X working as a virtual plant in parallel with the real plant.

10.3. RESULTS

The SBR technology's flexibility and high degree of automation favor implementing control strategies that can increase the productivity of the plant, optimize the operation, decrease the personnel necessities and provide stability and reliability in the process. Taking into account all these benefits different control strategies can be defined. According to the control hierarchy defined in Olsson and Newell (1999) different levels of control can be defined depending on the information needed and the operating instructions applied. In this case, a supervisory control system is proposed based on the three level architecture presented in Figure 10-1.

The lower level is the **DAC and monitoring system** which permits a defined cycle recipe to be executed and all the data coming from the SBR to be obtained. Moreover, it can contribute to improving the SBR performance by establishing internal control loops to maintain environmental parameters at a desired level. The medium level control is the **phase length optimizer system** in which the length of the reaction phases (aerobic and anoxic) can be adjusted in order to minimize energy consumption and increase the capacity of the plant. Finally, the highest level of control is the **cycle supervision system** which is responsible for evaluating the performance of the process in the actual operating conditions. Whenever the performance is undesirable, the supervisory control module is responsible for proposing corrective and preventive measures.

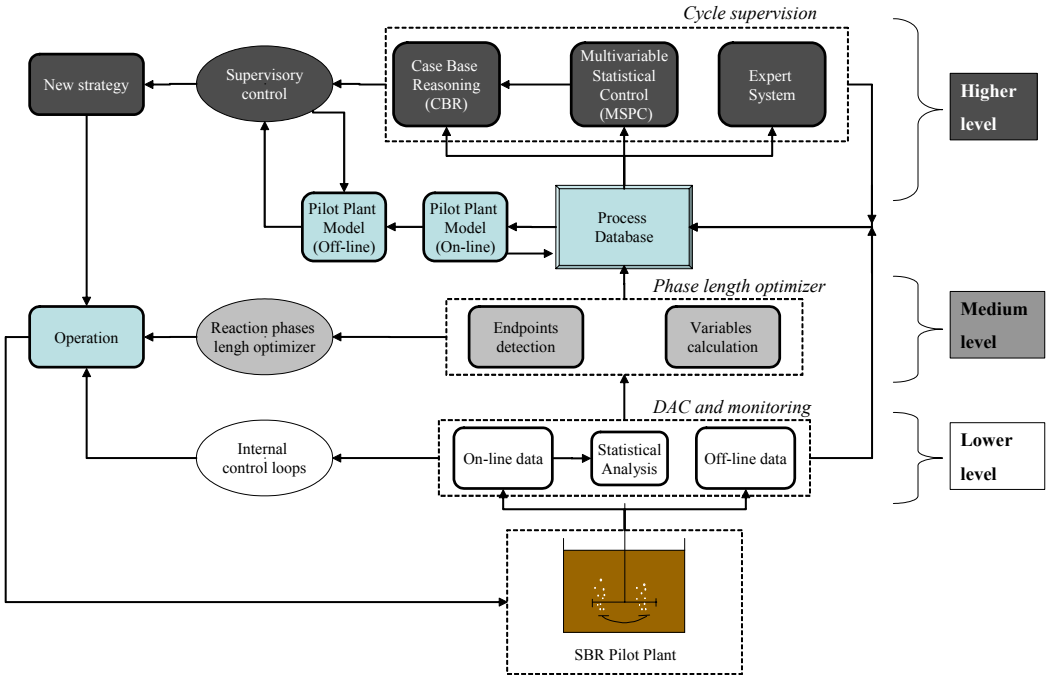


Figure 10-1. Three level architecture scheme of the supervisory control system.

Within this structure three more units play an important role: i) the Process Database, which is in charge of storing all the data coming from the three levels of control, ii) the models of the plant, and iii) the operation module that establishes the operating conditions at each time interval depending on the orders given by the three levels of control. A more specific explanation of each module that composes the supervisory control system is presented below.

10.3.1. Lower level control: DAC and monitoring system

The objectives of this module are running the plant following a defined cycle, and to monitor the process performance. The DAC system controls the process of enabling and disabling the devices and also gets on-line data from the sensors (e.g. pH, DO, ORP and temperature). Moreover, off-line data which is divided into analysis and qualitative observations can be introduced into the system by the plant operator. Using the gathered data a statistical analysis can be performed to obtain a first diagnosis that serves to detect abnormal functioning of the system (e.g. failures in the equipment).

Within this module a first level of control can be established using internal control loops, executed at each time interval. The purpose of these loops is to maintain the environmental parameters that influence the process at a desired level. Some of them can be easily measured (e.g. pH, temperature and dissolved oxygen) and thus controlled using On-Off, PID or Fuzzy procedures. One of the most common parameters to control is the dissolved oxygen concentration in the reactor. In the SBR pilot plant different DO controls have been successfully applied: On-Off and Fuzzy (Traoré *et al.,* 2005).

10.3.2. Medium level control: phase length optimizer

This module gets the data from the DAC system and controls the phase length of the reaction phases if the endpoints of the biological reactions are detected. Analyzing the evolution of the on-line data (pH, ORP, DO) and calculated data (OUR) results in identifying patterns that indicate the end of ammonia depletion (end of aerobic phases) and the end of denitrification (end of anoxic phases) (see Chapter 7). Hence, to obtain a system that can adjust the length of the phases two elements are necessary: calculation of the variables and the reaction endpoints detection.

Calculating the variables allows new variables to be obtained (e.g. OUR) from the parameters gathered in the lower level. The endpoint detection module requires the minimum, maximum or flexion points to be detected dynamically using filtering methods, derivatives and episode representation (Rubio *et al.*, 2004). Nevertheless, a simpler alternative implemented in SBR pilot plant is based on using fixed set-points for the controlled variables as presented in Chapters 8 and 9. This second alternative can be complemented with an optimizer to fine-tune the parameters of the controller according to a certain cost function. This can be achieved in the higher level control that supervises the process.

10.3.3. Higher level control: cycle supervision

In this higher level the advanced process control of the system is conducted at a cycle level. The main purpose is to check whether the current cycle and the operating conditions are the most suitable or not. Hence, this module is in charge of performing a diagnosis of the process performance, detecting possible operating problems and proposing a new cycle configuration, new operating conditions and/or parameters of the controllers if necessary. This layer uses artificial intelligence tools and it is composed of an advanced optimization module using Expert System (ES), Multivariable Statistical Process Control (MSPC) and Case Based Reasoning (CBR) tools.

10.3.3.1. Expert System (ES)

The ES uses the heuristic rules obtained from the knowledge which is codified using IF-THEN statements and can be presented as decision trees. This ES performs the evaluation of the nitrification and denitrification processes during the reaction phases. This is conducted once the cycle is finished, for all the reaction phases separately, by using the gathered data.

The decision trees used for the evaluation of nitrification and denitrification performance are presented in Figure 10-2 and Figure 10-3 respectively.

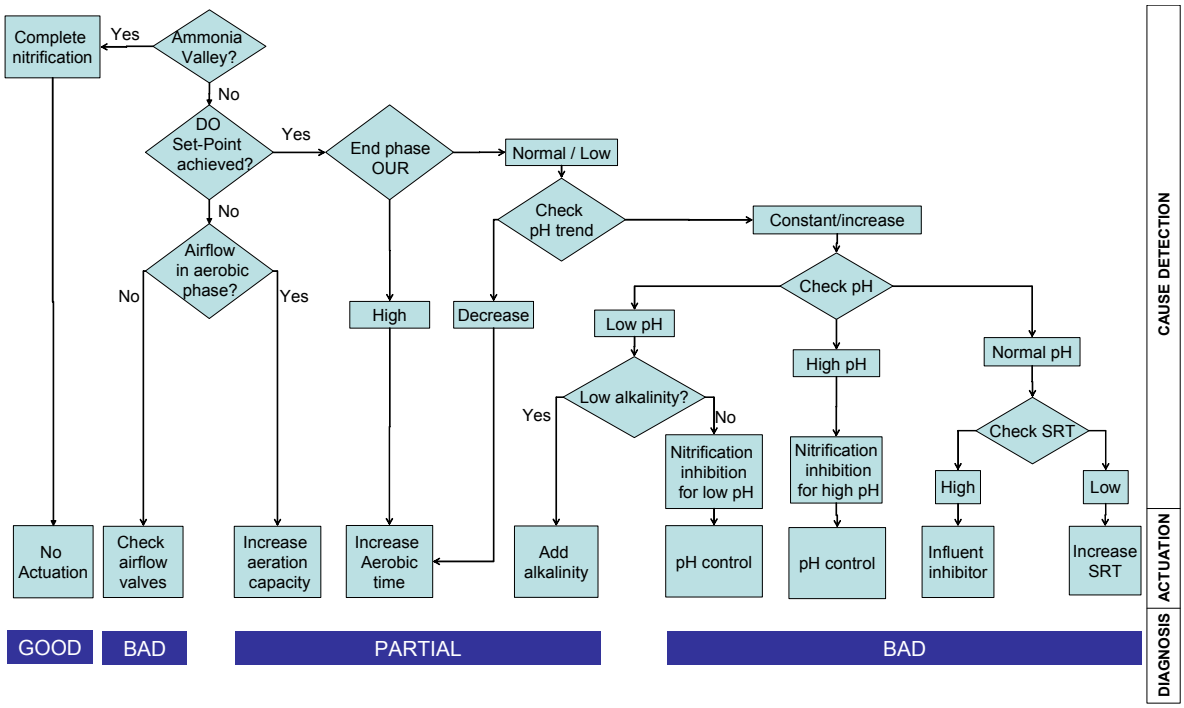


Figure 10-2. Decision tree for evaluating the nitrification performance.

The nitrification tree presented in Figure 10-2 is divided into three parts: i) the cause detection where the knowledge is structured, ii) the actuations derived from the reasoning and iii) the diagnosis to assess the performance of the SBR into three categories (Good, Partial or Bad).

In the scheme good nitrification is diagnosed when the Ammonia Valley is detected. If it is not detected the expert system may diagnose whether the system is under partial or bad functioning. Therefore, it checks sequentially whether the DO set-point is achieved or not, the value of the OUR at the end of the aerobic phase, the pH trend and finally the mean pH value of the phase.

Partial nitrification performance can be related to DO limitation that can be detected if the DO set-point is not achieved. Thus, more aerobic time might be necessary for high OUR values or even for low OUR values but combined with a decrease in the pH profile. Alternatively, low alkalinity can limit the nitrification process and is assessed by alkalinity measurements evaluated when having low pH values, constant/decreasing pH trend and normal/low OUR values.

Bad nitrification performance can be related to DO limitation when the airflow valve is not working and no DO is introduced in the system. Moreover, nitrification can be inhibited for both low and high pH. Alternatively, the presence of an inhibitor in the reactor may lead to bad nitrification performance and it would be related to low OUR values and normal pH values. Finally, the washout of the sludge implies bad nitrification and it can be directly related to low SRT of the system.

In order to asses the denitrification performance the decision tree presented in Figure 10-3 can be used. Similarly to the nitrification tree presents the cause detection reasoning, the actuations and the diagnosis.

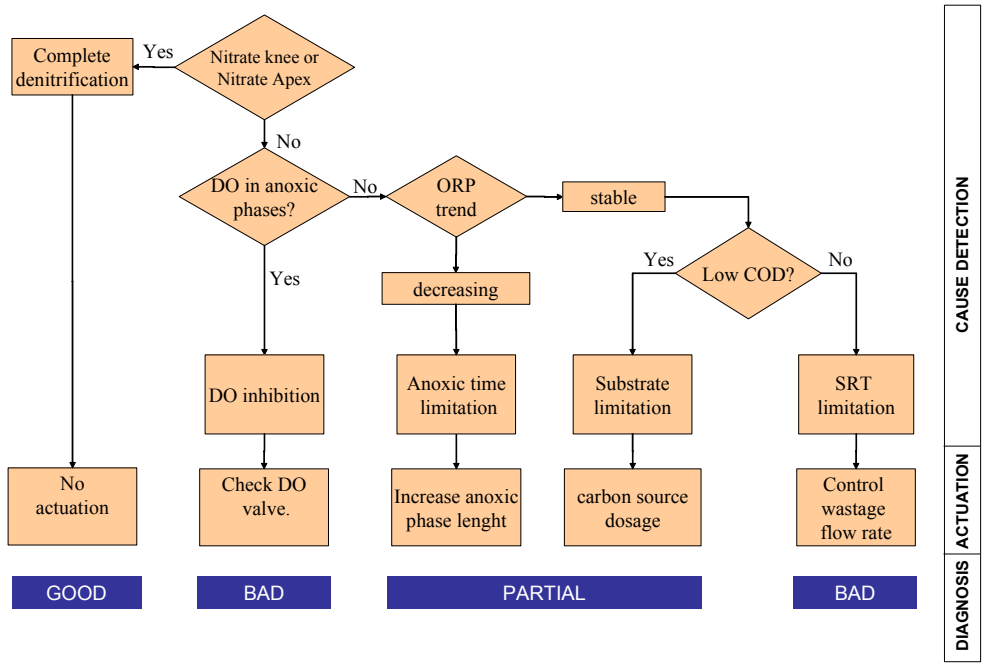


Figure 10-3. Decision tree for evaluation of the denitrification performance.

Good denitrification is assessed when the Nitrate Knee or the Nitrate Apex are detected, that indicate that the nitrates have been consumed. To assess partial or bad denitrification the tree sequentially checks the DO in the anoxic phases, the ORP trend and finally the influent COD.

Partial denitrification can be caused by anoxic time limitation and this is related to a decreasing ORP trend. Alternatively, denitrification can be limited by substrate what is detected by checking the influent COD. Bad denitrification can be caused by DO inhibition or alternatively by washout of the microorganisms related to the SRT limitation.

The presented decision trees have not been validated yet. Part of this validation can be conducted using a model-based approach and the rest using experimental procedures. The experience of expert systems in our research group applied to activated sludge systems can be found in Comas (2000) and R-Roda *et al.* (2002).

10.3.3.2. Multivariable Statistical Process Control.

Statistical control of batch processes can be conducted using the Multiway Principal Component Analysis (MPCA), which is the extension of PCA. MPCA is a widely used data-driven technique for monitoring batch processes and its purpose is to explain the variance-covariance structure of a multivariate dataset through a few linear combinations of the original variables with special properties in terms of variances (Nomikos *et al.*, 1994).

MPCA can be used alone or in combination with other tools. A combination of MPCA and an automatic fuzzy classification algorithm was developed to be applied in the SBR Plant (Ruiz *et al.*, 2004). In this supervisory control system MPCA is first used to drastically reduce the amount of data obtained for each SBR cycle. Then the Case-Based Reasoning tool (explained below) is used to perform situation assessment of the process. As a result, each SBR cycle can be classified according to its performance.

10.3.3.3.Case-Based Reasoning (CBR).

Case Based Reasoning is an approach to problem solving that is able to use specific knowledge of previous experiences. A new problem is solved by matching it with similar past situations that are recorded in the Case Library. CBR is based on four stages (see Figure 10-4) which are conducted once the cycle is finished or when detecting a problem in the lower level of control:

i) **Retrieve:** In this step, the new situation (cycle or part of it) is compared to the cases available in the Case Library. The objective is to find a past situation similar to the new one. The similarity of the new case with the cases in the library is computed by means of a distance function.

ii) **Reuse:** The information retrieved from the historical case is used to improve the current performance.

iii) **Revise:** Evaluate whether the solution retrieved from the historical case has a positive effect on the current performance of the plant. This evaluation can be conducted in the real plant or alternatively on the model that supports the supervisory control system. The revision is conducted by the plant manager, who has the detailed knowledge of the process. This evaluation is a source of new knowledge that can be introduced within the artificial reasoning as a new learned case.

iv) **Retain:** Update the CBR knowledge base with the new learned case. This involves adding the new learned case into the case library. This step permits the CBR system to improve the reasoning ability.

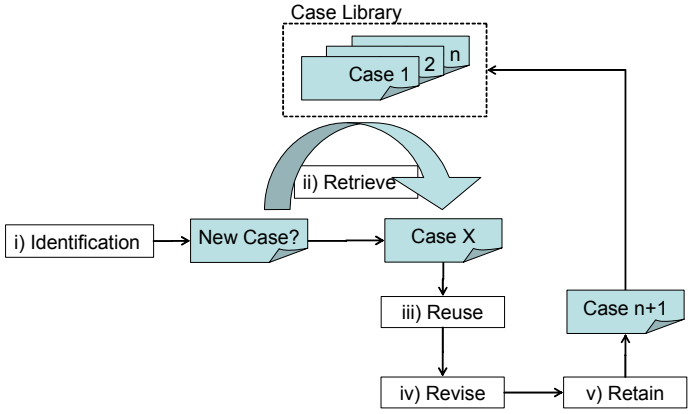


Figure 10-4. Steps in the CBR approach.

The key point of CBR is defining the cases. The proposed approach takes advantage of all available information using the particular information about the whole cycle (on-line and calculated variables, applied strategy, endpoint detection and, if available, the quality of the influent and the effluent). Moreover, in this case, the CBR is combined with the MPCA, in such a way that the MPCA is a preprocessing tool for the CBR system that compresses the dynamic information of process measured variables in a suitable form to be used to define cases. Therefore, it is possible to improve the fault detection tasks to obtain a more useful situation assessment system including capabilities such as diagnosis, estimation of unknown variables and strategy proposals. CBR experiences in our research group applied to the activated sludge process can be found in R-Roda *et al.* (1999) and Comas *et al.* (2005). Another experience found in the literature dealing with SBR can be found in Wiese *et al.* (2004).

Using the ES, the MSPC and CBR, a diagnosis of the current operational state and trend of the WWTP process can be performed. Furthermore, a recipe proposal of the suitable action plan is achieved. Finally, this layer can evaluate the proposed cycle recipe using an off-line mathematical model, which gets the current state from the on-line model and performs a long term simulation. In addition to this structure, the process and control engineer is involved in process management by defining the goals and the strategy to follow.

10.3.3.4. Complementary units

Three complementary modules are necessary within the supervisory control system, which interact with the different levels of the system: the process database, the model and the operation module.

- ***The process database.***

The process database is in charge of storing all the information coming from the other modules, which can be further processed. The database used is MySQL and is connected with labVIEW through the Open DataBase Connectivity (ODBC). This permits huge amounts of information to be handled without collapsing the functioning of the computer. The database is structured in two main groups which are i) the static data and ii) the dynamic data.

The static data contains the recipes and the sequences of recipes to make the SBR work, the configuration parameters of the program, and also the information about the current operation. The dynamic data includes the on-line data acquired with the DAC and monitoring system (on-line and calculated data), the data coming from the phase length optimizer (e.g. times to achieve endpoints), and the information generated by the cycle supervision system (problems detected and solutions proposed).

- ***Pilot plant models.***

It is necessary to run two models: the on-line model and the off-line model. The on-line pilot plant model works as a virtual plant, receiving the same input conditions as the real plant. This on-line model permits us to know the evolution of the state variables and detect possible dysfunctions when huge deviations between the process and the model are observed. Simulation software is on-line connected to LabVIEW® to get and return the information. The input conditions are sent using DataSocket protocol. The information obtained in the simulations can be sent to LabVIEW for further processing by using Dynamic Data Exchange (DDE) communication. The structure and the connection of the software allow the recalibration of the model to be performed when necessary. Hence, the input conditions (e.g. flows and influent wastewater composition) are saved by LabVIEW® in consecutive files what permits simulating the process from the desired situation in the past. Then, a manual adjustment of the model parameters or the model structure can be performed.

The off-line model is useful at the supervision level, taking the state variables values of the on-line model as the initial state, and simulating the results obtained from the diagnosis. A long-term simulation is advised because a change in the operating conditions may have effect at minimum three times the SRT. The off-line simulation results can be evaluated by using performance indices as presented in Vanrolleghem and Gillot (2002).

- ***Operation.***

The operation module is in charge of deciding the current operation depending on the responses generated by the three levels. The DAC and monitoring module and the phase length optimizer work at the same time establishing the internal control loops and the optimization of the phase lengths. Once the cycle is finished, a diagnosis of the current performance can be conducted and then a proposal for continuing or changing the operation is done. Moreover, the cycle supervision module can be activated if a failure is detected in the lower levels of control. Hence, a hierarchy between the different modules of the control system is established to have a list of priorities to face the operation of the SBR.

10.3.4. SBR supervision software

The SBR supervision software named SYCOTIN (**In**telligent **Co**n**t**rol **Sy**stem) has already been started and is continuously up-to-date. Its structure permits to easily add new modules as they are coded. In this point the main features of this software are presented. The lower and medium levels of control have been already coded and the higher level is under development.

The general menu allows the user to define the work plan, the work sequence, the parameters of the control strategy, to interact with the database and configure the connection with GPS-X,

apart from general settings and other specific tools. This software environment permits to easily access the process data and control the SBR operation. The main features of the SYCOTIN are:

- Work plans and work sequences:
  - Creating new work plans, defining the phases and its lengths
  - Loading existing work plans
  - Creating work sequences, from the work plans
- On-line data Acquisition
  - The data from the sensors are acquired each time interval
  - Window to include the calibration parameters of the sensors signal.
- Plotting the data
  - The current signal from the sensors is plotted.
- DataBase
  - Storing the data.
  - Consultation.
  - Report generation
- Control of the dissolved oxygen
  - Establish for each phase the desired set-point
  - Establish for each phase the desired type of control (No control, On-Off, PID or Fuzzy).
- Phase length optimizer
  - Establish the desired control variables (pH, ORP, DO, OUR) for each phase.
  - Establish the control parameters (t_{min}, t_{wait}, OUR_{min}, ORP_{min}…).
- GPS-X connection
  - Connection between GPS-X and LabVIEW® by using the Datasocket. A security system has been developed to overcome with problems with the network.

Two print screen examples of the user-friendly interfaces of the software used to develop this supervisory control system are presented below.

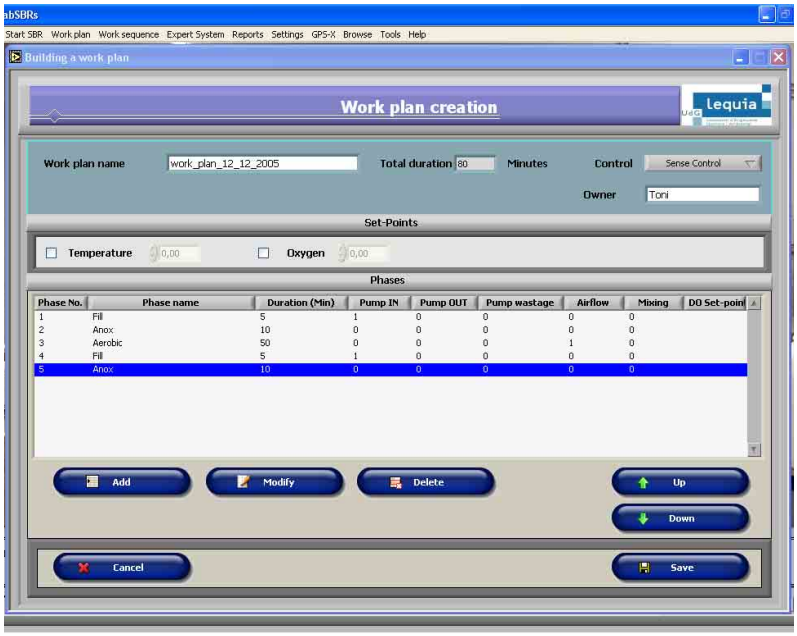


Figure 10-5. Print screen 1 of the supervisory control system interfaces, developed in LabVIEW® (work plan definition).

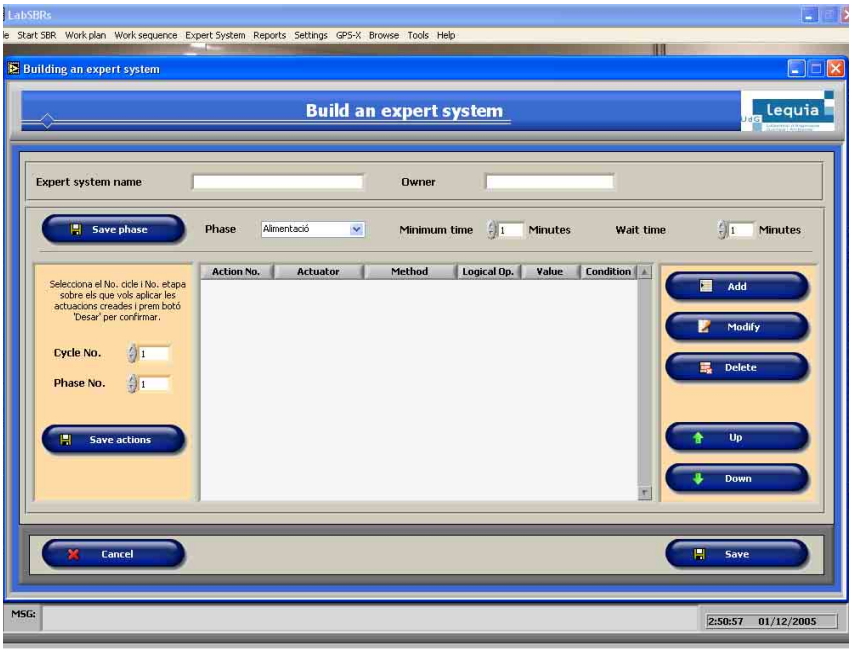


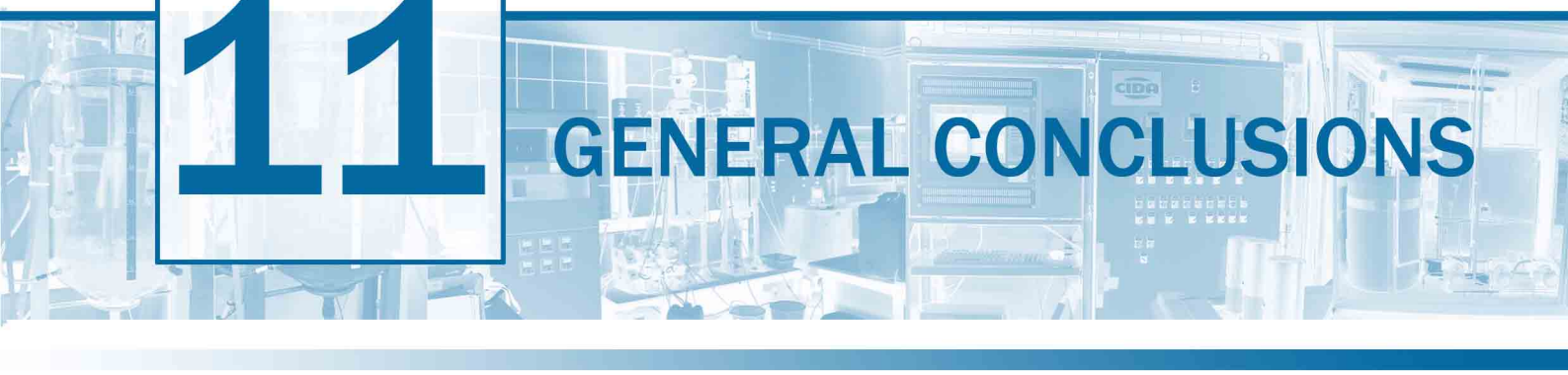
Figure 10-6. Print screen 2 of the supervisory control system interface (ES configuration).

10.4. FUTURE WORK

The future work is focused on finishing the supervisory control system presented in this Chapter. The different units (ES, MSPC and CBR) are under development and in a near future they have to be evaluated to test their effectiveness. After this evaluation the real possibilities of the supervisory system will be established. The advantage of a good planning in the LabVIEW® programming permits to update the software as soon a new module is obtained. However, the final aim of the project is to implement the supervisory control system in an SBR plant for a long-term period.

On the other hand, the obtained promising results encourage the extension of the system to the simultaneous removal of organic matter, nitrogen and phosphorus. This implies to abstract the knowledge from the phosphorus removal process and to apply this knowledge into the three levels of control. In the lower level, the desired conditions to achieve phosphorus removal have to be established. In the medium level, the patterns to determine the end of release and the end of phosphorus uptake have to be identified in order to adjust the length of the anaerobic, aerobic and anoxic phases. Finally, in the higher level it should be possible to face abnormal situations related to the phosphorus removal and adapting the operating cycle to the required conditions.

This future work is supported by a project (MCYT DPI2005-08922-C02-01, “Development of an intelligent control system applied to the SBR technology to remove organic matter, nitrogen and phosphorus”) financed by the Spanish Government. This, combined with the knowledge acquired encourages the conduction of the research in this subject.



11 GENERAL CONCLUSIONS

11. GENERAL CONCLUSIONS

It has been demonstrated that the productivity of the SBR plant can be increased, the energy consumption reduced, the personnel necessities decreased and the reliability on the process increased. This has been achieved by designing a control system for the SBR and with the help of calibrated models that can provide valuable information at a reasonable time-scale. The following main conclusions can be drawn from the research carried out in this thesis:

Calibration of ASM models to describe the carbon and nitrogen removal processes in the SBR

The analysis of the available calibration protocols permitted to handle the calibration task with guaranties of success. Moreover, some key points were identified to adapt the calibration protocols for SBR applications.

Two calibrated and validated models were obtained that properly describe the carbon and nitrogen removal processes:

- The first one (Chapter 5) was obtained to be used for evaluating control strategies. In this case, the use of only historical data was enough to achieve the goal of the study. Moreover, the final evaluation of the calibration allowed detecting some strengths and weaknesses to be used in further experiences. One of the key points for the success in the calibration was the modification of the simulation methodology transferring the experimental history into the model.

- The second model (Chapter 6) was obtained to support a supervisory control system. This experience considered the improvements detected in the calibration of the model 1. An accurate influent wastewater characterization was conducted and the b_H and Y_H parameters were successfully determined. This allowed decreasing the uncertainty in the influent wastewater characterization. The ARD was calculated to assess the fit between the experimental and simulated values. Low values were obtained for both the calibration and validation profiles. Moreover, the model was validated for a period of 70 days, describing properly the dynamics of the process. Hence, a suitable calibration procedure was obtained, directly applicable in the research of our group, to be used for further experiences and considering that the validity of the model is limited and periodic recalibrations may be needed.

Developing a real-time control system

In the second section of the thesis the control system for the SBR was successfully designed. This system was basically designed to work using the on-line sensors of DO, pH and ORP and the calculated OUR. Different steps were necessary to obtain the control system:

- The patterns in the on-line signals (DO, pH, ORP) and calculated variables (OUR) described in the literature were identified in several historical case studies to obtain a conceptual background for generating different ideas for controller. For the aerobic phase the identified key points were the AV, the αO_2, the α_{OUR} and the OUR_V. Regarding the anoxic phases, the NK and the NA were identified. The dissolved oxygen control during the aerobic phases influences the other variables (e.g. pH) and hence, to higher levels of control.

- A model-based approach was useful for designing and evaluating a control strategies to optimize the length of the reaction phases. The OUR and the ORP were chosen as the key parameters of control and the use of process indexes was useful tool to evaluate the control strategies. On the one hand, it was seen that implementing a DO controller improved the denitrification process leading to a reduction in the nitrite and nitrate concentration in the effluent and decreased the required aeration energy. On the other hand, the implementation of the on-line control strategy allowed increasing the capacity of the plant.

- The real-time control system was implemented in the semi-industrial pilot plant in order to optimize de length of the aerobic and anoxic phases. This was based on the OUR and the ORP variables, establishing a threshold value for these parameters that was directly related to the end of nitrification and denitrification processes. This control system was implemented for real-time control of a SBR treating urban wastewater working satisfactory for more than three months.

- Finally, a first approach to a supervisory control system was presented. This system was divided into three levels (low, medium and high). The lower level permits controlling the SBR at the desired conditions, the medium level is focused on the on-line adjustment of the length of the reaction phases. The higher level deals with the assessment of the process status and is able to propose corrective and preventive measures. This layer uses artificial intelligence tools and it is composed of an advanced optimization module using Expert System, Multivariable Statistical Process Control and Case Based Reasoning tools. These modules are under development and have to be validated in future work.

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12. REFERENCES

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