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CONCEPTUAL DESIGN OF WASTEWATER TREATMENT PLANTS USING MULTIPLE OBJECTIVES

Xavier FLORES ALSINA

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Xavier Flores Alsina

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IGNASI RODRÍGUEZ-RODA

Associate Professor at the Laboratory of Chemical and Environmental Engineering, University of Girona

RENÉ BAÑARES-ALCÁNTARA

Reader in Engineering Science at the Department of Engineering Science, University of Oxford

CERTIFY

That Mr. Xavier Flores Alsina has done the work presented in this thesis, "**Conceptual Design of Wastewater Treatment Plants using Multiple Objectives**" under our supervision. The thesis is submitted as part of the requirements to obtain a doctoral degree in Environmental Sciences (Physics and Environmental Technology).

We submit and sign the present certification to the Faculty of Sciences at the University of Girona for any intents and purposes for which it may be used.

Girona, March 2008

Ignasi Rodríguez-Roda　　　　René Bañares-Alcántara

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To Teresa Maria Alsina

"**Yup, life moves pretty fast.**

If you don't stop and take a look around once in a while,

you might miss it"

Ferris Bueller's Day Off (1986)

PREFACE

The implementation of EU Directive 91/271/EEC concerning urban wastewater treatment promoted the construction of new facilities and the introduction of nutrient removal technologies in areas designated as sensitive. The need to build at a rapid pace imposed economically sound approaches for the design of the new infrastructures and the retrofit of the existing ones. These studies relied exclusively on the use of heuristic knowledge and numerical correlations generated from simplified activated sludge models. Hence, some of the resulting wastewater treatment plants (WWTPs) were characterized by a lack of robustness and flexibility, bad controller performance, frequent microbiology-related solids separation problems in the secondary settler, high operating and maintenance costs and/or partial nutrient removal, which made their performance far from optimal. Most of these problems arose because of inadequate design, making the scientific community aware of the crucial importance of the conceptual design stage. Thus, these traditional design approaches should turn into more complex assessment methods in order to conduct integrated assessments taking into account a multiplicity of objectives an hence ensuring a correct plant performance. Despite the importance of this fact only a few methods in the literature addressed the systematic evaluation of conceptual WWTP design alternatives using multiple objectives. Yet, the decisions made during this stage are of paramount importance in determining the future plant structure and operation.

The main objective pursued in this thesis targets the development of a systematic conceptual design method for WWTP using multiple objectives, which supports decision making when selecting the most desirable option amongst several generated alternatives. This research work contributes with a modular and evolutionary approach combining techniques from different disciplines such as: a *hierarchical* decision approach, *multicriteria* decision analysis, preliminary multiobjective optimization using sensitivity functions, knowledge extraction and data mining techniques, *multivariate* statistical techniques and *uncertainty* analysis using Monte Carlo simulations. This is accomplished by dividing the design method into 4 different blocks: (1) *hierarchical* generation and *multicriteria* evaluation of the design alternatives, (2) analysis of *critical decision*s, (3) *multivariate* analysis and, finally, (4) *uncertainty* analysis.

The first block of the proposed method, supports the conceptual design of WWTP combining a *hierarchical* decision approach with *multicriteria* analysis. The *hierarchical* decision approach breaks down the conceptual design into a number of issues that are easier to analyze and to evaluate while the *multicriteria* analysis allows the inclusion of different objectives at the same time. Hence, the number of alternatives to evaluate is reduced while the future WWTP design and operation is greatly influenced by environmental, technical, economical and legal aspects. Also, the inclusion of a sensitivity analysis facilitates the study of the variation of the generated alternatives with respect to the relative importance of the objectives.

The second block, analysis of *critical decisions,* is tackled with sensitivity analysis, preliminary multiobjective optimization and knowledge extraction to assist the designer during the selection of the best alternative amongst the most *promising alternatives* i.e. options with a similar overall degree of satisfaction of the design objectives but with completely different implications for the future plant design and operation. The analysis provides a wider picture of the possible design space and allows the identification of desirable (or undesirable) WWTP design directions in advance.

The third block of the proposed method, involves the application of *multivariate* statistical techniques to mine the complex *multicriteria* matrixes obtained during the evaluation of WWTP alternatives. Specifically, the techniques used in this research work are i) cluster analysis, ii) principal component/factor analysis, and iii) discriminant analysis. As a result, there is a significant improvement in the accessibility of the information needed for effective evaluation of WWTP alternatives, yielding more knowledge than the current evaluation methods to finally enhance the comprehension of the whole evaluation process.

In the fourth and last block, *uncertainty* analysis of the different alternatives is further applied. The objective of this tool is to support the decision making when uncertainty on the model parameters used to carry out the analysis of the WWTP alternatives is either included or not. The uncertainty in the model parameters is introduced, i.e input uncertainty, characterising it by probability distributions. Next, Monte Carlo simulations are run to see how those input uncertainties are propagated through the model and affect the different outcomes. Thus, it is possible to study the variation of the overall degree of satisfaction of the design objectives, the contributions of the different objectives in the overall variance to finally analyze the influence of the relative importance of the design objectives during the selection of the alternatives.

Thus, in comparison with the traditional approaches the conceptual design method developed in this thesis addresses design/redesign problems with respect to multiple objectives and multiple performance measures. Also, it includes a more reliable decision procedure that shows in a systematic, objective and transparent fashion the rationale way a certain alternative is selected and not the others. The decision procedure provides to the designer/decision maker with the alternative that best fulfils the defined objectives, showing its main advantages and weaknesses, the different correlations between the alternatives and evaluation criteria and dealing with the uncertainty prevailing in some of the model parameters used during the analysis.

A number of case studies, selection of biological nitrogen removal process (case study #1), optimization of the setpoints in two control loops (case study #2), redesign to achieve simultaneous organic carbon, nitrogen and phosphorus removal (case study #3) and evaluation of control strategies at plant wide level (case studies #4 and #5), are used to demonstrate the capabilities of the conceptual design method.

RESUM

La implementació de la Directiva Europea 91/271/CEE referent a tractament d'aigües residuals urbanes va promoure la construcció de noves instal·lacions al mateix temps que la introducció de noves tecnologies per tractar nutrients en àrees designades com a sensibles. Tant el disseny d'aquestes noves infraestructures com el redisseny de les ja existents es va portar a terme a partir d'aproximacions basades fonamentalment en objectius econòmics degut a la necessitat d'acabar les obres en un període de temps relativament curt. Aquests estudis estaven basats en coneixement heurístic o correlacions numèriques provinents de models determinístics simplificats. Així doncs, moltes de les estacions depuradores d'aigües residuals (EDARs) resultants van estar caracteritzades per una manca de robustesa i flexibilitat, poca controlabilitat, amb freqüents problemes microbiològics de separació de sòlids en el decantador secundari, elevats costos d'operació i eliminació parcial de nutrients allunyant-les de l'òptim de funcionament. Molts d'aquestes problemes van sorgir degut a un disseny inadequat, de manera que la comunitat científica es va adonar de la importància de les etapes inicials de disseny conceptual. Precisament per aquesta raó, els mètodes tradicionals de disseny han d'evolucionar cap a sistemes d'avaluació mes complexos, que tinguin en compte múltiples objectius, assegurant així un millor funcionament de la planta. Tot i la importància del disseny conceptual tenint en compte múltiples objectius, encara hi ha un buit important en la literatura científica tractant aquest camp d'investigació.

L'objectiu que persegueix aquesta tesi és el de desenvolupar un mètode de disseny conceptual d'EDARs considerant múltiples objectius, de manera que serveixi d'eina de suport a la presa de decisions al seleccionar la millor alternativa entre diferents opcions de disseny. Aquest treball de recerca contribueix amb un mètode de disseny modular i evolutiu que combina diferent tècniques com: el procés de decisió jeràrquic, anàlisi multicriteri, optimació preliminar multiobjectiu basada en anàlisi de sensibilitat, tècniques d'extracció de coneixement i mineria de dades, anàlisi multivariant i anàlisi d'incertesa a partir de simulacions de Monte Carlo. Això s'ha aconseguit subdividint el mètode de disseny desenvolupat en aquesta tesis en quatre blocs principals: (1) generació jeràrquica i anàlisi multicriteri d'alternatives, (2) anàlisi de decisions crítiques, (3) anàlisi multivariant i (4) anàlisi d'incertesa.

El primer dels blocs combina un procés de decisió jeràrquic amb anàlisi multicriteri. El procés de decisió jeràrquic subdivideix el disseny conceptual en una sèrie de qüestions mes fàcilment analitzables i avaluables mentre que l'anàlisi multicriteri permet la consideració de diferent objectius al mateix temps. D'aquesta manera es redueix el nombre d'alternatives a avaluar i fa que el futur disseny i operació de la planta estigui influenciat per aspectes ambientals, econòmics, tècnics i legals. Finalment aquest bloc inclou una anàlisi de sensibilitat dels pesos que proporciona informació de com varien les diferents alternatives al mateix temps que canvia la importància relativa del objectius de disseny.

El segon bloc engloba tècniques d'anàlisi de sensibilitat, optimització preliminar multiobjectiu i extracció de coneixement per donar suport al disseny conceptual d'EDAR, seleccionant la millor alternativa

un cop s'han identificat decisions crítiques. Les decisions crítiques són aquelles en les que s'ha de seleccionar entre alternatives que compleixen de forma similar els objectius de disseny però amb diferents implicacions pel que respecte a la futura estructura i operació de la planta. Aquest tipus d'anàlisi proporciona una visió més àmplia de l'espai de disseny i permet identificar direccions desitjables (o indesitjables) cap on el procés de disseny pot derivar.

El tercer bloc de la tesi proporciona l'anàlisi multivariant de les matrius multicriteri obtingudes durant l'avaluació de les alternatives de disseny. Específicament, les tècniques utilitzades en aquest treball de recerca engloben: 1) anàlisi de conglomerats, 2) anàlisi de components principals/anàlisi factorial i 3) anàlisi discriminant. Com a resultat és possible un millor accés a les dades per realitzar la selecció de les alternatives, proporcionant més informació per a una avaluació mes efectiva, i finalment incrementant el coneixement del procés d'avaluació de les alternatives de disseny generades.

En el quart i últim bloc desenvolupat en aquesta tesi, les diferents alternatives de disseny són avaluades amb incertesa. L'objectiu d'aquest bloc és el d'estudiar el canvi en la presa de decisions quan una alternativa és avaluada incloent o no incertesa en els paràmetres dels models que descriuen el seu comportament. La incertesa en el paràmetres del model s'introdueix a partir de funcions de probabilitat. Desprès es porten a terme simulacions Monte Carlo, on d'aquestes distribucions se n'extrauen números aleatoris que es subsisteixen pels paràmetres del model i permeten estudiar com la incertesa es propaga a través del model. Així és possible analitzar la variació en l'acompliment global dels objectius de disseny per a cada una de les alternatives, quines són les contribucions en aquesta variació que hi tenen els aspectes ambientals, legals, econòmics i tècnics, i finalment el canvi en la selecció d'alternatives quan hi ha una variació de la importància relativa dels objectius de disseny.

En comparació amb les aproximacions tradicionals de disseny, el mètode desenvolupat en aquesta tesi adreça problemes de disseny/redisseny tenint en compte múltiples objectius i múltiples criteris. Al mateix temps, el procés de presa de decisions mostra de forma objectiva, transparent i sistemàtica el perquè una alternativa és seleccionada en front de les altres, proporcionant l'opció que més bé acompleix els objectius marcats, mostrant els punts forts i febles, les principals correlacions entre objectius i alternatives, i finalment tenint en compte la possible incertesa inherent en els paràmetres del model que es fan servir durant les anàlisis.

Les possibilitats del mètode desenvolupat es demostren en aquesta tesi a partir de diferents casos d'estudi: selecció del tipus d'eliminació biològica de nitrogen (cas d'estudi # 1), optimització d'una estratègia de control (cas d'estudi # 2), redisseny d'una planta per aconseguir eliminació simultània de carboni, nitrogen i fòsfor (cas d'estudi # 3) i finalment anàlisi d'estratègies control a nivell de planta (casos d'estudi # 4 i # 5).

RESUMEN

La implementación de la Directiva Europea 91/271/CEE referente al tratamiento de aguas residuales urbanas promovió la construcción de nuevas instalaciones al mismo tiempo que introdujo nuevas tecnologías para el tratamiento de nutrientes en áreas designadas como sensibles. Tanto el diseño de estas nuevas infraestructuras como el rediseño de las ya existentes, se llevó a cabo a partir de aproximaciones fundamentalmente basadas en objetivos económicos debido a la necesidad de terminar las obras en un periodo de tiempo relativamente corto. Estos estudios estuvieron basados en conocimiento heurístico o correlaciones numéricas que provienen de modelos determinísticos simplificados. Así, muchas de las estaciones depuradoras de aguas residuales (EDARs) resultantes se caracterizaron por carecer de robustez y flexibilidad, poca controlabilidad, con frecuentes problemas de separación de sólidos de origen microbiológico en los decantadores secundarios, elevados costes de operación y eliminación parcial de nutrientes. Muchos de estos problemas surgieron debido a un diseño inadecuado de manera que la comunidad científica se dio cuenta de la importancia de las etapas iniciales de diseño conceptual. Precisamente, los métodos tradicionales de diseño deben cambiar hacia sistemas de evaluación mas complejos que tengan en cuenta múltiples objetivos asegurando un mejor funcionamiento de las futuras plantas. A pesar de la importancia de este problema existe todavía un vacío importante en la literatura científica que trate el problema de diseño conceptual de EDARs con múltiples objetivos.

El objetivo que persigue esta tesis es el de desarrollar un método de diseño conceptual de EDARs teniendo en cuenta múltiples objetivos, de manera que sirva de herramienta de soporte a la toma de decisiones al seleccionar la mejor alternativa entre las diferentes opciones de diseño. Este trabajo de investigación contribuye con un método de diseño modular y evolutivo que combina diferentes técnicas como: el proceso de decisión jerárquico, análisis multicriterio, optimización preliminar multiobjetivo a partir de análisis de sensibilidad, análisis multivariante y análisis de incertidumbre a partir de simulaciones de Monte Carlo. Esto se ha conseguido subdividiéndolo en cuatro bloques principales: (1) generación jerárquica y análisis multicriterio de los alternativas de diseño, (2) análisis de decisiones criticas, (3) análisis multivariante y finalmente (4) análisis de incertidumbre.

El primero de los bloques subdivide el proceso de diseño conceptual en una serie de cuestiones más fácilmente analizables y evaluables, mientras que el análisis multicriterio permite la inclusión de diferentes objetivos al mismo tiempo. De esta manera se reduce el número de alternativas a evaluar y se garantiza que el futuro diseño y operación de la planta este influenciado por aspectos ambientales, económicos, legales y técnicos. Este bloque también incluye el análisis de sensibilidad de los pesos de los objetivos, de manera que es posible estudiar la variación de las alternativas de diseño cuando se cambia su importancia relativa.

El segundo de los bloques engloba técnicas de análisis de sensibilidad, optimización preliminar multiobjetivo y extracción de conocimiento para dar soporte al diseño conceptual de EDAR seleccionado la mejor alternativa una vez que se han identificado decisiones críticas. Las decisiones críticas son aquellas

cuyas opciones presentan un cumplimiento similar de los objetivos de diseño pero con implicaciones muy distintas para la futura estructura y operación de la planta. Este tipo de análisis proporciona una información más amplia del espacio de diseño y permite identificar direcciones deseables (o indeseables) a las que el proceso de diseño puede conducir.

El tercer bloque proporciona análisis multivariante de las matrices multicriterio obtenidas durante la evaluación de las alternativas de diseño. Concretamente las técnicas utilizadas en este trabajo de investigación engloban: 1) análisis de conglomerados, 2) análisis de componentes principales/análisis factorial y 3) análisis discriminante. Como resultado es posible un mejor acceso a los datos para realizar la selección de las alternativas, proporcionando más información para una evaluación más efectiva y finalmente incrementando el conocimiento del proceso de evaluación de las alternativas de diseño que se tienen que seleccionar.

En el cuarto y último bloque desarrollado en esta tesis, las diferentes alternativas de diseño son evaluadas teniendo en cuenta la incertidumbre. El objetivo de este bloque es estudiar la variación en la toma de decisiones cuando una alternativa es evaluada incluyendo o no la incertidumbre en los modelos que describen su comportamiento. La incertidumbre en los parámetros del modelo se introduce a partir de funciones de probabilidad. Después se llevan a cabo simulaciones de Monte Carlo donde de estas distribuciones se extraen números aleatorios que se sustituyen por los parámetros del modelo. Este tipo de análisis permite estudiar como esta incertidumbre se propaga y afecta el grado global de satisfacción de los objetivos de diseño, cuales son las contribuciones que los objetivos ambientales, legales, económicos y técnicos tienen en esta variación y finalmente el cambio en la selección de alternativas cuando hay una variación en la importancia relativa de los objetivos de diseño.

En comparación con las aproximaciones tradicionales de diseño, el método desarrollado en esta tesis trata problemas de diseño/rediseño teniendo en cuenta múltiples objetivos y múltiples criterios. Al mismo tiempo, el proceso de toma de decisiones muestra de forma objetiva, transparente y sistemática porque una alternativa es seleccionada y no las otras, proporcionando la opción que mejor cumple con los objetivos marcados, mostrando sus puntos fuertes y sus puntos débiles, las principales correlaciones entre objetivos y alternativas y finalmente teniendo en cuenta la posible incertidumbre inherente en los parámetros de los modelos que se utiliza durante los análisis.

Las posibilidades del método desarrollado se demuestran en esta tesis a partir de diferentes casos de estudio: selección del tipo de eliminación biológica de nitrógeno (caso de estudio #1), optimización de una estrategia de control (caso de estudio #2), rediseño de una planta para conseguir la eliminación simultanea de carbono, nitrógeno y fósforo (caso de estudio # 3) y finalmente análisis de estrategias de control a nivel de planta (casos de estudio # 4 y # 5).

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PhD THESIS

CHAPTER 1. INTRODUCTION

1.1. MOTIVATION

The increasing pace of industrialization, urbanization and population growth that our planet has faced over the last one hundred years has considerably increased environmental pollution and habitat destruction, and negatively affected water, air and soil qualities. In this the context within which wastewater treatment has become one the most important environmental issues of the day, insofar as it reduces or prevents pollution of natural water resources - i.e. inland surface waters, groundwater, transitional water and coastal water -promotes sustainable water re-use, protects the aquatic environment and improves the status of aquatic ecosystems.

The implementation of EU Directive 91/271/EEC concerning urban wastewater treatment promoted the construction of new facilities and the introduction of nutrient removal technologies in areas designated as sensitive. The need to build at a rapid pace imposed economically sound approaches for the design of the new infrastructures and the retrofit of the existing ones. These studies relied exclusively on the use of heuristic knowledge and numerical correlations generated from simplified activated sludge models (e.g. ATV, HSA Principles, Ten State Standards and Custom Models). Nevertheless, some of the resulting wastewater treatment plants (WWTPs) were characterized by a lack of robustness and flexibility, bad controller performance, frequent microbiology-related solids separation problems in the secondary settler, high operational costs and/or partial nitrogen and phosphorus removal. This made their performance far from optimal. Most of these problems arose because of inadequate design, making the scientific community aware of the crucial importance of the design stage (Vanrolleghem *et al*., 1996; Vidal *et al*., 2002; Dominguez *et al*., 2006; Rivas *et al*., 2008)

The new EU Water Directive (2000/60/EEC) establishes a new framework for Community action in the field of water policy. The Directive requires the development of management plans, where the major pressures and impacts on the receiving water are shown and measures to reach quality objectives are decided. In addition, one of the main characteristics of this new directive is the shift away from control of the point sources of pollution to integrated pollution prevention and control at river basin level, with the receiving water quality based on upstream pollution limits. This approach results in more freedom during the evaluation procedure – due to the expansion of the management limits – which can lead on the one hand to a better allocation of economic resources in pollution abatement, but on the other hand introduces a higher degree of complexity during the evaluation procedure because additional factors must be taken into account (Benedetti 2006).

For this reason, traditional design approaches have to become more complex assessment methodologies that address design/redesign problems with respect to multiple objectives and multiple performance measures. WWTPs need to ensure a sufficient degree of pollution removal in terms of organic matter and nutrients to comply with the legislative limits on water discharge while, at the same time, keeping construction and operating costs to a minimum. Also, the need to increase their effectiveness and reduce their environmental impact has led to consider some additional criteria to evaluate a plant's technical reliability and the potential damage to the water body caused by the treated effluent. Further, more attention has to be paid at the conceptual design level in order to ensure better WWTP performance. Decisions made during the conceptual design stage - e.g. sequence of aerobic, anoxic and aerobic sections, addition of certain chemical compounds and extra recycles - are of paramount importance in determining the whole plant performance – e.g. adaptation to short term and long term perturbations, potential risk of solids separation problems, aeration costs and effluent characteristics. Finally, a more reliable decision making procedure is necessary in which the selection of alternatives is based on communicable, systematic, objective and transparent procedures that allow a subsequent analysis of why one alternative was selected with respect to others. Considering the importance of the conceptual design/redesign of WWTPs, the existing literature in the field is still sparse and only a few systematic methodologies that tackle the complex task at the heart of the design problem are available to support the decision maker. The importance of conceptual design for WWTPs using multiple objectives and the lack of systematic methodologies to handle this complexity are the main motivations for this research work.

1.2. CHALLENGES IN THE CONCEPTUAL DESIGN OF WASTEWATER TREATMENT PLANTS

Certain key challenges have to be confronted to promote the further progress of conceptual design in wastewater treatment facilities:

- Reducing the number of process alternatives. Conceptual design is complex and ill-defined because of the large number of potential solutions - e.g. modifications of existing equipment, addition of new equipment, piping - that might be considered in order to accomplish the same goal (Douglas 1988). However, after thorough evaluation, a very high percentage of these alternatives prove to be unsuitable.
- Dealing with multiple criteria during the evaluation of alternatives. The different conceptual alternatives have to maximize the degree of satisfaction of different objectives (Hoffman *et al.,* 2003). The purpose of wastewater treatment is to remove pollutants that can harm the aquatic environment if they are discharged into it. Thus, the selected alternative needs to comply with current regulatory standards as well as minimize the environmental impact on the receiving water body (Copp 2002). Furthermore, both construction and operating costs have to be minimized. In particular energy savings must be looked at - e.g. aeration, pumping, heating and mixing. Chemicals such as metal salts for phosphorus precipitation, the external carbon source to enhance denitrification efficiency and the costs related to the collection and disposal of sludge (Vanrolleghem and Gillot, 2002) must also be considered. Finally, when technical reliability is maximized several additional more factors must be considered. First, the plant adaptation to different types of perturbations, i.e. good disturbance rejection. Very few WWTPs receive a constant influent either in quantity or quality, but are subject to daily, weekly and annual variations (Gernaey *et al.,* 2006). Secondly, when the plant has instrumentation, control and automation, it is important to evaluate the performance of the controller and the degree of adaptability to different perturbations under different design

or operating conditions (Olsson and Newell, 1999). Thus, the selected alternative must maintain the operating variables within an operating space delimited by a set of constraints, which may be process (biomass, oxygen requirements), equipment (maximum pumping rates) or safety (effluent requirements) related. Last of all, it is important to include all naturally occurring microbiology-related solid separation problems caused by microorganisms population imbalances between filamentous and floc-forming bacteria, leading to problems of bulking and foaming or causing undesirable operating conditions which could, for example, lead to rising sludge (Wanner 1994, Jenkins *et al.,* 2003). Consequently, wastewater engineers have to take into account design factors (organic load, the anaerobic ratio, anoxic and aerobic time) and operating factors (sludge retention time) that could have a crucial influence on changes to multispecific populations integrating activated sludge systems.

- Handling *critical decisions* arising during the conceptual design of WWTPs. Certain decisions are *critical* because of their influence on the whole design process, i.e. they influence many other decisions and hence have a strong impact on future process structure and operation, with a set of possible solutions that result in a similar degree of satisfaction of the design objectives. Decision making for these *critical decisions* is especially difficult when several design objectives (as detailed in the previous challenge) must be taken into account, due to a lack of support tools for managing the interplay and the apparent ambiguity emerging from the alternatives evaluated in a *multicriteria* fashion. The ability to look ahead to future design stages might lead to different decisions (Smith 2005). Unfortunately, looking ahead is not possible with the current tools, and instead, decisions are based on incomplete knowledge.
- Extracting meaningful knowledge during the evaluation of WWTP alternatives. Biological processes in WWTPs present complex relationships between design/operating variables (e.g. anaerobic/anoxic/aerobic retention times, temperature in the anaerobic digesters, flow rates) and process parameters (effluent ammonium, nitrate, etc). Some of these present synergies (interdependences) such as aeration energy and nitrification efficiency, but others are subjected to a clear trade-off (e.g. sludge retention time and nitrification efficiency against risk of bulking). Thus, the result is a hugely complex evaluation matrix consisting of a large number of physicochemical, operational and technical parameters which are often difficult to interpret and drawing meaningful conclusions
- Including *uncertainty* during the decision making process. *Uncertainty* is a central concept when dealing with biological systems like WWTPs that are subject to pronounced natural variations (Grady *et al.,* 1999). Although wastewater models are well characterized, some parameters used during the analysis of the alternatives present *uncertainties* such as the fractions in which the different compounds arrive at the facility or the effect of either temperature or toxic compounds on the kinetic parameters. Hence, an understanding of these parameters, their inherent *uncertainty*, the way they are propagated through the model, the effect on the different outcomes and on the whole decision-making process is essential for the correct analysis of a WWTP. The assessment and presentation of the *uncertainty* is widely recognized as an important part of the analysis of complex water systems (Beck., 1987)

The challenges listed above demonstrate the complexity associated with the conceptual design of a WWTP. These complexities give rise to a number of important questions. The research work in this thesis attempts to provide with answers to the following questions:

How can the time-consuming evaluation process of a large number of conceptual design alternatives be reduced?

How can an optimal solution be found that maximizes the degree of satisfaction of the different objectives included in the evaluation procedure?

How can the designer be provided with a tool to support the management of the interplay and apparent ambiguity emerging from a multicriteria evaluation of WWTP alternatives?

How can future desirable (or undesirable) design directions be detected?

How can tools be found that are efficient at discovering groups of conceptual design alternatives with similar performance and identifying the main features for either a specific or a group of alternatives?

How the interpretation of the complex interactions amongst multiple criteria be facilitated?

How can structure be given to the decision making process, and all the knowledge generated during it reused?

How can the designer be provided with a tool to handle the uncertainty inherent in the early stages of WWTP conceptual design and allow the study of its effect on overall decision making?

1.3. THESIS STATEMENT

The first hypothesis of this thesis is that the complex problem of the conceptual design of WWTPs can be broken down into a number of simpler steps that follow a predefined order: reaction, separation and recirculation. Such a breakdown facilitates analysis and evaluation of the different design alternatives that are generated without having to obtain a complete solution to a problem when an alternative has shown to be non viable at higher levels of hierarchy.

The second hypothesis is that each alternative under evaluation can be formulated as a vector of different criteria and represented as an n-dimensional performance score profile. All the features that characterize each alternative can be summarized into a metric (weighted sum) that will give their overall degree of satisfaction according to the defined design objectives and overall process performance.

The third hypothesis is that a combination of sensitivity analysis, preliminary multiobjective optimization and knowledge extraction provides additional information with which to confront the problem of *critical decisions*. Thus, a better picture of the design space obtained by unravelling future desirable (or undesirable) directions during plant design will be possible.

The fourth hypothesis is that *multivariate* statistical techniques can mine the intensive *multicriteria* evaluation matrixes and provide aggregate indicators that enhance the understanding of the evaluation procedure. These techniques will unravel the natural association between conceptual design alternatives; design/operating variables and evaluation criteria, thereby highlighting information not available at first glance.

The fifth and final hypothesis is that the Monte Carlo simulation technique is a practical way to imitate the deviation in model outputs as a consequence of variance in model inputs during the analysis of biological WWTPs using deterministic models. It is based on the specification of input probability functions in the models' *uncertainty* parameters. A set of sampling values is randomly generated from the defined probability functions, thereby enabling the inclusion of the variation of those parameters in the decision making.

The main objective pursued in this thesis targets the development of a systematic WWTP conceptual design method that specifically addresses the identified challenges. The method evaluates conceptual design alternatives using multiple objectives, and tackles the analysis of *critical decisions* by providing further information about future design stages in the design. It can also be used as an exploratory tool for both analysis and interpretation of the *multicriteria* data matrices. Finally, it takes into explicit account the *uncertainties* prevailing around the model parameters used during the evaluation of the alternatives

1.4. CONTRIBUTIONS TO RESEARCH

The thesis offers a number of contributions in the field of the conceptual design of WWTPs.

- An evaluation methodology that combines a *hierarchical* decision approach with *multicriteria* decision making analysis. The *multicriteria* method allows the inclusion of different objectives such as environmental, economic, technical and legal while the hierarchy reduces the design problem to a set of issues that follow a predefined order (reactor, separation and recirculation). Furthermore, a sensitivity analysis of the weights is introduced in the decision making procedure as a tool to study the variation of the selected alternative when the relative importance of the design objectives is changed.
- A systematic procedure that assists the designer in tackling *critical decisions* during the decision making process. This methodology involves preliminary multiobjective optimization, the characterization of alternatives and the evaluation of trade-offs. Preliminary multiobjective optimization allows the comparison of the most *promising alternatives* when they are close to the optimum. The characterization of alternatives identifies both their strong and weak points. Finally, the evaluation of the trade-offs balances the improvement in the criteria identified as weak with the loss of overall process performance, thereby supporting the decision maker in selecting the alternative with the highest chance of success.
- A *multivariate* analysis-based methodology with which to mine the *multicriteria* matrices obtained during the evaluation of WWTP alternatives. Cluster analysis (CA), Principal Component/Factor Analysis (PCA/FA) and Discriminant Analysis (DA) are applied to the evaluation matrix data set obtained from simulation of the alternatives generated. This combination of techniques serves as an excellent exploratory tool for both analysis and interpretation of *multicriteria* matrices, making it possible i) to determine clusters of alternatives with similar behaviour, ii) to find and interpret hidden, complex and causal relation features in the data set and iii) to identify important discriminant variables for a single control strategy or a group.

- Finally, a systematic procedure is presented that supports the *multicriteria* evaluation of wastewater treatment alternatives under *uncertainty.* The proposed approach shows the variation in the decision making process depending on whether or not *uncertainty* in the model parameters is included. The *uncertainty* in these parameters, i.e. input *uncertainty,* is introduced and characterised by probability distributions based on available process knowledge. Next, Monte Carlo simulations are run to see how these input uncertainties are propagated through the model and how they affect different outcomes. Thus, i) the variation in the overall degree of satisfaction of the objectives defined for the WWTP-generated alternatives is quantified, ii) the contributions of environmental, legal, technical and economic objectives to the existing variance are identified and, finally, iii) the influence of the relative importance of the objectives during the selection of alternatives is analyzed.

1.5. THESIS OUTLINE

The thesis is structured in three main parts as shown in **Figure 1.1.** The first part comprises **Chapters 1** to **3** and describes the research scope, the main thesis objectives, the contributions to research, made in this thesis, the characteristics of current WWTP design methodologies, the position of the proposed approach amongst other design methods, a summary of the structure of the new method, and finally a brief introduction to the different wastewater treatment processes and models used as case studies.

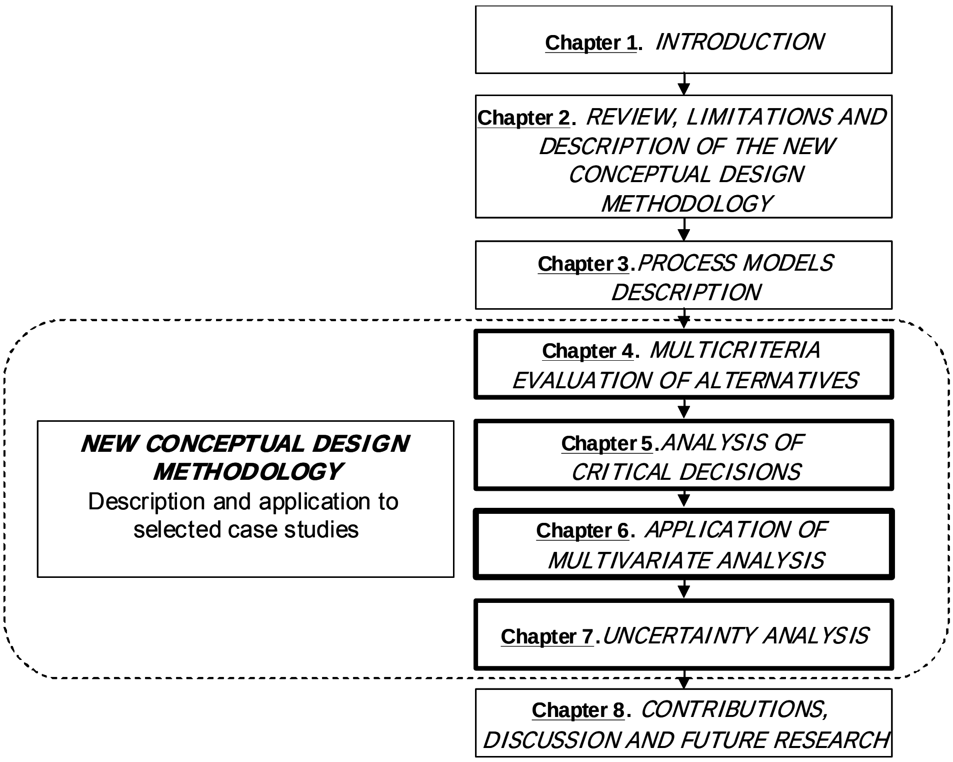

Figure 1.1. Outline of the thesis

The second part comprises **Chapters 4** to **7**, in which the new conceptual design approach is introduced step by step. Each chapter consists of an introductory part containing basic knowledge required for the comprehension of the chapter where the central concepts are laid out, followed by a practical part where these concepts are applied (case studies). At the end of each chapter conclusions are drawn concerning the overall thesis objectives. **Chapter 4** explains how the different alternatives generated by a *hierarchical* decision process are selected on the basis of several different design objectives. Two examples are shown to demonstrate the usefulness of the proposed approach. In the first, the type of biological nitrogen removal process in an existing organic carbon and nitrification activated sludge plant is selected while in the second, the set points of two PI control loops for both aeration and internal recycle in a nitrogen removal activated sludge plant are optimized. **Chapter 5** analyses the problem of *critical decisions* identified in **Chapter 4:** optimizing the most *promising alternatives*, identifying their strong and weak points and, finally, evaluating the trade-off between the improvement of the criteria identified as the option's weak points and the loss of overall process performance. This systematic procedure is applied to the redesign of the previous nitrogen removal activated sludge plant to achieve simultaneous organic carbon, nitrogen and phosphorus removal. In **Chapter 6** the analysis and the interpretation of the evaluation procedure is improved with *multivariate* statistical tools. The *multivariate* statistical techniques are applied to the results of twelve simulated control strategies in a WWTP with biological nitrogen removal. In the last research chapter (**Chapter 7**) the *uncertainty* in model parameters is introduced within the evaluation procedure by means of Monte Carlo simulations. Its usefulness is shown through another case study in which *uncertainty* in the ASM1 model parameters - i.e. influent fractions and kinetic parameters - is included when evaluating different control strategies.

In the final section, **Chapter 8**, the entire approach is re-examined and the results of the different case studies summarized. Overall conclusions are then drawn and suggestions for future research are made.

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

PhD THESIS

CHAPTER 2. LITERATURE REVIEW, LIMITATIONS OF CURRENT APPROACHES AND DESCRIPTION OF NEW CONCEPTUAL DESIGN METHOD

2.1. CONCEPTUAL DESIGN IN CHEMICAL PROCESSES

Conceptual design in chemical processes is performed during the implementation of new technologies, the specification of equipment dimensions and operating conditions, the creation of new facilities and the retrofit of existing processes. It normally involves several design tasks which are performed sequentially, starting from data gathering, process synthesis and case based development (Seider *et al*., 2004).

A good classification scheme for the many methods that have been suggested for conceptual design in chemical processes was presented in Gundersen (1989). Those methods comprise knowledge-based systems (expert systems – artificial intelligence), design methods based on heuristic rules, optimization methods stemming from operation research, and pinch methods. Some prominent examples in these categories were introduced by Kirkwood *et al*. (1988) (expert systems), Douglas (1988) (heuristic method), Kocis and Grossman (1989) (MINLP optimization of process flowsheets) and Linnhof *et al.* (1982) (pinch technology for minimization of energy use or maximization of energy reuse) based on the earlier work of Linnhof and Flower (1978).

All the conceptual design methods for the complete design of a process flowsheet follow a *hierarchical* procedure to a certain degree. At the first level the reaction system needs to be selected, at the second level the separation system to separate and recycle products is conceived, at the third level the heat exchanger network is devised, and at the last level the required utility systems are determined (Smith, 2005). Iterations between the different levels are necessary in all the methods.

2.2. CONCEPTUAL DESIGN OF WWTP APPROACHES

Conceptual design generally follows a succession of different phases, from the definition of project objectives and requirements to the implementation of the most reasonable solution (Grady *et al*., 1999). The first step involves the identification of the most reasonable potential alternative based on the current state of knowledge. The costs and the scope of these potential solutions are then estimated by calculating the bioreactor size, aeration energy, solid wastage etc. Next, the potential advantages and disadvantages of a particular solution are considered and a decision is made whether to evaluate each one in more detail or not. A particular alternative solution is dropped when its potential advantages are not sufficient to warrant further consideration, and more study is devoted to those remaining. The conceptual design stage is characterized by the fact that little process knowledge is available when the most important decisions have to be taken. Each iteration loop results in more refined information, which allows a better estimate of the sizes and costs of the alternatives. Thus, degrees of freedom steadily decrease while process knowledge is constantly gathered, and the costs involved in eliminating errors made in earlier stages rapidly increase. Consequently, the use of more refined techniques is called for. For all the phases of process development, the literature gives a large number of design and decision making tools available to support the decision maker (i.e. the process engineer in charge of process development).

After entering the operating phase, WWTPs are usually in use over long periods of time in order to make the often large construction costs viable. In order to maintain a competitive position, a WWTP needs to adapt. Typical examples of external and internal conditions and the incentives they imply include legislation changes (e.g. permitted limits of BOD_5 ,TSS, COD, TN and TP), new technology (new reactor, new chemical compounds) or simply changes in plant capacity (e.g. increased population). The redesign task is called retrofit and includes a combination of different types of modifications such as the addition of new equipment, the decommissioning of old equipment, the refitting of equipment even though the flowsheet structure is unchanged, and the alteration of the piping which connects the different equipment (Fisher *et al*., 1987). Solving a retrofit problem is similar to developing a new process: it also consists of several sequential steps that start with the identification of the retrofit incentive and continue with plant redesign and final implementation

In the literature two different approaches to solving WWTP design problems can be found: (1) the qualitative knowledge-based approach integrating expert systems and heuristic rules and (2) the numerical-based approach integrating simulations and optimization methods. Both approaches have their advantages and weaknesses but are complementary to each other. During the 90s most of the reported conceptual design applications were still based on one or another of them. In more recent times, WWTP conceptual design methods combining the advantages of both approaches have been introduced in an attempt to eliminate their inherent weaknesses.

The qualitative-knowledge based approach. These methods usually start from a base case of the investigated process and are then modified following a defined procedure where heuristic rules or wastewater treatment process insights are used to make the decisions at each level. This knowledge is obtained by daily experience of plant operation and historical know-how in specific process technologies, even though better technologies might be available.

The numerical-based approach. The numerical-based approach makes use of structural optimization strategies to analyze, evaluate and select the best possible alternative for a given conceptual design problem. Normally it is supported by mathematical models that describe the different processes to be implemented in the plant. Because of the large number that have to be evaluated; these methods require that the alternatives are properly pre-selected to ensure the feasibility of the structural optimization.

The purpose of the following review is to introduce the most important existing conceptual design methods, classified in terms of the different design approaches.

2.2.1. Applications of the qualitative knowledge-based approach

Most of the reported applications of the qualitative knowledge-based approach focus on the selection of different WWTP alternatives. One of the earliest works in this field is that presented by Krovidy and Wee (1993), where the design of wastewater treatment systems was formulated as a heuristic search problem using case based reasoning.

Freitas *et al.,* (2002) presented a design methodology to support engineers in the conceptual design of wastewater treatment facilities and help them to improve creativity and effectiveness. The system is presented as an expert system coupled to a relational database and external programs integrated as a knowledge-based management system. Chin-Tien and Jehng-Jung (1996) developed an expert system to find the appropriate treatment technology for a given waste stream. The system was intended to serve as a decision support tool for a designer to determine optimal treatment process sequences for various contaminants at different concentration levels.

In Rodriguez-Roda *et al.,* (2000), the advantages of using design history to support the design and retrofit of WWTPs were demonstrated. Using design history it was possible to :(1) automatically evaluate the compliance of alternative design proposals with respect to the design objectives; (2) study the influence of the weight of the arguments in the selection of the most adequate proposal; (3) document the decision making process; and (4) assist the designer in the search for specific items within the historical records. Finally, it is important to mention Panebianco and Pahl-Wostl (2003), who introduced an agent-based modelling approach to improve the understanding and dissemination of small-scale technologies in wastewater treatment. The conceptual agent-based model that was developed allowed representation of the complex dynamics of the socio-technical system, and was particularly suited for supporting collective learning and decision making.

2.2.2. Applications of the numerical-based approach

In this section are included all the traditional design approaches normally used for consultancies and engineering companies. These methods are based on simplified activated sludge models or safety factors. In literature can be found several design manuals summarizing these approaches such as: Ramalho (1997), Grady (1999), Qasim (1999), Metcalf & Eddy (2003).

Also, in literature can be found more sophisticated approaches including mathematical modelling during the design phase, where process alternatives are evaluated via dynamic simulations. For example, in the model study carried out in Salem *et al*., (2002), different alternatives for the upgrade of a biological N removal plant were evaluated with the objective to evaluate the potential of bioaugmentation in the return sludge line. Hao *et al*., (2001) used WWTP model simulations to compare the traditional University of Cape Town (UCT) bio P removal plant layout with an innovative alternative two-stage WWTP configuration (A_2O). The latter fully exploited the capabilities of the denitrifying polyphosphate accumulating organisms (PAOs) by introducing a separate nitrifying biofilm reactor in the process. Also, the work of Yuan *et al.,* (2000) is worth mentioning; after evaluating the sludge storage concept via ASM1 simulations, it was demonstrated that around 20% of the reactor volume could be saved. Other approaches, such as that presented in Coen *et al.,* (1996), aimed at upgrading WWTPs for biological N removal and evaluated the possibilities for improved biological N removal within an existing WWTP configuration, while Ladiges *et al.,* (1999) predicted the effect of a change of load on WWTP performance. During scenario evaluations with bio-P models, evaluation of different alternatives often results in a trade-off between bio-P capacity and nitrification, where increased DO concentrations will promote nitrification but negatively influence PAO storage products due to these products' aerobic decay (Çinar *et al*., 1998). Finally, Gernaey *et al.,* (2002) illustrated different implementations of chemical P precipitation in an existing N removal WWTP.

Other approaches focusing more on process synthesis can be found, for example, in the recent publication of Rivas *et al.,* (2008), where a mathematical formulation for the optimum design of activated sludge WWTPs using a non linear optimization method is presented, and the work carried out by Alasino *et al.,* (2007), where the process structure and operating conditions are optimized using a rigorous model. Francisco and Vega (2007) proposed a norm-based approach for the integrated design of WWTPs, i.e. design parameters were obtained simultaneously with the parameters of the controller.

More systematic approaches combining a certain degree of methodology and dynamic simulations can be found in Vidal *et al,*. (2002), where different technologies were implemented in an existing WWTP following a hierarchy of decisions, and evaluation of the alternatives that were generated was by multiple criteria. Finally, it is important to mention the work carried out by Benedetti *et al.,* (2006), where the design and upgrade of WWTPs is addressed by balancing costs and the risk of exceeding standards

2.3. LIMITATIONS OF CURRENT CONCEPTUAL DESIGN APPROACHES

In this section, the main limitations of current conceptual design methods are addressed, and the desired attributes of the new conceptual design method proposed in this thesis are summarized. Perhaps one of the most important limitations of the approaches that are currently available – with the exception of the conceptual design presented by Vidal *et al.* (2002) – is that there is as yet no unified systematic strategy to deal with wastewater treatment problems with multiple objectives.

Great progress has been made in the fields of energy saving (Ferrer *et al*., 1996), analysis of control performance (Gernaey and Jørgensen, 2004), waste minimization (Wei *et al*., 2003), increasing plant adaptation to short term perturbations (Pons and Corriou, 2002; Comas *et al*., 2006a) and decreasing microbiology-related solids separation problems (Comas *et al.,* 2006b). However, combining these objectives to obtain a solution that maximizes the degree of satisfaction of all of them has only been dealt with sparsely.

Further limitations are:

- Most of the published approaches do not present systematic procedures for generating different alternatives. There is no point in examining alternatives at higher levels of detail (e.g. location of the anaerobic reactor in a denitrifying plant for biological phosphorus removal, or including an additional recirculation system from the anoxic to the anaerobic reactor) if at lower levels of detail the alternative is not viable - e.g. biological phosphorus removal is not feasible compared to chemical precipitation.

- The subtle difference between a traditional (bio)chemical process and WWTPs is that the main objective is economic, even if environmental factors are important. Thus, traditional design approaches incorporating economic objectives, such as fixed capital investment, net present value (NPV), operating cost and payback period presented in the traditional wastewater engineering handbooks, e.g. US EPA 1982, have to evolve into more complex assessment methods taking into account multiple objectives including environmental, economic, technical and legal aspects.
- There is no clear strategy to proceed when *critical decisions* are required during the design process. The lack of efficient tools for further analysis of the design space does not allow a look-ahead step to see how the plant design might look in the future, thus forcing the designer to decide on an alternative on the basis of an incomplete picture.
- The experience gathered during the plant's design process is generally not taken into account. Although there are some methods based on heuristic rules, these have been systematically derived from the perspective of reviews of the literature, such as the work presented in Rodriguez-Roda *et al.* (2000). They do not reflect the available specific process-knowledge, e.g. the relationships between design variables and different evaluation criteria discovered during sensitivity analyses.
- There are some clear limitations with the current tools used to find correlations amongst criteria and alternatives (Gernaey *et al*., 2007). First and foremost, the association between criteria and alternatives is only based on two criteria. e.g. effluent quality index and operting costs. Secondly, this approach is not capable of discovering the main features amongst multiple criteria. Finally, it is not possible to know whether or not the criteria used to find this association is really discriminant with respect to the rest of the criteria. Therefore, other tools capable of handling both complexity and ambiguity among the other criteria during *multicriteria* evaluation are necessary for further evaluations.
- Finally, there is a lack of methodologies that take into account the *uncertainty* of the model parameter used to evaluate the different WWTP alternatives in the early stages of design. Even though the topic of *uncertainty* has been tackled previously in the literature, e.g. Rousseau *et al.* (2001), Bixio *et al.* (2002), Benedetti *et al.* (2006), the published works present certain limitations. For example, multiple objectives are not taken into account during the evaluation procedure. Also, the causes of the variation in the different outcomes, i.e. criteria - whether or not the input model *uncertainty* parameter is included - are not determined. Finally, the issue of how decision making might change if the *uncertainty* is included or not is only briefly dealt with. Clearly, there is a need to fill this gap by providing tools to support the decision makers that have to deal with this kind of multicriteria problems in the wastewater field.

From these findings it can be concluded that an ideal conceptual design method for WWTPs should be capable of addressing design/redesign problems with respect to multiples objectives and multiple performance measurements, i.e. evaluation criteria such as economic and environmental impact. Furthermore, the method should take advantage of all the knowledge generated during the design procedure, i.e. process specific knowledge, to increase understanding of the rationale behind the selected alternatives, and predict future WWTP design directions in a communicable, systematic, objective and transparent fashion. An ideal conceptual design method should also be able to discover the multiple and complex correlations among criteria and alternatives in order to improve both analysis and evaluation procedure. Finally, it should include the possibility of considering the *uncertainty* in the model parameters ('model inputs') already in the early stages of the design, studying its influence over the whole decision making procedure.

2.4. DESCRIPTION OF THE NEW CONCEPTUAL DESIGN METHOD

In this section a concise overview of the proposed conceptual design method for WWTPs is given. This method is specially aimed at handling the complexity of dealing with multiple objectives. A review of the current methods for WWTP design highlights two general principles in approaching a conceptual design problem: the qualitative knowledge-based approach and the numerical approach. It is obvious that a good conceptual design method should include elements of both approaches in a sensible manner. In view of the combinatorial problem emerging from the systematic generation of conceptual design alternatives, the generation step has to be broken down in several subproblems. The qualitative knowledge-based approach shows clear advantages for the preselection of the most *promising alternatives* since the *hierarchical* decision process can act as an efficient filter. The numerical approach, on the other hand, is well suited for the decision process when only a few alternatives remain. Thus, the proposed method uses the qualitative knowledge-based method for the generation of alternatives while the numerical-based approach is used for their evaluation. The conceptual design method proposed in this thesis is therefore structured in four blocks (see **Figure 2.1).**

- ***Hierarchical* generation and *multicriteria* evaluation of the design alternatives.** First and foremost it is assumed that the design problem can be reduced to a set of issues that follow a predefined order: reaction, separation and recirculation. Next, each alternative under evaluation can be formulated as a vector of scores in which the elements are criteria used to quantify the degree of satisfaction of the different design objectives. The initial state in the exploration (*Step 1*) involves the collection and analysis of all the information necessary to carry out the conceptual design. This initial state includes the study of the facility location, the composition of the wastewater that has to be treated, the applicable legislation and if there is a restriction affecting the design process (budget or space availability). *Step 2* includes the definition of the design objectives, the evaluation criteria used to measure the degree of satisfaction of the objectives and the different weighting factors assigned to determine the relative importance of the objectives. Finally in *Step 3* the issues to be solved are identified, the alternatives are generated, the evaluation criteria for each particular issue are selected, the alternatives from which to finally select the best alternative are evaluated according to their performance, and the relative importance is determined for the defined objectives.

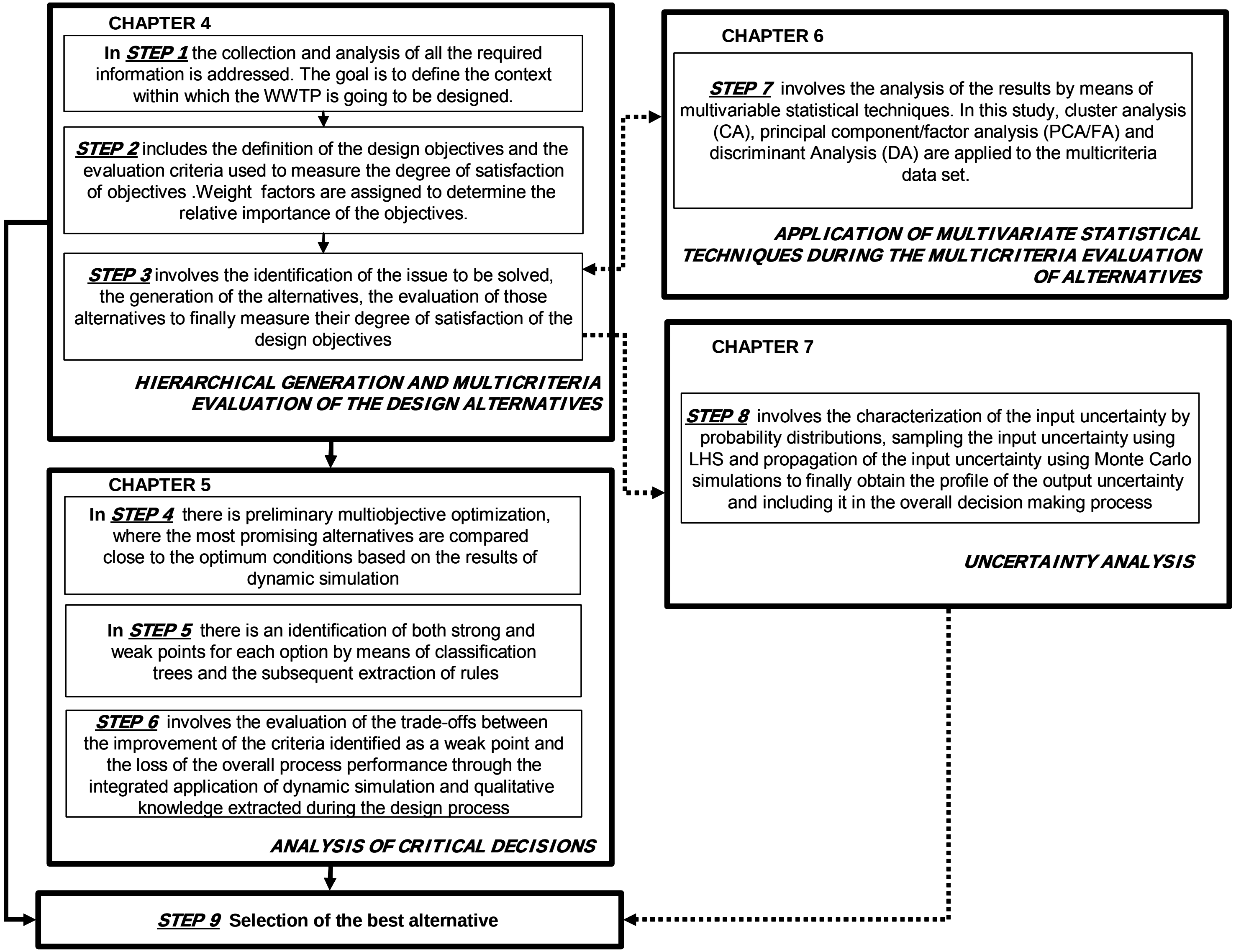

Figure 2.1. Simplified structure of the proposed conceptual design method (see text for explanations)

- **Analysis of *critical decisions*.** The second block of the proposed design method is only applied to those decisions considered to be *critical*. By *critical decisions* we mean those (i) with a great influence on the overall design process and (ii) involving a set of options, i.e. the most *promising alternatives*, which satisfy the design objectives to a similar degree. The approach is suited for handling the *critical decisions* that arise during the conceptual design of WWTPs and it is comprised of three different steps. In *Step 4,* the most *promising alternatives* are compared close to the optimal conditions on the basis of the results of dynamic simulation. *Step 5* involves identification of the strong and weak points of each alternative by means of classification trees and the subsequent extraction of rules for each alternative. Finally, in *Step 6*, there is an evaluation of the trade-off between improvement of the criteria identified as weak points of the option and the loss of overall process performance through the integrated application of dynamic simulation and qualitative knowledge extracted during the design process
- **Application of *multivariate* statistical techniques.** The third block of the proposed method is used to support the *multicriteria* analysis of the different WWTP alternatives by means of *multivariate* statistical techniques (*Step 7*). This block is not always used, but to improve both analysis and interpretation of large and complex *multicriteria* datasets. In this study, cluster analysis (CA), principal component/factor analysis (PCA/FA) and discriminant analysis (DA) are applied to the matrix data set obtained when several alternatives are evaluated by dynamic simulation. These techniques allow i) natural groups or clusters of alternatives with similar behaviour to be determined, ii) complex, casual and complex relation features in the data set to be found and interpreted and iii) important discriminant variables within a single alternative or a group of alternatives to be identified.
- ***Uncertainty* Analysis.** The last of the blocks is used to study how the decision making changes when *uncertainty* in the model parameters used to evaluate the generated alternatives is either included or not. As in the previous case, this block is optional and only used when the robustness of a decision needs to be evaluated (*Step 8*). In *Step 8.1* there is the identification and quantification of the input *uncertainty* i.e. model parameters to take into account during the decision procedure by means of probability distributions. Input *uncertainty* is sampled using the Latin Hypercube Sampling method in *Step 8.2*. Finally the input *uncertainty* is propagated through the whole WWTP model to obtain the output *uncertainty* and i) quantify the variation in the overall degree of satisfaction of the design objectives for the generated WWTPs alternatives, ii) the identification of the contributions of environmental, legal, technical and economic objectives to the existing variance and finally iii) the analysis of the influence of the relative importance of the design objectives during the selection of alternatives is analyzed.

The method developed in this thesis is applied to several case studies: i) enhancement of the efficiency of the biological nitrogen removal process (case studies #1 & #2); ii) simultaneous organic carbon, nitrogen and phosphorus removal (case study #3); and iii) overall plant wide performance involving particularly nitrogen removal, primary and secondary settling, anaerobic digestion, thickening and dewatering (case studies #4 & #5). Block 1 (*hierarchical* generation and *multicriteria* evaluation) is performed for the selection of the biological nitrogen removal process in an organic carbon removal and nitrification WWTP (case study #1), for set point optimisation of the two PI control loops (case study #2) and for retrofitting to achieve simultaneous organic carbon, nitrogen and phosphorus removal (case study #3) in a nitrogen removal WWTP. The analysis of *critical decisions* (block 2) is only developed for the simultaneous organic carbon, nitrogen and phosphorus-removal case study (case study #3). The capabilities of *multivariate* statistical techniques (block 3) and *uncertainty* analysis (block 4) are demonstrated using the whole WWTP (case studies #4 & #5).

The proposed conceptual design method includes a number of elements found in different disciplines. The *hierarchical* decision process (Douglas, 1988; Smith, 2005) is used to break down the design problem into a number of issues that are easier to analyze and evaluate, while *multicriteria* decision analysis (Vincke, 1992; Belton and Stewart, 2002) allows the inclusion of different objectives at the same time during the decision procedure. Also, for the analysis of *critical decision*s, preliminary multiobjective optimization based on sensitivity functions (Douglas *et al*., 1985) and knowledge extraction by means of rules (Quinlan 1993), provide the designer with a better picture of the design space and information about undesirable (or desirable) directions that the plant could take. Finally, both *multivariate* statistical (Johnson and Wichern, 1992; Hair *et al*., 1998) and *uncertainty* analysis based on Monte Carlo simulations (McKay *et al*., 1979; Iman *et al*., 1981) complement the evaluation procedure by unravelling the association between design/operating variables and alternatives, highlighting information not available at first glance and studying the effect of the model parameters in the decision making depending on whether or not *uncertainty* is included.

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

PhD THESIS

CHAPTER 3. DESCRIPTION OF PROCESS MODELS

3.1. OVERVIEW

This chapter describes the different process models chosen to demonstrate the capabilities of the proposed conceptual design method for WWTPs: the biological nitrogen removal process (case studies # 1 & #2), ii) phosphorus removal (case study # 3) and iii) overall plant wide WWTP performance involving in particular: nitrogen removal, primary and secondary settling, anaerobic digestion, thickening and dewatering (case studies ·#4 & #5). A detailed description of the different (bio)chemical processes is given in section 3.2 (biological nitrogen removal process), section 3.3 (simultaneous carbon, nitrogen and phosphorus removal) and section 3.4 (plant wide WWTP perfomance).

As **Figure 2.1** shows**,** some of the steps in the conceptual design method require knowledge of the dynamic behaviour at a characteristic design/operating point. The simulation of process performance is carried out by means of dynamic modelling with a commercial flowsheet simulator. Further, quantification of the criteria used to evaluate the degree of satisfaction of the different objectives is needed. The equations used for these criteria can be found at the end of **Chapters 4**, **5**, **6** and **7** of this thesis.

A WWTP simulator environment can be described as software that allows the modeller to simulate a WWTP configuration. A fairly detailed overview of simulator environments can be found in Olsson and Newell (1999) and Copp (2002). Current process simulator environments can be classified as either general purpose simulator or specific WWTP simulator (Gernaey *et al.*, 2004). General purpose simulator environments normally have great flexibility but the modeller has to supply the models that must be used to perform a specific WWTP configuration. This can be very time consuming. However, it is important to spend sufficient time on model implementation and debugging to avoid the risk of running a lot of simulations with a model that turns out to be erroneous for the specific application task. As a consequence, general purpose simulator environments require skilled users that fully understand the implications of each line of code in the models. Specific WWTP simulator environments usually contain an extended library of predefined process unit models, for example a perfectly mixed ASM1 or ASM2d bioreactor, and a one-dimensional 10-layer settler model. The process configuration can be usually constructed by connecting process unit blocks. Pop up windows allow the model parameters to be modified.

The dynamic simulation performed in this thesis was carried out in a MATLAB/Simulink environment, a popular example of a general-purpose simulator.

3.2. BIOLOGICAL NITROGEN REMOVAL PROCESS IN WWTPs

3.2.1. Biological nitrogen removal process description

The removal of organic carbon can be accomplished in a number of aerobic suspended growth or attached (fixed film) growth treatment processes. Both require sufficient contact time between the wastewater and the heterotrophic microorganisms, and sufficient concentrations of oxygen and nutrients. During the initial biological uptake of the organic material, more than half is oxidized and the remainder is assimilated as new biomass, which may be further oxidized by endogenous respiration. The stoichiometry of each oxidation, and synthesis and endogenous respiration, can be seen in **equations 3.1** and **3.2** respectively (Metcalf & Eddy, 2003)

$$\underset{organic\ \ matter}{COHNS} + O_2 + nutrients \xrightarrow{bacteria} CO_2 + NH_3 + \underset{cells}{C_5H_7NO_2} + other \quad end \quad products \qquad \text{(eq 3.1)}$$

$$\underset{cells}{C_5H_7NO_2} + 5O_2 \xrightarrow{bacteria} 5CO_2 + 2H_2O + NH_3 + energy \qquad \text{(eq 3.2)}$$

For both suspended and attached growth processes, the excess of biomass produced every day is removed and processed to maintain proper operation and performance. The biomass is separated from the treated effluent by settling.

When the aerobic conditions are maintained, autotrophic bacteria can grow by obtaining energy from ammonia and nitrite oxidation using bicarbonate as a carbon source. The process is called nitrification and occurs in two steps: i) the aerobic oxidation of ammonium to nitrite by means of ammonium oxidizing bacteria (AOB) and ii) the aerobic oxidation of nitrite into nitrate by means of nitrite oxidizing bacteria (NOB). **Equations 3.3** and **3.4** offer further details about the stoichiometry of these reactions (Metcalf & Eddy, 2003).

$$NH_4^+ + \frac{3}{2}O_2 \xrightarrow{AOB} NO_2^- + H_2O + 2H^+ \qquad \text{(eq 3.3)}$$

$$NO_2^- + \frac{1}{2}O_2 \xrightarrow{NOB} NO_3^- \qquad \text{(eq 3.4)}$$

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 gas (the denitrification process), and thus removing the soluble nitrogen from the system as stated in **equation 3.5** (Metcalf & Eddy, 2003).

$$\begin{aligned} &NO_3^- + 0.345C_{10}H_{19}O_3N + H^+ + 0.267HCO_3^- + 0.267NH_4^+ \xrightarrow{bacteria} \\ &\xrightarrow{bacteria} 0.655CO_2 + 0.5N + 0.612\underset{cells}{C_5H_7NO_2} + 2.3H_2O \end{aligned} \qquad \text{(eq 3.5)}$$

Hence, the classical nitrogen removal systems require a sequence of aerobic and anoxic conditions in which nitrification and denitrification processes can occur respectively.

3.2.2. Biological nitrogen removal process model

The Activated Sludge Model No 1 (ASM1, Henze *et al.*, 2000) can be considered as the reference model, since it was generally accepted by the WWTP community and later on in the industry. The list of the variables considered by the ASM1 is summarized in **Table 3.1** and the main correlation between the main process and these state variables is represented in **Figure 3.1.** As shown in **Figure 3.1,** two groups of microorganisms are considered in the ASM1: heterotrophic biomass (X_H) and autotrophic biomass (X_A). Heterotrophic organisms can grow by oxidizing soluble organic substrate (S_S) under aerobic or anoxic conditions using oxygen (S_O) or nitrate (S_{NO}) as an electron acceptor. This substrate comes with the influent wastewater but it can also be the result of hydrolysis of the particulate organic substrate (X_S).

Autotrophic microorganisms only grow under aerobic conditions (S_O), by consuming the influent ammonium (S_{NH}) originated from consecutive hydrolysis and ammonification processes or soluble (S_{ND}) or particulate (X_{ND}) organic nitrogen.

Table 3.1. State variables for the IWA activated sludge model N #1

State variable description	State symbol	Units
Soluble inert organic matter	S_I	g (COD)·m^{-3}
Readily biodegradable substrate	S_S	g (COD)·m^{-3}
Particulate inert organic matter	X_i	g (COD)·m^{-3}
Slowly biodegradable substrate	X_S	g (COD)·m^{-3}
Active heterotrophic biomass	X_H	g (COD)·m^{-3}
Active autotrophic biomass	X_A	g (COD)·m^{-3}
Particulate products arising from biomass decay	X_P	g (-COD)·m^{-3}
Dissolved oxygen	S_o	g (COD)·m^{-3}
Nitrate nitrogen	S_{NO}	g N·m
Ammonium	S_{NH}	g N·m
Soluble biodegradable organic nitrogen	S_{ND}	g N·m
Particulate biodegradable organic nitrogen	X_{ND}	g N·m
Alkalinity	S_{ALK}	Mole HCO_3^-·m^{-3}

For a full description of the ASM1 model, as well as a detailed explanation of the matrix format used to represent it, see **Table 3.2.** By using this representation, it is possible to identify the model's various parameters. The matrix representation shows the stoichiometry relationships that relate the state variables (i) to the process equations (j). To ensure a consistent application of the models for all the alternatives evaluated both kinetic and stoichiometry parameters are set.

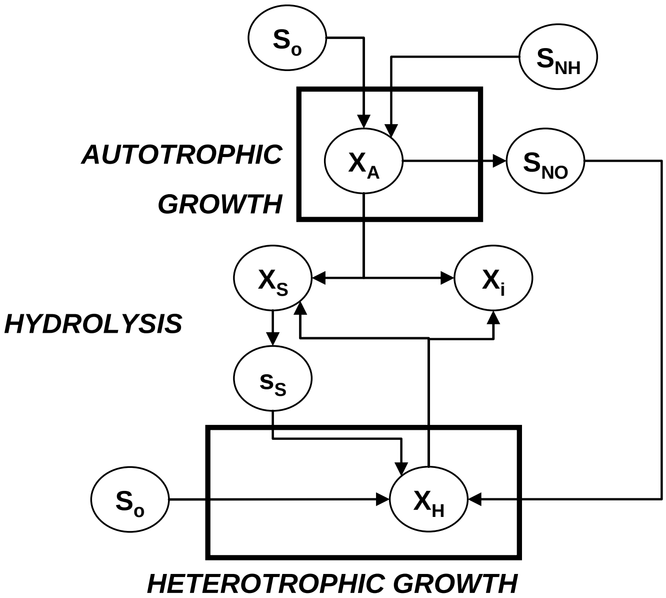

Figure 3.1. Substrate flow for autotrophic and heterotrophic biomass in ASM1 (Gernaey *et al.*, 2004)

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Table 3.2. Matrix Representation of the ASM1 showing the processes, the components, process rates equations and stoichiometry (Henze *et al.*, 2002)

Component V_{ij} / i; j / Process	S_I	S_s	X_I	X_s	X_H	X_A	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*			$-\frac{1-Y_H}{Y_H}$		$-i_{XB}$			$-\frac{i_{XB}}{14}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{S_O}{K_{OH}+S_O}\right)X_H$
2.Anoxic heterotrophic growth		$-\frac{1}{Y_H}$							$\frac{1-Y_H}{2.86Y_H}$	$-i_{XB}$			$\frac{1-Y_H}{14 \cdot 2.86Y_H}-\frac{i_{XB}}{14}$	$\mu_{mH}\left(\frac{S_S}{K_S+S_S}\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_H$
3.Aerobic autotrophic growth						*1*		$-\frac{4.57-Y_A}{Y_A}$	$\frac{1}{Y_A}$	$-i_{XB}-\frac{1}{Y_A}$			$\frac{i_{XB}}{14}-\frac{1}{7Y_A}$	$\mu_{mA}\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\frac{S_O}{K_{OA}+S_O}\right)X_A$
4.Heterotrophic death				$1-f_p$	-1		f_p					$i_{XB}-f_p.i_{XP}$		$b_H X_H$
5.Autotrophic death				$1-f_p$		-1	f_p					$i_{XB}-f_p.iX_P$		$b_A X_A$
6.Ammonification										*1*	-1		$\frac{i_{XB}}{14}$	$k_a S_{ND} X_H$
7.Hydrolysis of organics		*1*		-1										$k_H\frac{X_S/X_H}{K_X+X_s/X_H}\left(\frac{S_O}{K_{OH}+S_O}+\eta_h\frac{K_{OH}}{K_{OH}+S_O}\frac{S_{NO}}{K_{NO}+S_{NO}}\right)X_H$
8.Hydrolysis of organic nitrogen											*1*	-1		$\rho_7(X_{ND}/X_s)$
Conversion rate	$r_j=\sum_j v_{ij}\rho_j$													

Stoichiometric parameters: Heterotrophic yield: Y_H Mass N/Mass COD in biomass: i_{XB} Autotrophic yield: Y_A Mass N/Mass COD: i_{XP} Fraction of biomass yielding particulate products: f_P	Kinetic parameters: Heterotrophic growth 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

3.3. PHOSPHORUS REMOVAL PROCESS IN WWTPs

3.3.1. Phosphorus removal process description

The removal of phosphorus from wastewater involves the incorporation of phosphate into TSS and the subsequent removal of those solids in the secondary settler. Phosphorus can be incorporated into either biological solids (e.g. microorganisms) or chemical precipitates. The fundamentals of both chemical and biological phosphorus removal are explained in the following sections.

3.3.1.1. Biological phosphorus removal

In biological phosphorus removal, excess P is incorporated into the cell biomass, which is then removed from the process as a result of sludge wasting. Phosphorus accumulating organisms (PAOs) are encouraged to grow and consume phosphorus in the systems that use a reactor configuration providing PAOs with a competitive advantage over other bacteria. In the anaerobic zone, acetate is produced by the fermentation of soluble biodegradable organic material. This material comes from influent wastewater but is also a result of the hydrolysis of the particulate organic material. Next, using energy available from the stored polyphosphates, the PAOs assimilate acetate and produce intracellular polyhydroxybutyrate (PHB) storage products. Some glycogen contained in the cell is also used in this step. Concurrent with the acetate uptake is the release of orthophosphate and counterions (magnesium, potassium and calcium cations). The PHB content in PAOs increases while the polyphosphate content decreases during the acetate uptake. In the aerobic/anoxic zones the stored PHB is metabolized, providing energy from oxidation and carbon for new cell growth. Subsequently, the energy released from PHB oxidation is used to form polyphosphate, such that soluble orthophosphate is removed from the solution and incorporated into polyphosphates within the bacterial cells. Cell growth occurring due to PHB utilization and the formation of new biomass, with a high concentration of polyphosphate storage materials, account for net phosphorus removal. Finally, as a portion of the biomass is wasted, stored phosphorus is removed from the activated sludge plant for ultimate disposal with the waste sludge.

3.3.1.2. Chemical phosphorus removal

The chemical precipitation of phosphorus is brought about by the addition of the salts of multivalent ions that form precipitates of sparingly soluble phosphates. The multivalent metal ions most commonly used are calcium (Ca^{+2}), aluminium (Al^{+3}) and iron (Fe^{+3}). Calcium is usually added in the form of $Ca(OH)_2$ to precipitate phosphorus in the form of hydroxylapatite $Ca_{10}(PO_4)_6(OH)_2$, as shown in **equation 3.6.**

$$10Ca^{+2} + 6PO_4^{-3} + 2OH^- \longleftrightarrow \underset{hydroxylapatite}{Ca_{10}(PO_4)_6(OH)_2} \quad \text{(eq 3.6)}$$

Because of lime's reaction with the alkalinity of the wastewater, the quantity of lime required will, in general, be independent of the amount of phosphate present, and will instead depend primarily on the alkalinity of the wastewater.

The basic reactions involved in the precipitation of phosphorus with aluminium and iron are represented in **equation 3.7** and **3.8** (Metcalf & Eddy, 2003).

$$Al^{+3} + H_nPO_4^{n-3} \longleftrightarrow AlPO_4 + nH^+ \qquad \text{(eq 3.7)}$$

$$Fe^{+3} + H_nPO_4^{n-3} \longleftrightarrow FePO_4 + nH^+ \qquad \text{(eq 3.8)}$$

These reactions are deceptively simple and must be considered in the light of many competing reactions and their associated equilibrium constants, and the effects of alkalinity, pH, trace elements and ligands found in wastewater.

3.3.2. Phosphorus removal process model

The Activated Sludge Model No 2d (ASM2d) was selected as a model for phosphorus removal, both biological and chemical, with simultaneous nitrification and denitrification in activated sludge systems. The ASM2d is based on the ASM2 (Henze *et al*., 2000), expanded to include the denitrifying activity of the phosphorus accumulating organisms (PAOs).

The model comprises 19 state variables and takes into account 21 processes. The relations between the state variables and the processes considered are represented by means of a matrix (see Henze *et al*. (2000) for further details about the matrix).

Table 3.3. State variables of the Activated Sludge Model No 2d (ASM2d)

State variable description	State symbol	units
Fermentation products, considered to be acetate	S_A	g (COD)·m^{-3}
Alkalinity of the wastewater	S_{ALK}	Mole HCO_3^-·m^{-3}
Fermentable, ready biodegradable substrates	S_F	g (COD)·m^{-3}
Inert soluble organic material	S_I	g (COD)·m^{-3}
Dinitrogen N_2	S_{N2}	g N·m^{-3}
Ammonium plus ammonia nitrogen	S_{NH4}	g N·m^{-3}
Nitrate plus nitrite nitrogen (NO_3^- + NO_2^-)	S_{NO}	g N·m^{-3}
Dissolved oxygen	S_O	g (-COD)·m^{-3}
Inorganic soluble phosphorus	S_{PO}	g P·m^{-3}
Readily biodegradable substrate	S_S	g (COD)·m^{-3}
Nitrifying organisms	X_A	g (COD)·m^{-3}
Heterotrophic organisms	X_H	g (COD)·m^{-3}
Inert particulate organic material	X_I	g (COD)·m^{-3}
Metal hydroxides	X_{MeOH}	g TSS·m^{-3}
Metal phosphate	X_{MeP}	g TSS·m^{-3}
Phosphate accumulating organisms	X_{PAO}	g (COD)·m^{-3}
Cell internal storage product of phosphorus accumulating organisms	X_{PHA}	g (COD)·m^{-3}
Polyphosphate	X_{PP}	g P·m^{-3}
Slowly biodegradable substrates	X_S	g (COD)·m^{-3}
Total suspended solids	X_{TSS}	g TSS·m^{-3}

The basic principle of biological phosphorus removal in the ASM2d model is illustrated in **Figure 3.2:** the P accumulating organisms (X_{PAO}) are modelled with an internal structure, where all the organic products are lumped into one model component (X_{PHA}). X_{PAO} organisms can only grow (i.e. form new biomass) using cell internal organic storage material (X_{PHA}) as substrate, with oxygen (S_O) or nitrate (S_{NO}) as the electron acceptor. The storage process does not depend on the electron acceptor's condition, but is possible when fermentation products such as acetate (S_A) are available. In practice, this means that the storage process will only take place in the anaerobic section of the activated sludge plant, since fermentation products are typically only available under anaerobic conditions in a plant that is operated properly.

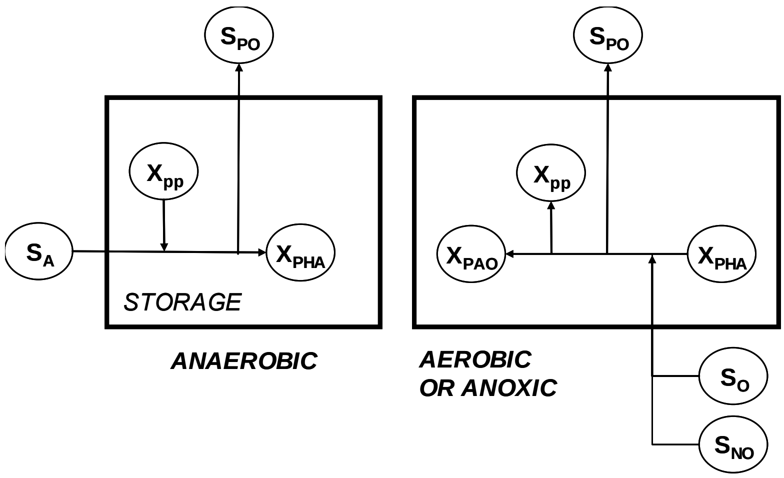

Figure 3.2. Illustration of the basic principles behind biological P removal as included in the ASM2d model (Gernaey *et al.*, 2004)

The precipitation and redissolution of the phosphate model is based on the assumption that it is a reverse process, which would be in equilibrium at steady state, as represented in **equation 3.9.**

$$X_{MeOH} + S_{PO} \longleftrightarrow X_{MeP} \qquad \text{(eq 3.9)}$$

3.4. SETTLING PROCESS

3.4.1. Settling process description

Solids separation is the final step in the production of a well clarified, stable effluent low in organic matter and suspended solids. As such, the settling process represents a critical step in the operation of an activated sludge treatment process. The separation of the solids from wastewater is carried out by gravity, where heavier suspended solids are separated from water by gravitational settling. These solids tend to form a sludge blanket with concentrated sludge at the bottom of the tank that can be returned to the inlet of the plant to treat more wastewater or removed (wasted) for further treatment and disposal, composing the waste sludge line

3.4.2. Settling process model

As with the biological process model, international acceptability was the overriding criterion for the settling model selection. The double exponential settling velocity function of Takács *et al*. (1991) is based on the solid flux concept, and is applicable to both hindered and flocculent settling conditions. **Equation 3.10** shows the Takács double exponential velocity function. As in the biological model, the parameters used in the function have been fully defined in order to avoid unbiased comparisons.

$$v_{sj} = v_0 e^{-r_h X_j^*} - v_o e^{-r_o X_j^*} \qquad \text{(eq 3.10)}$$

$$0 \le v_{sj} \le v_0^{'}$$

where $v_{s,j}$ is the settling velocity in layer j ($m \cdot day^{-1}$), X_j^* is the suspended solids concentration in layer j ($g \cdot m^{-3}$), subject to the limiting condition that ($X_J^* = X_j - X_{min}$), X_j is the suspended solids concentration in layer j ($g \cdot m^{-3}$) and X_{min} is the minimum attainable suspended solids concentration ($g \cdot m^{-3}$) calculated from $X_{min} = f_{ns} \cdot X_{in}$ [where X_{in} is the mixed liquor suspended solids concentration entering the tank and f_{ns} is the non-settleable fraction].

3.5 PLANT WIDE WWTP PROCESS

3.5.1. Plant wide WWTP process description

A typical WWTP usually includes primary treatment and secondary treatment to remove organic matter and suspended solids from wastewater and the sludge line. A typical example of a WWTP is showed in **Figure 3.3**

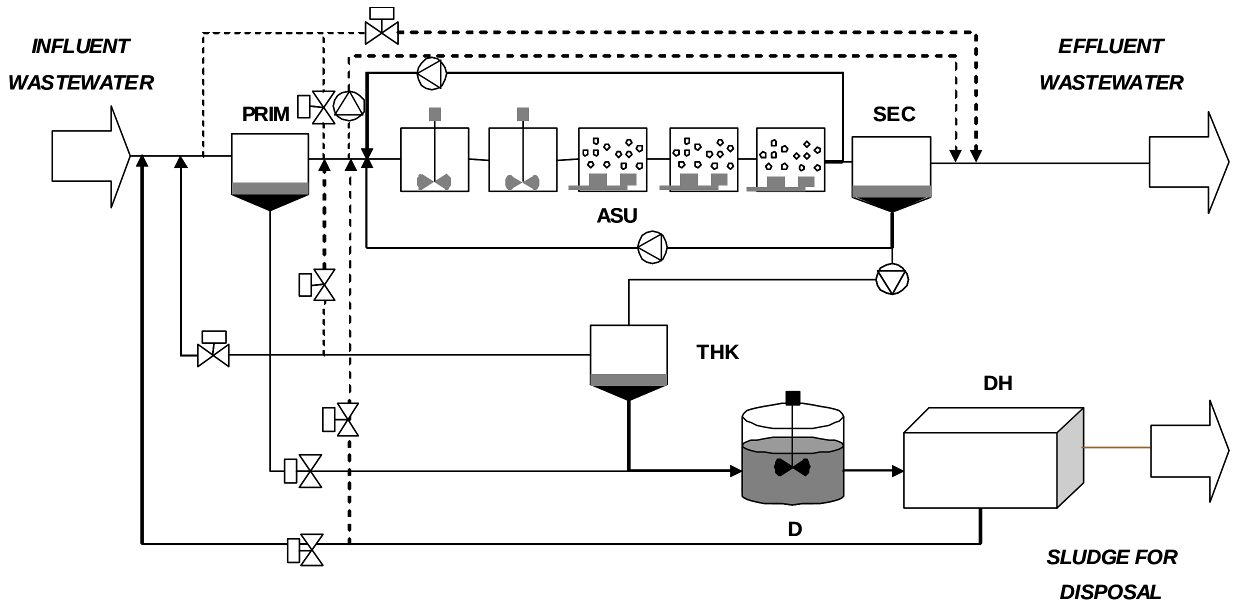

Figure 3.3. Flow diagram of a plant-wide WWTP

Primary treatment (PRIM) is designed to physically remove solid material from the incoming wastewater. Coarse particles are removed by screens or reduced in size by grinding devices. Inorganic solids are removed in grit channels and many of the organic suspended solids are removed by sedimentation. Overall, the primary treatment removes almost one half of the suspended solids in the raw wastewater. The wastewater that flows to the secondary treatment is called the primary effluent.

As previously stated, secondary treatment usually consists of a biological conversion of dissolved and colloidal organic compounds into stabilized, low energy compounds, and new cells of biomass, caused by a very diversified group of microorganisms in the presence of oxygen, and the respiration of these microorganisms. This mixture of microorganisms (living biomass), together with inorganic as well as organic particles contained in the suspended solids, constitutes the so-called activated sludge (ASU). This mixture is kept moving in wastewater by the stirring of aerators, turbines or rotators, which simultaneously supplies the oxygen required for the biological reactions. Some of the organic particles can be degraded by subjecting them to hydrolysis whereas others are non-degradable (inert). This mixture of microorganisms and particles has the ability to bioflocculate, that is, to form aggregates that are called activated sludge flocs, if there is a balanced population between floc-formers and filamentous bacteria. The activated sludge floc provides the sludge with the capacity to settle and separate from treated water in the clarifier. A biological reactor followed by a secondary settler or clarifier (SEC) constitutes the activated sludge process, which is the best known, most widely used process for secondary wastewater treatment. Organic matter that enters an activated sludge process has only three outlets: carbon dioxide, excess sludge and the effluent.

The problems of dealing with the excess sludge are complex because 1) it is composed largely of substances responsible for the offensive character of untreated wastewater, 2) the portion of biosolids produced from biological treatment requiring disposal is composed of the organic matter content in the wastewater but in another form, and it too will decompose and become offensive and 3) only a small part is solid matter. The objective of sludge treatment is to reduce the water and biodegradable organics content in the waste sludge and to render the processed solids suitable for reuse or final disposal.

The principal methods used for solids processing consist of thickening (THK) and dewatering (DH), used primarily to remove moisture from solids, and digestion (D), used primarily to treat or stabilize the organic material in the solids.

3.5.2. Plant wide WWTP process model

This section describes the different models comprising the WWTP under study. In **Figure 3.4** there is a representation of the different models at plant wide level. The activated sludge reactor and secondary settling models are identical to the ones described previously in Sections 3.3.2 and 3.4.2 and will not be discussed further.

3.5.2.1. Primary clarifier model

The proposed primary clarifier is modelled based on the approach presented by Otterpohl and Freund (1992) and Otterpohl *et al.* (1994). It is described as a completely mixed tank with separation of the effluent into a waste stream and a sludge stream. The concentration of incoming solids is based on an empirical expression that takes into account hydraulic retention time and the ratio of particulate to total COD. The model parameters are defined so as to produce a TSS concentration in the sludge stream equal to 3% of the average dry weather influent wastewater and a TSS removal efficiency of 50%. During dynamic simulations the primary sludge waste flow rate is set to be proportional to the influent flow rate and the concentration of particulate components is allowed to vary. The concentrations of soluble components are not affected and are equal in both the overflow (influent of the activated sludge tanks) and the underflow (primary sludge) streams.

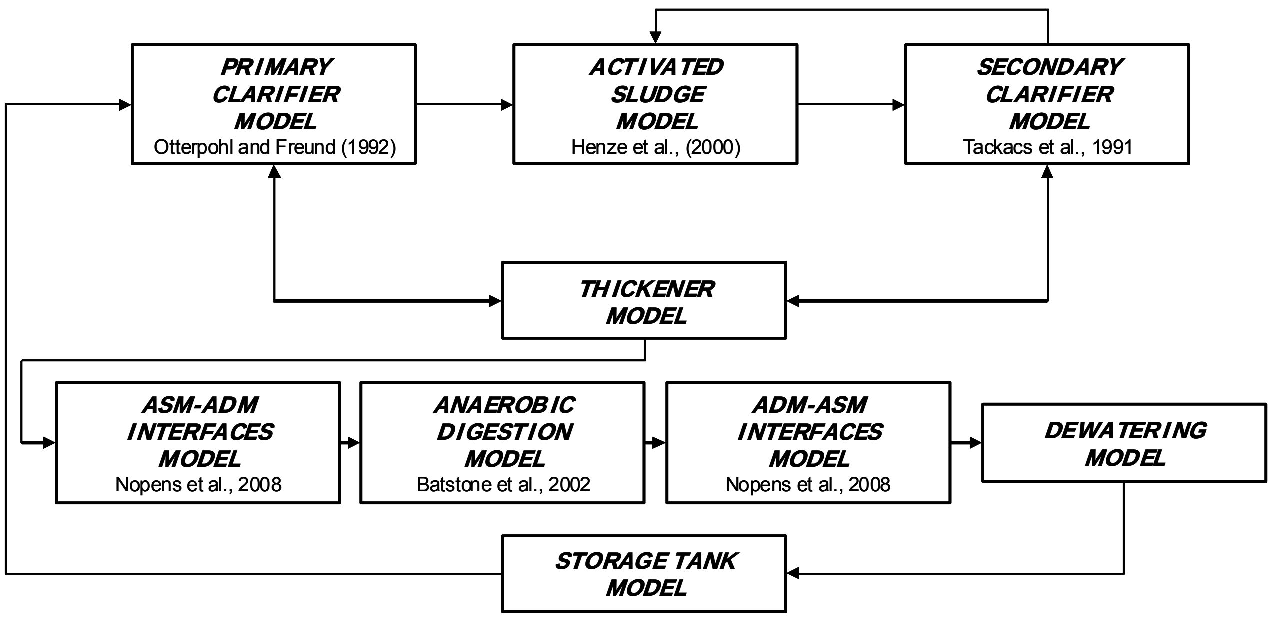

Figure 3.4. Schematic representation of the different models at plant wide level

3.5.2.2. Thickener unit

The wastage flow from the secondary clarifier is fed to the thickener. The plant does not take into account changing sludge characteristics but rather assumes sludge with good settling qualities. In accordance with this simplification, the thickener is modelled as an ideal, continuous process with no biological activity. Of the particulate material entering the thickener unit, 98% is assumed to settle and end up in the thickened sludge stream. The concentrations of soluble components are equal in both outward streams. During dynamic conditions the underflow TSS concentration (7%) is maintained through instantaneous flow rate adjustments.

3.5.2.3. Anaerobic digestion model

The Anaerobic Digestion Model No 1 (ADM1) by Batstone *et al*. (2002) is a published and recognized dynamic anaerobic digestion model. It includes biological reactions in the water phase as well as liquid-gas interactions and gas production. **Figure 3.5** gives a representation of the main processes considered by the model. It is structured with disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis steps. Extracellular solubilization steps are divided into disintegration and hydrolysis, of which the first is a largely non-biological step that converts composite particulate substrate (X_c) to inerts (X_i and S_i), particulate carbohydrates (X_{ch}), protein (X_{ch}) and lipids (X_{li}). The second is enzymatic hydrolysis of particulate carbohydrates, proteins and lipids to monosaccharides (S_{su}), amino acids (S_{su}) and long chain fatty acids (S_{fa}) respectively. Disintegration is mainly included to describe degradation of the composite material with lumped characteristics, while the hydrolysis steps are there to describe well defined, relatively pure substrates (such as cellulose, starch and protein feeds).

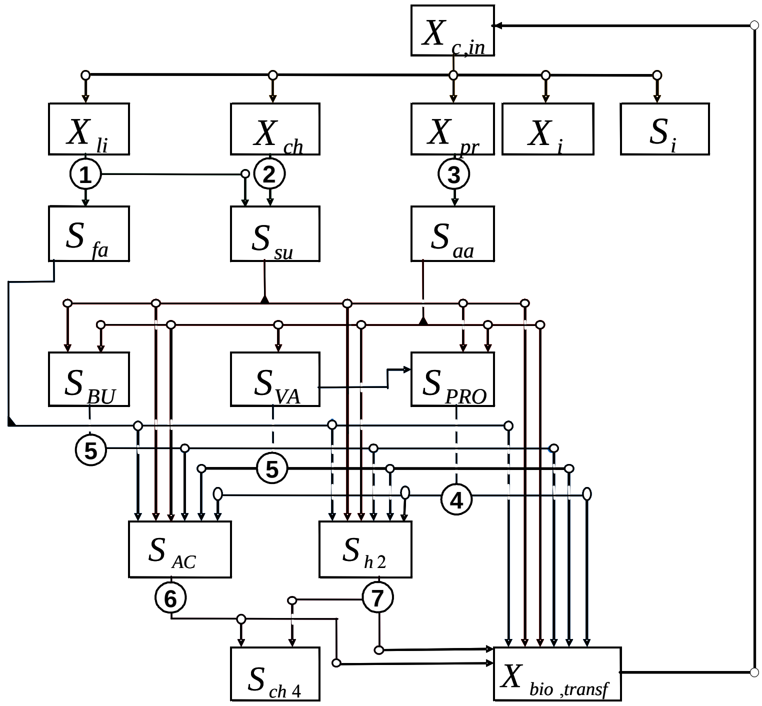

Figure 3.5. Representation of the biochemical reactions in the anaerobic digestion model (ADM1): (1) acidogenesis from sugars, (2) acidogenesis from amino acids, (3) acetogenesis from LCFA, (4) acetogenesis from propionate, (5) acetogenesis from butyrate and valerate, (6) aceticlastic methanogenesis and (7) hydrogenotrophic methanogenesis (from de Gracia *et al.*, 2007)

Two separate groups of acidogens (X_{su} and X_{aa}) degrade monosaccharides (S_{su}) and amino acids (S_{aa}) to mixed organic acids (S_{pro}, S_{va} and S_{bu}), hydrogen (S_{h2}) and carbon dioxide. The organic acids (S_{pro}, S_{va} and S_{bu}) are subsequently converted to acetate (S_a), hydrogen (S_{h2}) and carbon dioxide by acetogenic groups (X_{c4} and X_{fa}) that utilize LCFA (S_{fa}), butyrate and valerate (S_{c4}), and propionate (S_{pro}). The hydrogen produced by these organisms is consumed by a hydrogen-utilizing methanogenic group (X_{h2}), and the acetate by an aceticlastic methanogenic group (X_{ac}). Death of biomass is represented by a first-order kinetics. Inhibition functions include pH, hydrogen, and free ammonia. Mechanisms included to describe physico-chemical processes are acid base reactions (to calculate the concentration of hydrogen ions, free ammonia and carbon dioxide) and non-equilibrium liquid-gas transfer. Solids precipitation is not included. Kinetic and stoichiometric parameters in the anaerobic digestion are set to default values based on a mesophilic regime. Some of the state variables taken into account in the ADM1 model are summarized in **Table 3.4**.

3.5.2.4. Dewatering unit.

Efficient dewatering is essential for overall plant performance and must be included. However, as it is typically a mechanical process (several types of equipment based on somewhat different principles are available), it is modelled as an ideal, continuous process with no biological activity. Of all particulate matter entering the dewatering unit, 98% is assumed to be concentrated into the sludge stream and subsequently removed. The concentrations of soluble components are equal in both outward streams. During dynamic conditions the TSS concentration (28%) is maintained through instantaneous flow rate adjustments.

Table 3.4. State variables of the Anaerobic Digestion Model No 1 (ADM1)

State variable description	State symbol	units
Composites	X_c	kg (COD)·m^{-3}
Carbohydrates	X_{ch}	kg (COD)·m^{-3}
Proteins	X_{pr}	kg (COD)·m^{-3}
Lipids	X_{li}	kg (COD)·m^{-3}
Particulate inerts	X_i	kg (COD)·m^{-3}
Soluble inerts	S_i	kg (COD)·m^{-3}
Monosaccharides	S_{su}	kg (COD)·m^{-3}
Amino acids	S_{aa}	kg (COD)·m^{-3}
Total LCFA	S_{fa}	kg (COD)·m^{-3}
Total valerate	S_{vs}	kg (COD)·m^{-3}
Total butyrate	S_{bu}	kg (COD)·m^{-3}
Total propionate	S_{pro}	kg (COD)·m^{-3}
Total acetate	S_{ac}	kg (COD)·m^{-3}
Hydrogen	S_{h2}	kg (COD)·m^{-3}
Methane	S_{ch4}	kg (COD)·m^{-3}
Inorganic carbon	S_{ic}	M
Inorganic nitrogen	S_{IN}	M
Biomass	$X_{su\text{-}h2}$	kg (COD)·m^{-3}
Cations	S_{cat}	M
Anions	S_{an}	M

3.5.2.5. ASM/ADM model interfaces

Interfacing the state variables in the activated sludge system models with those in the anaerobic digester and vice versa is an important issue to resolve for the correct assessment of the whole system. The model interfaces are based on the work of Copp *et al*. (2003) and the further modifications reported in Nopens *et al*. (2008). These modifications allow the interface to deal with the differences in primary and secondary sludge composition (and the concomitant differences in biogas yield) to guarantee charge continuity, and to reduce the accumulation of inerts in the system. This means that (i) X_S and biomass fractions are treated differently, (ii) mapping of ASM1 variables no longer leads to composite material (X_C) in the ADM1 but rather directly to lipids, carbohydrates and proteins, thereby omitting the disintegration step and iii) inorganic carbon can be calculated directly in this so-called modified-Copp interface (Nopens *et al.*, 2008).

3.5.2.6. Reject wastewater storage tank

A storage tank for process water (nitrogen rich supernatant from sludge dewatering) is also included to allow the dosage of this influent source to the biological step (either to the inlet of the primary clarifier or the inlet of the activated sludge system). The tank is modelled as a completely mixed tank reactor without describing any type of biological reaction. A pump is used to transport the water from the storage tank to the activated sludge plant.

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

PhD THESIS

Part of this chapter has been published as:

Flores X., Bonmati A., Poch M., Bañares-Alcantara R. and Rodríguez-Roda I. Hierarchical decision process combined with multicriteria analysis support conceptual design of activated sludge plants. In Proceedings of 14th European Symposium on Computer-Aided Process Engineering (ESCAPE-14). Lisbon, Portugal. 2004.

Flores X., Poch M., Rodríguez-Roda I., Bañares-Alcántara R. and Jiménez L. Hierarchical decision process: a key to activated sludge process redesign. In proceedings of 15th European Symposium on Computer-Aided Process Engineering (ESCAPE-15). Barcelona, Spain. 2005.

Flores X., Bonmatí A., Poch M., Rodríguez-Roda I., and Bañares-Alcántara R. Selection of the activated sludge configuration during the conceptual design of activated sludge plants using multicriteria analysis. 2005. Ind. Eng. Chem. Res. 44(10):3556.

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CHAPTER 4. *HIERARCHICAL* GENERATION AND *MULTICRITERIA* EVALUATION OF WASTEWATER TREATMENT PLANT ALTERNATIVES

This chapter presents the first block of a proposed conceptual design method which combines a *hierarchical* decision process (Douglas 1988, Smith 2005) with *multicriteria* analysis (see for example Vincke 1992, Belton and Stewart 2002). The *hierarchical* decision process determines the direction of the design process and an evaluation method, expressed as a *multicriteria* problem, to resolve the different issues that arise during the decision procedure. The proposed systematic procedure comprises several steps: i) initial state in the exploration where all the available information to carry out the evaluation is collected, ii) definition of objectives and the criteria used to quantify their degree of satisfaction, and finally iii) a decision procedure involving identification of the issue to be resolved, the generation of alternatives and the evaluation of those alternatives to finally select one according to its performance and the relative importance of the defined objectives.

The quantification procedure for comparing the competing alternatives is systematized using different sources of information, such as dynamic simulation (to quantify effluent quality, sludge production, aeration energy, etc.), model-based cost estimations (investment costs), and some knowledge-based diagrams retrieved from the literature for criteria that cannot be evaluated numerically (e.g. risk of bulking, foaming and rising). Standard value functions are proposed to normalize the effect of the quantified criteria. The overall degree of satisfaction of the different proposed objectives is calculated by a weighted sum, consisting of the addition of the normalized values for all the generated criteria multiplied by their weight.

This chapter is organized as follows: first, a brief description of the proposed procedure is presented; next, the methodology is applied to the case studies, in which a decision procedure is developed to select the type of biological nitrogen removal process in an organic carbon removal and nitrification activated sludge wastewater treatment plant (WWTPs), and to optimize the set points of two control loops implemented in a nitrogen removal activated sludge WWTP. The results of the first case study show that for this given scenario, postdenitrification is the structural modification to be implemented because it has the best values in both environmental and legal objectives although it does not satisfactory accomplish the economic aspects i.e. high operating costs. Nevertheless, during the sensitivity analysis it can be seen that as soon as economic objectives gain in importance the recommended solution switches from post- to predenitrification because although the predenitrification system implies a higher construction cost it is cheaper to operate than postdenitrification with an external carbon source. On the other hand, with respect to the second case study, the combination of set points that ensures a better degree of satisfaction of the control objectives, no matter their relative importance, are low DO and high NO set points respectively.

4.1. METHODOLOGY

This section details the proposed procedure to support the conceptual design of WWTPs, which combines the *hierarchical* decision process with *multicriteria* analysis. Under this procedure, the design problem is reduced to a set of (Z) issues $[I = \{I_1,..,I_Z\}]$ that follow a predefined order: reaction, separation and recirculation.

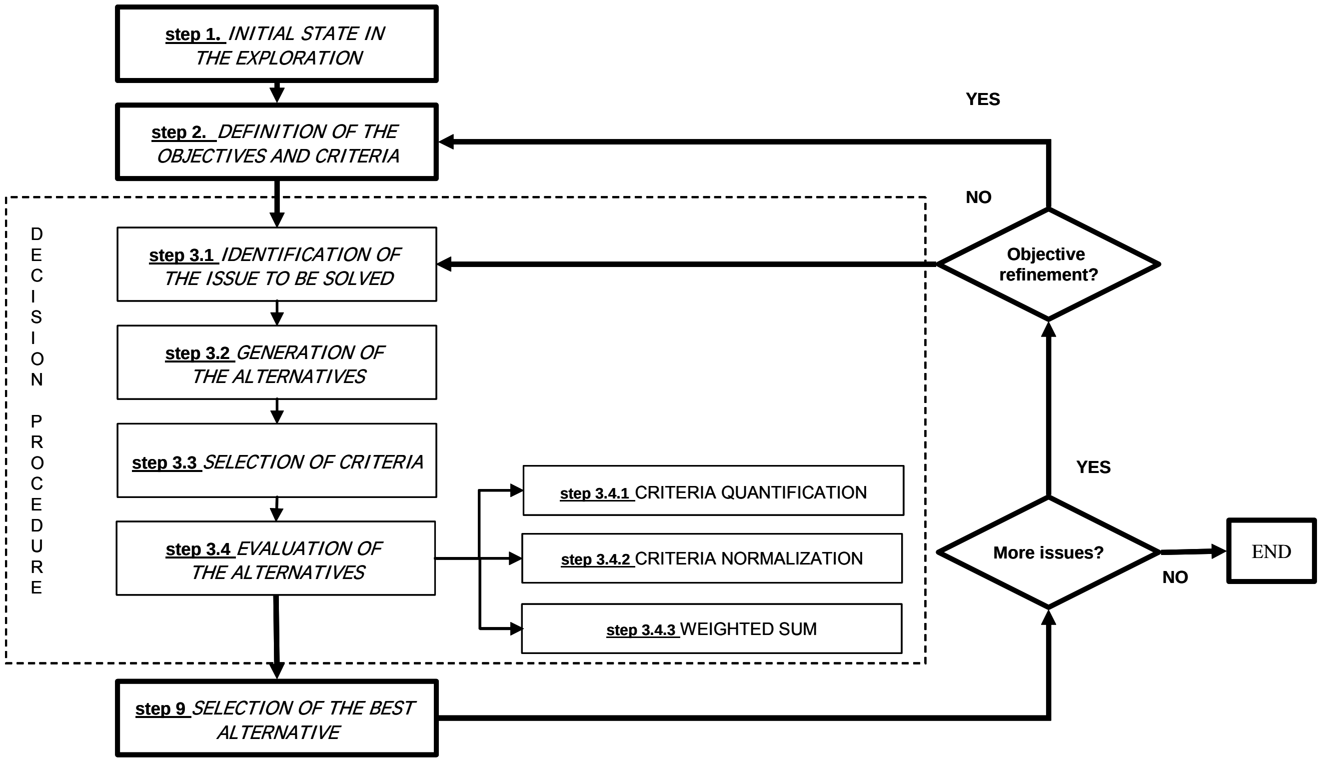


Figure 4.1. Flow diagram of the first block of the conceptual design method (see text for explanations)

The flow diagram, shown in **Figure 4.1**, is subdivided into three main blocks. It is important to point out that this figure is no more than an extended snapshot of the first block of the proposed conceptual design method summarized in **Figure 2.1**.

In *Step 1* the collection and analysis of all the required information is addressed. The goal is to define the context within which the WWTP needs to be designed. The initial state in the exploration includes the study of the location site of the facility, the composition of the wastewater that has to be treated, the applicable legislation and, finally, whether there is any restriction affecting the design process (e.g. budget or land occupation). *Step 2* includes the definition of design objectives $[OBJ = \{OBJ_1,..,OBJ_P\}]$ and the evaluation criteria $[X = \{X_1,..,X_W\}]$ used to measure the degree of satisfaction of the objectives. Weight factors $[w = \{w_1,..,w_P\}]$ are assigned to determine the relative importance of the objectives and normalized to sum 1 in order to avoid unbiased comparisons$[\sum_{k=1}^{P} w_k = \sum_{i=1}^{W} w_i = 1]$.

In *Step 3* there are a number of tasks: identification of the issue to be resolved I_l (*Step 3.1*); generation of the alternatives $[A = \{A_1,...,A_m\}]$ (*Step 3.2*); selection of a subset of criteria $[X = \{X_1,...,X_n\}]$ defined for this issue (*Step 3.3*), and evaluation of the proposed alternatives (*Step 3.4*). This evaluation is approached as a *multicriteria* method and comprises: quantification (*Step 3.4.1*), normalization (*Step 3.4.2*) of the evaluation criteria, and a weighted sum (*Step 3.4.3*). All the criteria [X] are quantified by dynamic simulation or model-based costs estimations. The quantification of an option A_j with respect to criterion X_i is indicated as $x_{j,i}$. Thus, each option under evaluation can be formulated as a vector of scores and represented as an n-dimensional performance score profile $[A_j = (x_{j,i},\ldots, x_{j,n})]$. Value functions [v ($X_i$)] map the score profiles of all alternatives into a value $v(x_{j,i})$ normalized from 0 to 1. The 0 and 1 values are associated with the worst (x_{i*}) and the best (x_i^*) situation respectively whilst a mathematical function is used to evaluate the intermediate effects. The collection of the best $[x^* = (x_1^*,\ldots,x_n^*)]$ and the worst $[x_* = (x_{1*},\ldots,x_{n*})]$ scores for all criteria determine the best $[v(x^*) = (v(x_1^*),\ldots,v(x_n^*))=1]$ and the worst $[v(x_*) = (v(x_{1*})\ldots v(x_{n*}))= 0]$ profiles. Finally, a weighted sum is used to obtain a unique value for each option (**equation 4.1**). This sum is calculated by adding the product of each normalized criterion $v(x_{j,i})$ multiplied by its corresponding weight (w_i). The alternatives are ranked according to the score obtained.

$$s(A_j) = v(x_{j,1})\cdot w_1 + \ldots + v(x_{j,i})\cdot w_i + \ldots + v(x_{j,n})\cdot w_n = \sum_{i=1}^{n} v(x_{j,i})\cdot w_i \qquad \text{(eq 4.1)}$$

The alternative with the highest score is the one with the highest degree of satisfaction of the objectives considered, and the one recommended for implementation, although the final decision will rest on the designer. The same methodology is applied to deal with each new issue that arises until the conceptual design of the wastewater treatment process is completed. Objectives are not fixed, but can evolve through time, thus allowing for the initial design objectives to be refined. This decision procedure follows the logical order based on the *hierarchical* decision process. The whole design process is organized as a decision network where the evaluated issues represent the nodes and the evaluated alternatives the branches.

4.2. CASE STUDY # 1: SELECTION OF BIOLOGICAL NITROGEN REMOVAL PROCESS IN AN ORGANIC CARBON REMOVAL AND NITRIFICATION WWTP

The case study shows the application of the proposed approach to support the conceptual redesign of an existing activated sludge plant. To be precise, the type of biological nitrogen removal process is selected for an organic carbon removal and nitrification plant. A full decision procedure is developed to resolve a single issue relating to reactor configuration. Once this issue is resolved, the design process will continue identifying and successively solving new issues, such as type of secondary settler, the implementation of automatic control strategies, etc., until the whole conceptual design is achieved.

4.2.1. *Step 1*. Initial state in the exploration

Certain information about the initial plant is available to define the design context. Council Directive 91/271/EEC concerning urban wastewater treatment is the relevant water legislation. The plant is to be located in an ecologically sensitive area. Hence, under the legislation it has to remove organic matter, suspended solids and nitrogen before the treated water is discharged into the environment (to avoid eutrophication).

The plant to be redesigned is the IWA nitrifying activated sludge plant (Copp, 2003). It comprises five aerobic continuously stirred tank reactors (CSTRs) in series and a secondary settler. All the aerobic reactors (AER 1, 2, 3, 4, & 5) have a volume of 1200 m^3 while the secondary settler has a total volume of 6000 m^3 (see **Figure 4.2**). In the aerobic section of the plant the organic matter and ammonia (ammonia is the common form of nitrogen in the influent wastewater) are oxidized to carbon dioxide and nitrate.

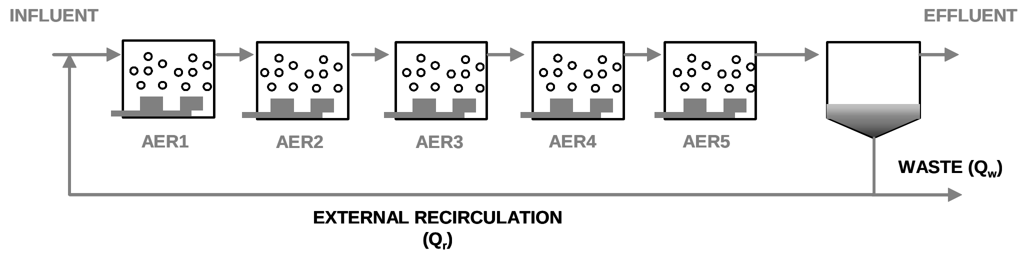


Figure 4.2. Flow diagram of the plant to be redesigned

The influent wastewater composition is the same as that proposed in the Benchmark Simulation Model N°1 (BSM1). The BSM1 is a standardized simulation and evaluation example including plant layout, simulation models and model parameters. There is also a detailed description of the disturbances to be applied during the testing and evaluation of criteria in order to check the relative effectiveness of control strategies in an activated sludge plant (Copp, 2002). The average dry weather wastewater to be treated has a flow rate of 18500 $m^3 \cdot day^{-1}$ (see profile in **Figure 4.3a**) with an organic and nitrogen load of 6500 kg $COD \cdot day^{-1}$ and 680 kg $N \cdot day^{-1}$ respectively (see **Figure 4.3b**). Finally, the budget is restricted to $3 \cdot 10^6$ € for investment and $1 \cdot 10^6$ € $\cdot year^{-1}$ for operation. Limited space in the plant means that the reactor volume cannot be increased.

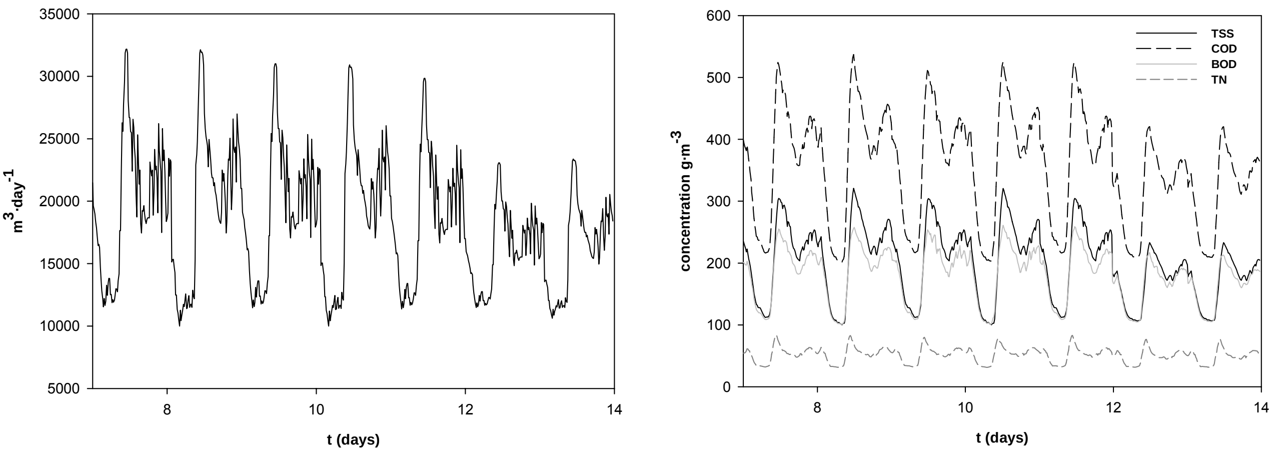


Figure 4.3. Influent wastewater flow (a) and components (b) profile

4.2.2. *Step 2*. Definition of the design objectives and criteria

Design objectives and the criteria (see **Table 4.1**) used to quantify their degree of satisfaction are defined in the second stage of the methodology as shown in the flow diagram in **Figure 4.1**. Different weighting factors are assigned to each objective according to the context defined within the initial state in the exploration. Equal importance for the four redesign objectives is assumed in our case study, thus w_P= 0.25.

Table 4.1. Objectives, criteria and references

OBJECTIVE (OBJ_k)	CRITERION (X_i)		REFERENCES
OBJ_1: minimize environmental impact	X_1 : impact on water		Flores *et al.*, 2006; Copp, 2002 Gernaey and Jorgensen 2004
OBJ_2: minimize economic cost	X_2 : construction costs X_3 : operating costs		US EPA 1982 Vanrolleghem and Gillot, 2002
OBJ_3: maximize technical reliability	X_4 : robustness		Vanrolleghem and Gillot, 2002 Flores *et al.*, 2006
	X_5 : flexibility		Vanrolleghem and Gillot, 2002 Flores *et al.*, 2006
	X_6 : control performance		Stephanopoulos, 1984
	X_7: risk of microbiology-related solids separation problems	$X_{7\text{-}1}$: foaming risk $X_{7\text{-}2}$: bulking risk $X_{7\text{-}3}$: rising risk	Comas *et al.,* 2006b
OBJ_4: meet the European directive	X_8 : TIV (time in violation) COD X_9 : TIV BOD_5 X_{10} : TIV TSS X_{11} : TIV TN X_{12} : TIV TP		Copp, 2002

4.2.3. *Step 3*. Decision procedure

4.2.3.1.*Step 3.1*. Identification of the issues to be resolved

The decision procedure starts with the identification of the issues to be resolved. The only issue addressed in the first case study is the selection of a biological nitrogen removal process (I_I, I =1). All of the processes include an aerobic zone in which biological nitrification occurs, i.e. ammonium oxidation to nitrate nitrogen. Some anoxic volume or time must be included to reduce the oxidized nitrogen to nitrogen gas. This reduction requires an electron donor, which can be supplied in the form of influent wastewater organic matter, endogenous respiration or an external carbon source.

4.2.3.2. *Step 3.2*. Generation of the alternatives

The three proposed modifications (m =3) focus on enhancing nitrogen removal and cover the different types of biological nitrogen removal processes taking place in single sludge configurations. These configurations are grouped according to whether the anoxic zone is located before, after or within the aerobic nitrification zone, i.e. predenitrification, postdenitrification or simultaneous nitrification denitrification (Metcalf & Eddy 2003). In option (A_1) the initial contact between wastewater and return activated sludge is in the anoxic zone (K_La-1 & K_La-2 = 0 day^{-1}) followed by the aerobic zone (K_La-3, K_La-4 & K_La-5 = 240 day^{-1}). This configuration is provided with an internal recycling system from the aerobic zone to the anoxic zone (Q_{intr} = 99366 $m^3 \cdot day^{-1}$). In (A_2) the anoxic zone (K_La-4 & K_La-5 = 0 day^{-1}) follows the aerobic zone (K_La-1, K_La-2 & K_La-3 = 240 day^{-1}). The postdenitrification design is operated with an exogenous carbon source addition (Q_{carb} = 5 $m^3 \cdot day^{-1}$) to provide an electron donor for nitrate consumption. Finally in (A_3) the nitrification and denitrification processes occur in the same tank (K_La-1, K_La-2, K_La-3, K_La-4 & K_La-5 = 240 / 0 day^{-1}). Hence, the aeration is turned on and turned off every half part of the total hydraulic retention time. i.e. influent wastewater is 50 % of the time in anoxic conditions and 50 % of the time in aerobic conditions.

4.2.3.3. Step 3.3. Selection of the criteria

A set of criteria (n = 10) is selected from **Table 4.1** to evaluate the three alternatives generated: X_1 (Impact on water), X_2 (Construction costs), X_3 (Operating costs), X_4 (Robustness), X_5 (Flexibility), X_7 (Risk of separation problems), X_8 -X_{11} (time in violation, TIV).

4.2.3.4. Step 3.4. Evaluation of the alternatives

CRITERIA QUANTIFICATION

Criteria X_1, X_3-X_5, X_7- X_{11} are quantified by dynamic simulation while criteria X_2 is calculated by means of economic model estimations. Simulations are performed with the MatLab-Simulink© environment. The IWA Activated Sludge Model no 1 (ASM1) was chosen as a biological process model (Henze *et al.*, 2000). The model includes 13 components (state variables) and describes biochemical carbon removal with simultaneous nitrification and denitrification by means of 8 processes. Through material balances over a CSTR, a set of ordinary differential equations is derived. The double exponential settling velocity of Takács *et al*. (1991), based on the solid flux concept, was selected as a fair representation of the settling process with a ten-layer discretization. The kinetic, stoichiometric and settling model parameters used are reported by Copp (2002). Further details about the models can be found in **Chapter 3**.

MatLab-Simulink© is used to calculate construction costs. Construction costs are estimated using the CAPDET model (US EPA, 1982). Default parameters for unit costs (excavation, concrete walls, concrete slabs, handrails, etc.), equipment (pumps and driving units, vertical mixers) and construction labour rates are used for the cost estimations.

Once the criteria are quantified, we obtain the score profile for each design option considered. The score profiles are presented in **Table 4.2.** Note that for this case study, X_8, X_9 and X_{10} have the same values, so these criteria are not useful for discriminating between competing alternatives.

Table 4.2. Score profiles for the alternatives generated in the first case study

OBJ_K	$x_{j.i}$	A_1	A_2	A_3	UNITS
OBJ_1	$x_{j.1}$	83.01	89.96	76.76	%
OBJ_2	$x_{j.2}$	554000	135000	65000	€
	$x_{j.3}$	749312	861461	862864	€·year^{-1}
OBJ_3	$x_{j.4}$	12.25	13.83	13.47	-
	$x_{j.5}$	16.94	15.37	14.41	-
	$x_{j.7-1}$	89.14	86.28	93.56	%
	$x_{j.7-2}$	56.29	60.47	56.16	%
	$x_{j.7-3}$	74.30	0.00	54.69	%
OBJ_4	$x_{j.8}$	0.00	0.00	0.00	%
	$x_{j.9}$	0.00	0.00	0.00	%
	$x_{j.10}$	0.00	0.00	0.00	%
	$x_{j.11}$	69.34	0.00	100.00	%

It should be emphasized that the results of the quantified criteria depend greatly on the model selected. When modelling activated sludge plants, there is a lack of agreement on the best model to apply to a given case. The representation of biomass decay (Siegrist *et al.*, 1999), the modelling of nitrogen removal (Gujer *et al*., 2001) and the oversimplification of the settling models (i.e. non reactive in most cases, despite the fact that a significant amount of biomass is often stored at the bottom of the secondary clarifier, e.g. Gernaey *et al*., 2006) are subjects still under discussion.

CRITERIA NORMALIZATION

Once quantified, the effect of each criterion X_i on the competing alternatives A_j is normalized by means of value functions between 0 and 1, which are associated with the worst (x_{i*}) and the best (x_i^*) situations respectively, while a mathematical function $v(X_i)$ is proposed to evaluate the intermediate effects. The difference between the best (x_i^*) and the worst (x_{i*}) situation is defined as the evaluation domain range (R_i).

To normalize X_3, for instance, the worst (x_{3*}) situation is reached when the operating costs budget defined in the initial state of exploration (*Step 1* of the proposed methodology) is achieved ($1·10^6$ €·year^{-1} for this case study), while the best situation (x_3^*) is defined by setting its value at $7·10^5$ €·year^{-1}. A linear function is proposed to evaluate the evaluation range (R_3) between x_{3*} and x_3^*.

Another example is the normalization of the impact on water criterion (X_1) where the evaluation domain (X_1) comprises two hypothetical situations: a total (x_1^* = 100%) reduction and no (x_{1*} = 0%) reduction of the polluted load entering the plant. As in the last case, a linear function is used to evaluate the intermediate situations.

Table 4.3. Extreme values and functions proposed to normalize the effect of selected criteria in this case study.

Criterion (X_i)	Worst value (x_{i*})	Best value (x_i^*)	Value function $v(X_i)$
X_1	0 %	100 %	$v(X_1) = 0.01·X_1$
X_2	$3·10^6$ €	0 €	$v(X_2) = 3.33·10^{-7}·X_2 + 1$
X_3	$1·10^6$ €·year^{-1}	$7·10^5$ €·year^{-1}	$v(X_3) = 3,33·10^{-6}·X_3 + 3.33$
X_4	0	20	$V(X_4) = 0.05·X_4$
X_5	0	20	$v(X_5) = 0.05·X_5$
X_{7-1}	100 %	0 %	$v(X_{7-1}) = - 0.01·X_{7-1} + 1$
X_{7-2}	100 %	0 %	$v(X_{7-2}) = - 0.01·X_{7-2} + 1$
X_{7-3}	100 %	0 %	$v(X_{7-3}) = - 0.01·X_{7-3} + 1$
X_8	100 %	0 %	$v(X_8) = - 0.01·X_8 + 1$
X_9	100 %	0 %	$v(X_9) = - 0.01·X_9 + 1$
X_{10}	100 %	0 %	$v(X_{10}) = - 0.01·X_{10} + 1$
X_{11}	100 %	0 %	$v(X_{11}) = - 0.01·X_{11} + 1$

As mentioned in the methodology section, the best $[x^* = (x_1^*,\ldots,x_n^*)]$ and the worst $[x_* = (x_{1*},\ldots,x_{n*})]$ scores for all criteria determine the best $[v(x^*) = (v(x_1^*),\ldots,v(x_n^*))=1]$ and the worst extreme profiles $[v(x_*) = (v(x_{1*})\ldots v(x_{n*}))= 0]$. Thus, for the criteria used in this case study, the corresponding extreme profiles are:

$$[(x_{i*}) = (x_{1*}= 0\ \%,\ x_{2*}= 3·10^6\ €,\ x_{3*}= 1·10^6\ €·year^{-1},\ x_{4*}= 0,\ x_{5*}=0,\ x_{7\text{-}1*}= 100\ \%,\ x_{7\text{-}2*}= 100\ \%,\ x_{7\text{-}3*}= 100\ \%,\ x_{8*}= 100\ \%,\ x_{9*}= 100\ \%,\ x_{10*}= 100\ \%,\ x_{11*}= 100\ \%)\ ]$$

$[(x_i^*) = (x_1^* = 100\ \%, x_2^* = 0\ €, x_3^* = 7{\cdot}10^5 €{\cdot}year^{-1}, x_4^* = 20, x_5^* = 20, x_{7\text{-}1}^* = 0\ \%, x_{7\text{-}2}^* = 0\ \%, x_{7\text{-}3}^* = 0\ \%, x_8^* = 0\ \%, x_9^* = 0\ \%, x_{10}^* = 0\ \%, x_{11}^* = 0\ \%)\ ]$

respectively. Once the extreme values are obtained, the mathematical models to evaluate the range for all the criteria are proposed. **Table 4.3** shows the extreme profiles and the value functions used in this case study.

WEIGHTED SUM

A weighted sum is finally calculated to obtain a single value for each alternative using **equation 4.1**. The alternatives are ranked according to the score obtained. The alternative with the highest score is recommended, but the final decision rests with the designer.

It should be mentioned that the analysis of the results is based on deterministic parameter values, i.e. model parameters are set at their default value. Even though the activated sludge models are well characterized, some process parameters can present *uncertainty*, such as influent fractions arriving at the facility or the effect of temperature and toxic compounds. The importance of this fact and its potential impact on the decision making process is realized, and will therefore be dealt with in **Chapter 7**.

Table 4.4. Normalized values, weights and scores obtained for the three alternatives

OBJ_K	$v(x_{j,i})$	A_1	A_2	A_3	w_i
OBJ_1	$v(x_{j,1})$	0.83	0.90	0.77	0.25
OBJ_2	$v(x_{j,2})$	0.82	0.96	0.98	0.075
	$v(x_{j,3})$	0.83	0.46	0.45	0.175
OBJ_3	$v(x_{j,4})$	0.61	0.69	0.67	0.083
	$v(x_{j,5})$	0.89	0.81	0.76	0.083
	$v(x_{j,7\text{-}1})$	0.11	0.14	0.06	0.028
	$v(x_{j,7\text{-}3})$	0.44	0.40	0.44	0.028
	$v(x_{j,7\text{-}3})$	0.26	1.00	0.45	0.028
OBJ_4	$v(x_{j,8})$	1.00	1.00	1.00	0.0625
	$v(x_{j,9})$	1.00	1.00	1.00	0.0625
	$v(x_{j,10})$	1.00	1.00	1.00	0.0625
	$v(x_{j,11})$	0.31	1.00	0.00	0.0625
$\sum_{i=1}^{n} v(x_{j,i}) \cdot w_i$		**0,74**	**0.79**	**0.68**	**1**

4.2.4. *Step 9*. Selection of the best alternative

At first sight, the results of the weighted sum in **Table 4.4** lead us to the following conclusion: according to the defined objectives, the recommended alternative is A_2 with a score of 0.79, with the rejected alternatives A_1 in second place (score = 0.74) and A_3 (score = 0.68) in third place. Even though alternative A_2 gets a better score in the weighted sum than its competitors, the future design and operation of the plant would be very different depending on whether A_1 or A_2.were selected. The topic of *critical decisions*, i.e. alternatives with a similar degree of satisfaction of the design objectives but with great influence on the future configuration and operation of the plant, is dealt with in detail in **Chapter 5**.

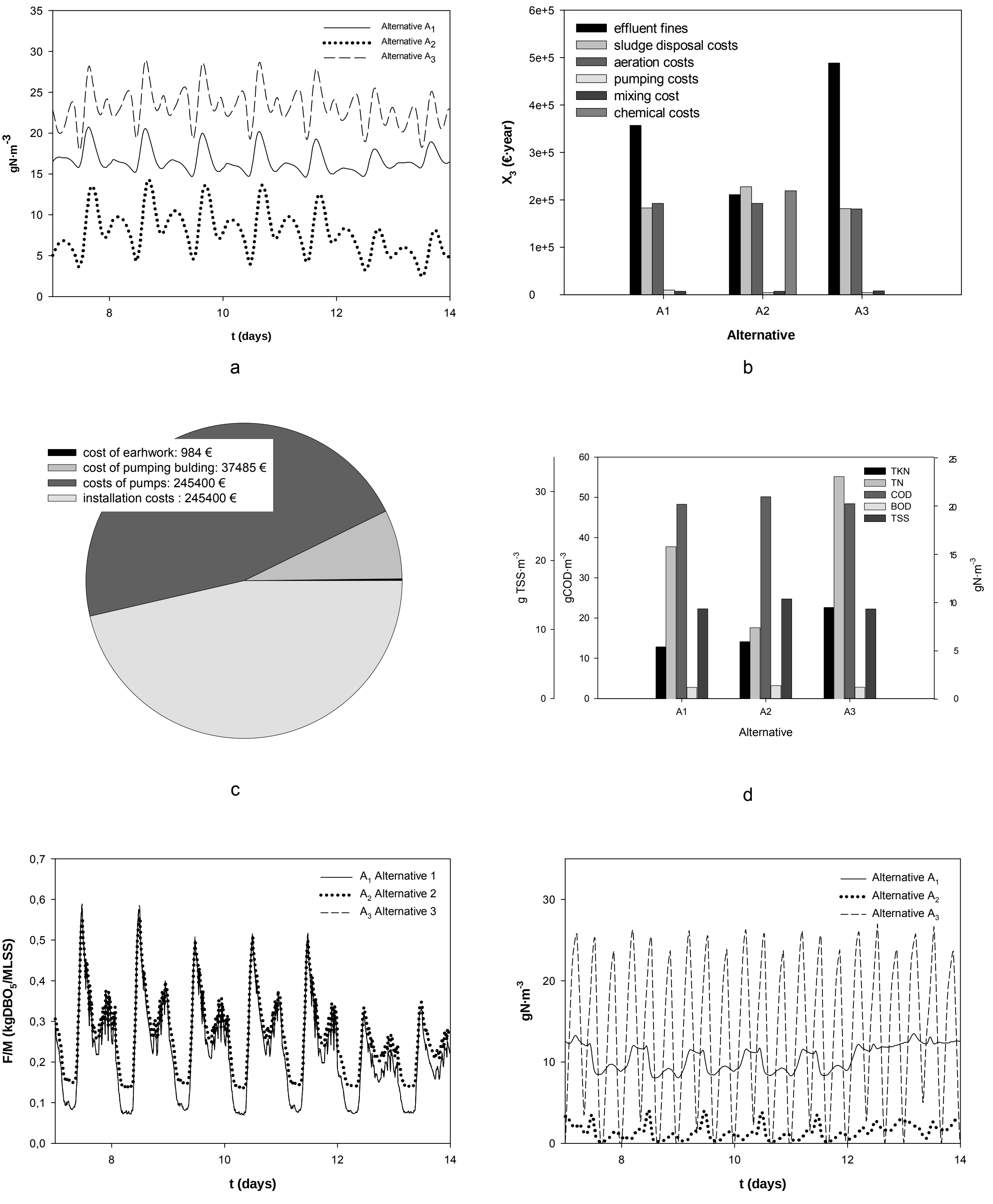


Figure 4.4. Representation of some of the evaluation criteria for the three alternatives evaluated: (a) dynamic effluent TN, (b) breakdown of operating costs, (c) pie chart of construction costs for alternative A_1, (d) average effluent pollutant composition (e) F/M ratio and (f) effluent nitrate composition

Alternative A_3 was the least favoured nitrogen removal process due to its low scores in objectives OBJ_1 (*minimize environmental impact*), OBJ_2 (*minimize economic costs*) and OBJ_4 (*comply with the limits set by European Directive 91/271*). This was mainly due to low denitrification rates achieved in the biological reactor and caused by both low hydraulic retention time and low concentrations of the soluble organic substrate in the influent, resulting in poor quality of the treated effluent (Mefcalf & Eddy, 2003) as shown in **Figures 4.4a, 4.4d** and **4.4f**. On the other hand, as can be seen from **Figure 4.4b** this alternative offers the lowest aeration and pumping costs and does not need the addition of a chemical compound. It would, however, result in heavy fines for the plant due to the high environmental impact (see **equation A4.8** in the criterion quantification section). Finally it is important to point out that alternative A_3 has the lowest construction costs ($x_{3,2}$) because it implies minor structural modifications. Its upgrading consists only of the installation of vertical impellers to keep the reactors mixed during the anoxic phase, the impeller support platform, the man-hour requirements and the crane rental. (See **equation A4.6** in criteria quantification section).

The predenitrification configuration (A_1) is in second place because it obtains good scores in some of the criteria used to quantify the degree of satisfaction for all the objectives considered (from OBJ_1 to OBJ_4), and is the most balanced of the three alternatives. The lack of soluble organic matter in the influent and low reactor retention time are compensated for in this alternative by an internal recirculation system, increasing the return of nitrates to the anoxic section and thus enhancing overall nitrogen removal efficiency (**Figure 4.4a, 4.4d** and **4.4f**). Nevertheless the plant presents relatively high construction costs ($x_{1,2}$) due to the installation of a recirculation system and its associated equipment, as shown in the pie chart in **Figure 4.4c** (for further details see **equation A4.5** in the criteria quantification section). As a result, this alternative is penalized in terms of satisfaction of OBJ_2 (*minimize economic costs*). However, it should be pointed out that the A_1 configuration presents the lowest operating costs ($x_{1,3}$), as shown by the breakdown of the three competing alternatives in **Figure 4.4b**.

In the end, the alternative A_2 was selected as the structural modification to be implemented. It has the best values in both environmental ($x_{2,1}$) and legal ($x_{2,8} – x_{2,11}$) criteria maximizing the degree of satisfaction of OBJ_1 and OBJ_4 (See **Figure 4.4a** and **4.4f**), although it does not satisfactorily accomplish $OBJ_{2,}$ basically due to high operating costs ($x_{2,3}$). These high operating costs are a result of the periodic purchase of an external carbon source for postdenitrification (see details in the operating cost breakdown depicted in **Figure 4.4b**) and the highest sludge production of all the alternatives due to this extra addition of organic compounds. On the other hand, construction costs are low for this alternative because it only consists of a storage tank, feed pump and a pipe system. The purchase costs of two turbine flocculating devices (one for each tank) to mix the anoxic reactors without introducing oxygen to the wastewater (see **equation A4.6**) are included. The good values obtained by this configuration for some of the technical criteria - such as low rising risk - are derived from an improvement in overall nitrogen reduction and a reduction of the amount of nitrate arriving in the secondary settler (see **Figure A4.3**).

There is not much variation from one configuration to another in terms of bulking, foaming and plant adaptation to short term and long term perturbations. The main reason for the low variation in bulking and foaming risk is the low variation in the F/M ratio for all the evaluated alternatives (see **Figure 4.4.e** and the knowledge flow diagrams at the end of this chapter). Finally, the similarity in terms of adaptability of the three plants to all the evaluated alternatives (see **equation A4.17** and **A4.18**) can be seen from the results in **Table 4.5**.

Table 4.5. Sensitivities to perturbations (S_i), calculation of the robustness (X_4) and flexibility (X_5) criteria

	A_1	A_2	A_3
S_1 (rain event)	0.07326	0.07387	0.07088
S_2 (storm event)	0.10705	0.09203	0.09588
S_3 (nitrogen impact event)	0.10705	0.04174	0.04790
$X_4 = \frac{1}{\sqrt{\frac{1}{3}\sum_{i=1}^{3} S_i^2}}$	**12.25**	**13.83**	**13.47**
S_5 (step increase in flow)	0.00503	0.00396	0.00435
S_6 (step increase in organic matter)	0.10085	0.11255	0.12004
S_7 (step increase in nitrogen)	0.01589	0.00161	0.00306
$X_5 = \frac{1}{\sqrt{\frac{1}{3}\sum_{i=1}^{3} S_i^2}}$	**16.94**	**15.37**	**14.41**

Both the analysis and interpretation of the *multicriteria* matrixes obtained during the evaluation procedure can be improved using *multivariate* statistical techniques (further information in **Chapter 6**). These techniques can help the designer to find a correlation between criteria and alternatives, thereby enhancing and facilitating understanding of the whole decision making process.

4.2.5. Sensitivity analysis

In conceptual design the context in which decisions are taken greatly influences the selection of the best option. In the proposed methodology the context is defined by the design team according to the weighting factor assigned to each objective. Giving more or less weight to a determined objective will clearly restrict some of the alternatives generated during the decision procedure. In order to determine the significance of the context in our case study, a simplified weight sensitivity analysis is described. The results show the influence of the different design objectives (assuming a change in the design context) on the final result.

The first example consists of a sensitivity analysis of objectives OBJ_1 (*minimize environmental impact*), OBJ_2 (*minimize economic costs*) and OBJ_3 (*maximize technical reliability*). The weight for objective OBJ_4 (*comply with legal limits*) stays constant, i.e. $w_4 = 0.25$, while the remaining 0.75 (as mentioned above the sum of all the weights has to be 1) is distributed amongst the weights of objectives 1 (w_1), 2 (w_2) and 3

(w_3). The weighted sum $s(A_j)$ for the three competing alternatives is recalculated to obtain the rank-order of scores. From the results shown in **Figure 4.5a** we can see that high values for w_1 (thus prioritizing the *minimization of the environmental impact*) clearly favour A_2 (postdenitrification with an external carbon source) ahead of A_1 (predenitrification) and A_3 (simultaneous denitrification). For example, $w_1 = 0.75$, $w_2 = w_3 = 0$ and $w_4 = 0.25$ results in scores of $s(A_1)= 0.83$, $s(A_2) = 0.93$ and $s(A_3)= 0.76$.

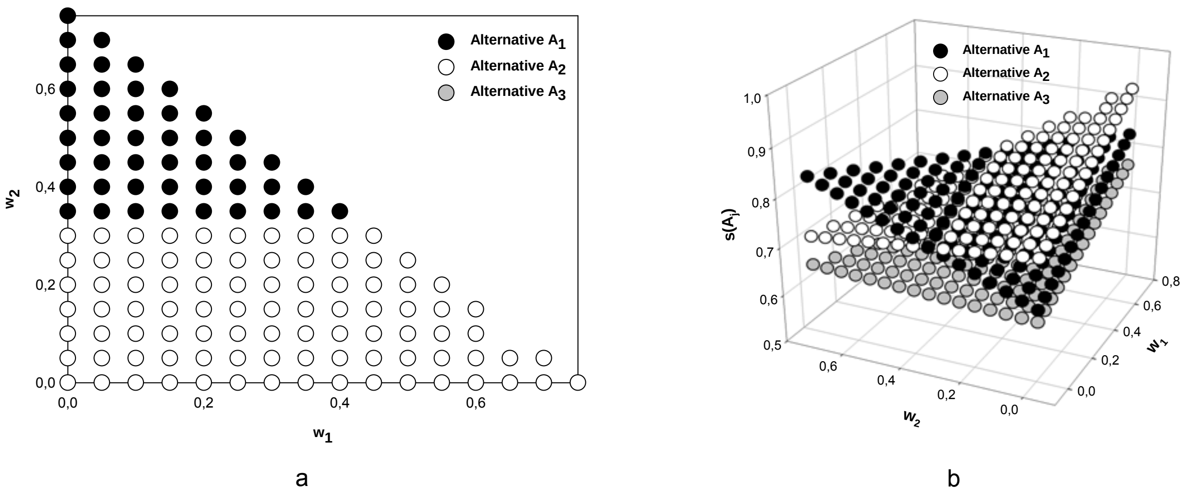


Figure 4.5. Sensitivity analysis of w_1, w_2 and w_3 (a,b)

As w_2 increases in value, however, A_2 and A_3 become roughly equivalent with predenitrification finally coming out best as shown in **Figure 4.5b**. At the same time the analysis shows how sensitive an alternative is to a change in weight. For instance, in this example there is a pronounced variation in the scores of A_1 and A_2 when the relative importance of OBJ_2 (*minimize economical costs*) is increased. This means that A_2 can significantly improve the fulfilment of OBJ_1 (*minimize environmental impact*) at the expense of sacrificing (to an extent) its economic feasibility, and vice versa.

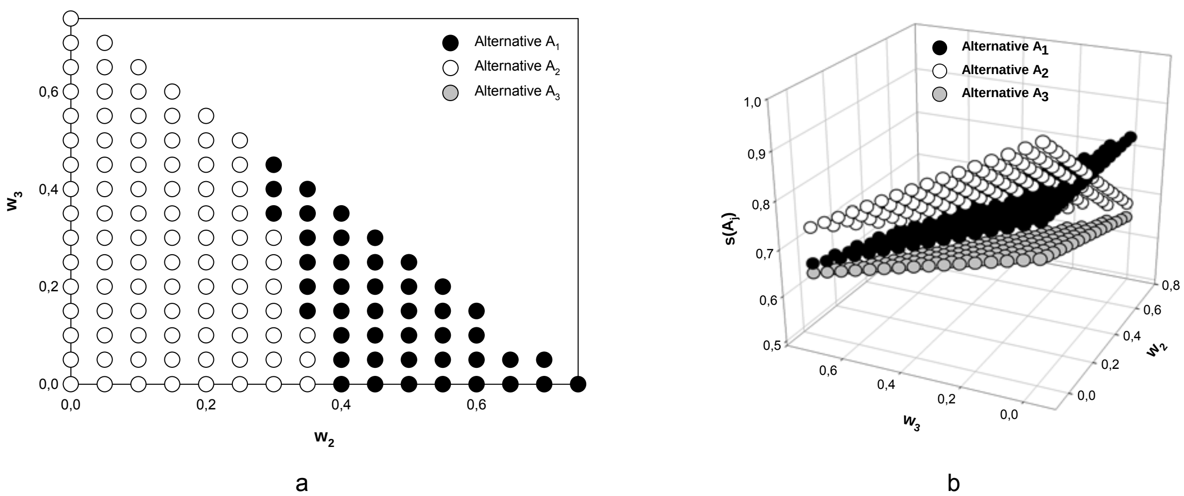


Figure 4.6. Sensitivity analysis of w_2, w_3 and w_4 (a,b)

On the other hand, if the sensitivity analysis is carried out amongst OBJ_2 (*minimize economic costs*), OBJ_3 (*maximize technical reliability*) and OBJ_4 (*comply with the limits set by European Directive)* the solution switches between alternatives A_1 and A_2, as shown in **Figure 4.6**. If economical costs (OBJ_2) are prioritized at the expense of technical characteristics (OBJ_3) and the attainment of European standards in terms of effluent discharges (OBJ_4), the most favoured option would be A_1 (with a score of 0.82 in the weighted sum of $s(A_1)$) while A_2 closely followed by A_3 would clearly be rejected ($s(A_1) = 0.68$ and $s(A_2) = 0.65$). But if the maximization of technical reliability is prioritized ($w_3 = 0.75$, $w_2 = 0$ and $w_4 = 0$) the alternative selected would be A_2 (with a score of 0.73), and A_1 and A_3 would be rejected (with scores of $s(A_1)$ 0.65 and $s(A_3)$ 0.63 respectively). The same happens when OBJ_4 is prioritized; the option with the best effluent quality (A_2) is recommended as the best candidate.

The interpretation of these response surfaces is quite straightforward, but limited to three objectives, i.e. we are limited to the third dimension. This problem of dealing with multiple objectives during a sensitivity analysis is dealt with in **Chapter 5** by means of classification trees.

4.3. CASE STUDY # 2: SET POINT OPTIMIZATION OF TWO PI CONTROL LOOPS IN A NITROGEN REMOVAL WWTP

The second case study presents another application of the methodology that optimizes the control loops for both aeration and internal recycling in a nitrogen removal activated sludge plant. As in the first case study, each block of the procedure, together with numerical details, is discussed in the section that follows until the combination of set points is found that maximizes the degree of satisfaction of the control objectives selected.

4.3.1. *Steps 1* & *2*. Initial state in the exploration and definition of the control objectives and criteria

The IWA/COST simulation benchmark WWTP (Copp, 2002) is the predenitrifying activated sludge plant under study. The plant has a modified Ludzack-Ettinger configuration (see for example Metcalf & Eddy 2003) with five reactors in series (tanks ANOX1 & ANOX2 are anoxic with a total volume of 2000 m^3, while tanks AER3, AER4 & AER5 are aerobic with a total volume of 4000 m^3). These are linked by internal recirculation between the 3rd aerobic (AER3) tank and the 1st anoxic (ANOX1) tank. Also the plant presents a 10-layer secondary settling tank (with a total volume of 6000 m^3) and two PI control loops. The first loop (DO) controls the dissolved oxygen in the 3rd aerobic tank (AER3) through manipulation of the aeration flow (K_La), and the second loop (NO) controls the nitrate in the 2nd anoxic tank (ANOX2) by manipulating the internal recycle flow rate (Q_{intr}) A schematic representation of the plant can be found in **Figure 4.7.**

In the aerobic section of the plant the organic matter and ammonia (ammonia is the form of nitrogen most commonly found in the influent wastewater) are oxidized to carbon dioxide and nitrate. The nitrate transported by internal recirculation is reduced to nitrogen in the anoxic section. This reduction requires an electron donor, which is supplied in the form of influent wastewater. This plant has the same regulations concerning urban wastewater treatment legislation, the same influent wastewater composition and the same operating cost restrictions as those presented in case study 1. **Table 4.1** summarizes control objectives, the set of criteria used to measure their degree of satisfaction and the references.

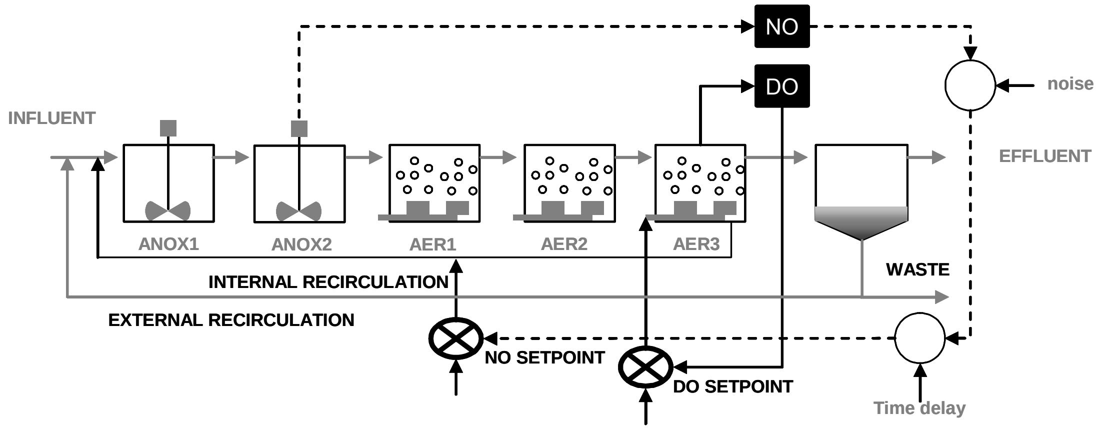


Figure 4.7. Schematic representation of the activated sludge plant with controllers

4.3.2. *Step 3*. Decision procedure

The optimization of both controllers exemplifies the usefulness of the proposed procedure. Each block of the procedure, together with numerical details, is discussed in the sections that follow. The different states of the controllers result in 272 possible alternatives *[A={A_1,…,A_{272}}]*. The NO and DO set points have a range of 0.25 to 4 gN·m^{-3} and 0 to 4 g (-COD)·m^{-3}. The main features of the controllers are summarized in **Table 4.6.**

Table 4.6. Main features of the controllers to be optimized by the proposed procedure

Oxygen controller for the third aerobic reactor		
Controller type	PI with anti-windup	
Proportional gain (K)	500	m^3(g -COD)$^{-1}$·d^{-1}
Integral time constant (Ti)	0.001	d
Anti wind up time constant (Tt)	0.0002	d
Controlled variable	S_O in AER3	
Set point	[0 – 4]	g (-COD)·m^{-3}
Manipulated variable	K_La 5	d^{-1}
Max deviation of MV (max-min)	300	d^{-1}
Nitrate controller for the second anoxic reactor		
Controller type	PI with anti-windup	
Proportional gain (K)	15000	m^3(g N)$^{-1}$·d^{-1}
Integral time constant (Ti)	0.05	d
Anti wind up constant (Tt)	0.03	d
Controlled variable	S_{NO} in ANOX1	
Set point	[0.25-4]	g N·m^{-3}
Manipulated variable	Q_{intr}	m^3·d^{-1}
Max deviation of MV (max-min)	92336	m^3·d^{-1}

The DO sensor is assumed to be ideal, with no delay or noise while the NO sensor has a time delay of 10 minutes and white, normally distributed, zero mean noise (standard deviation of 0.1 g·m^{-3}). External recirculation, waste flow rate and aeration flow rate in the first and second aerobic reactors are constant with respective values of 18446 (Q_r), 385 (Q_w) $m^3 \cdot day^{-1}$ and 240 (K_La 3 & 4) day^{-1}. Reactor 1 (ANOX1) & 2 (ANOX2) are not aerated but fully mixed (K_La 1 & 2 = 0 d^{-1}).

These combinations of set points are evaluated using the four control objectives *[OBJ={OBJ_1,…,OBJ_4}]* defined in **Table 4.1**. For this case study we assume equal importance for all the control objectives, hence $w_p = 0.25$ (p = 1 to 4). Next, a set of criteria from **Table 4.1** is used to evaluate all the combinations: X_1 (impact on water), X_3 (operating costs), X_4 (robustness), X_5 (flexibility), X_6 (control performance), X_7 (risk of separation problems), $X_8 – X_{11}$ (time in violation, TIV).

All the criteria are calculated by dynamic simulation. The simulations are performed with the MatLab-Simulink© environment. The IWA Activated Sludge Model no 1 (ASM1) was chosen as a biological process model (Henze *et al*., 2000). As mentioned previously, the model includes 13 components (state variables) and describes the biochemical carbon removal with simultaneous nitrification and denitrification by 8 processes. From material balances in a CSTR, a set of ordinary differential equations is derived. The double exponential settling velocity of Takács *et al.* (1991), based on the solid flux concept with a ten-layer discretization, was selected as a fair representation of the settling process. All the dynamic simulations follow a steady state simulation to ensure a consistent initial point and prevent the influence of starting conditions in the dynamic modelling. Only the data generated during the last seven days are used to quantify the criteria.

Once all the simulations have been carried out, more than a dozen three dimensional surfaces are created. **Figure 4.8** shows a selection of the surfaces for the criteria X_1 (a), X_3 (b), X_{6-2} (c), X_{7-2} (d), $X_{7,3}$ (e) and X_{11} (f). **Figure 4.8a** indicates that the best degree of satisfaction for OBJ_1 (*minimize environmental impact*) is found when the DO and NO set points are 0.25 g (-COD)$\cdot m^{-3}$ and 4 g N$\cdot m^{-3}$ respectively. This is mainly due to the improvement in the denitrification process, achieved by reducing the quantity of oxygen and increasing the quantity of nitrate and organic matter in the anoxic zone arriving from the aerobic reactor via the internal recycle. **Figure 4.9** shows the dynamic profile of both effluent TKN and TN for different combinations of DO and NO set points. As can be seen in **Figure 4.9a,** the higher the DO concentration, the lower the TKN effluent concentration, mainly due to the improvement in the nitrification process. It is important to emphasize the incremental improvement in nitrification efficiency when the DO set point is moved from 0.5 to 2 g (-COD)$\cdot m^{-3}$. However there is only a very small increment in the effluent ammonium, when the DO setpoint is moved from 2 to 4 g (-COD)$\cdot m^{-3}$. Variations in the NO set point do not make any difference to the TKN profile, as can be seen in **Figure 4.9c**. On the other hand, **Figure 4.9b** shows that the higher the DO concentration, the higher the quantity of nitrate transported to the anoxic zone, but also the higher the concentration of oxygen and the lower the concentration of organic matter, resulting in lower denitrification efficiency. Finally, **Figure 4.9d** also shows the effect of recirculation on overall nitrogen removal. If the NO set point is increased from 1 to 2.5 g N$\cdot m^{-3}$, the result is higher denitrification efficiency because the quantity of nitrate arriving at the anoxic zone increases. Nevertheless, as soon as the set point values increase, some oxygen is also transported to the anoxic zone, thereby inhibiting the denitrification process

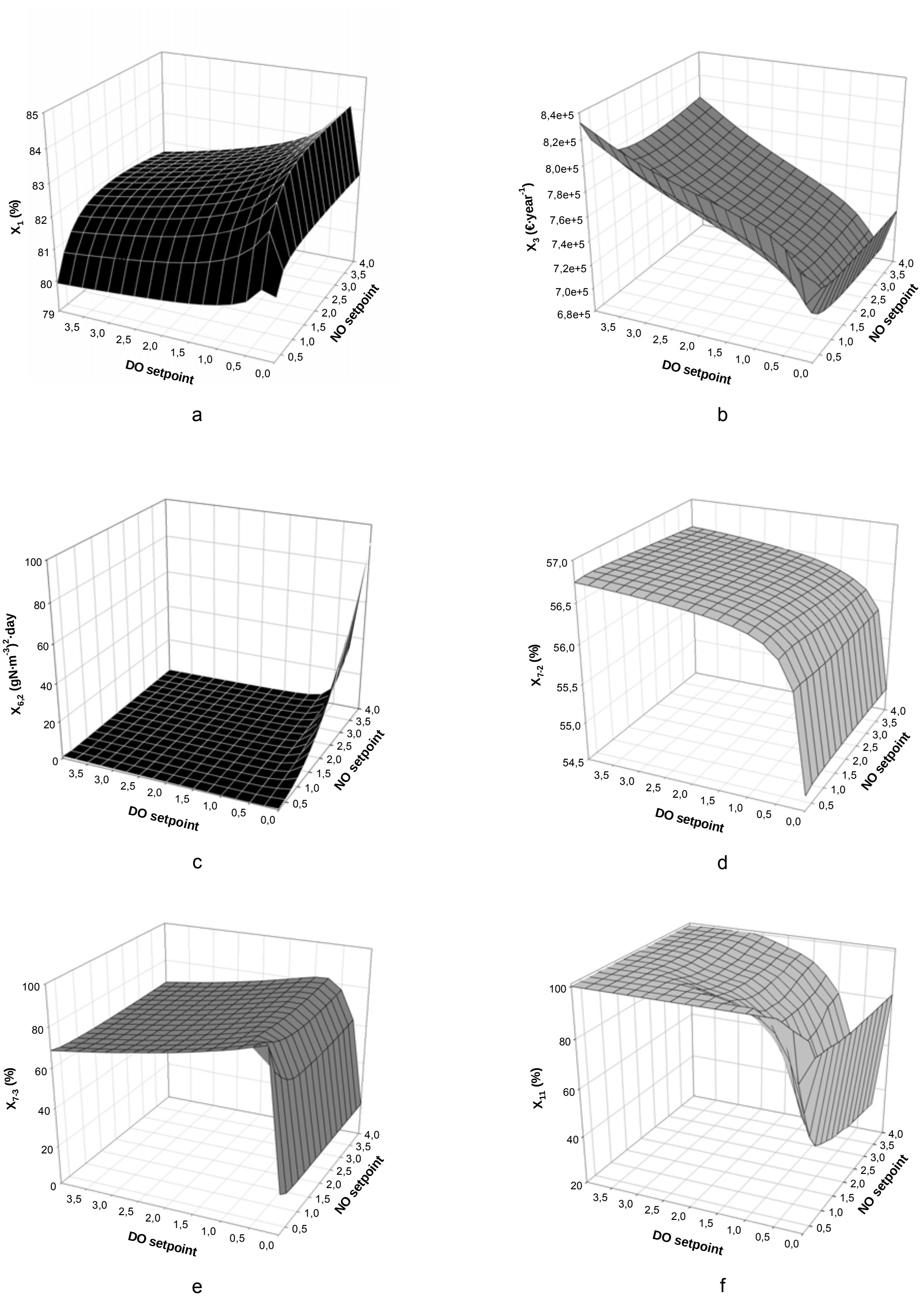


Figure 4.8. Representations of some of the evaluation criteria: (a) impact on water (X_1), (b) operating costs (X_3), (c) nitrate control performance ($X_{6,2}$), (d) foaming risk, (e) rising risk ($X_{7,3}$) and (f)time in violation (TIV) for TN (X_{11})

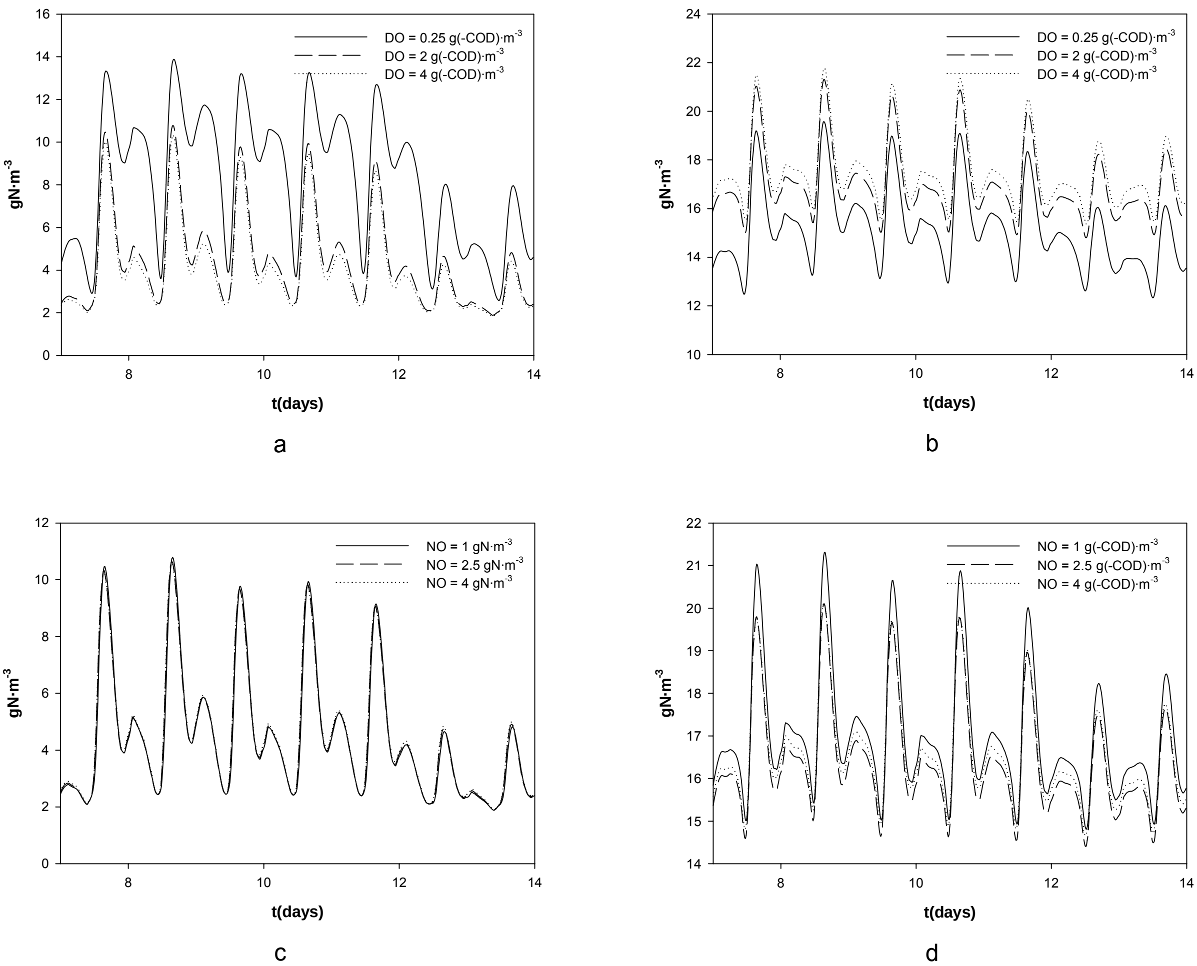


Figure 4.9. Dynamic profiles of both TKN (a,c) and TN (b,d) for different set point combinations (a – b) when the NO set point is constant (NO = 1 g N·m^{-3}) and the DO set point is changed; and (c-d) when the DO set point is constant (DO = 2 g (-COD)·m^{-3} and the NO set point is changed.

The operating costs are minimized when the DO and the NO set points are 0.25 g (-COD)·m^{-3} and 3.25 g N·m^{-3} respectively, as depicted in **Figure 4.8b**. A higher DO set point implies an increased supply of air and thus an increase in aeration costs (α_{AE}·AE in **equation A4.8**). Furthermore and as previously mentioned, this combination of set points increases the quantity of nitrate sent to ANOX1 and minimizes the consumption of organic matter in AER3, thereby improving the whole nitrogen removal process and reducing the fines levied as a result of environmental impact. Finally, it is important to note that although higher NO set points imply a high recirculation flow rate (α_{PE} PE in **equation A4.8**), the benefits obtained compensate for this drawback.

With respect to the NO controller performance (**Figure 4.8c**), performance is better if the nitrate set point is low. At high NO set point values the recirculation flow rate of nitrates from the aerobic zone is not sufficient to maintain the desired set point in the second anoxic reactor i.e. the recycle flow rate reaches saturation (maximum flow rate = 92336 m^3·day^{-1}) (see **Table 4.6**). Furthermore, it is important to point out that the higher the DO concentration in the aerobic zone, the lower the volume of mixed liquor that has to be pumped via internal recirculation; this is due to an increase in nitrification efficiency, which explains the dramatic decrease in control performance in this section, as shown in **Figure 4.8**.

The dynamic behaviour of the controller can be observed in **Figure 4.10** where the difference between the value of the controlled variable (in this case nitrate concentration in the second anoxic reactor ANOX2) and the desired set point is depicted. **Figure 4.10a** describes the negative effect of low DO concentrations on overall control performance due to a decrease in the nitrification rate, while **Figure 4.10b** shows the inability of the controller to reach the NO set point due to the limitation on the manipulated variable (actuator saturation). Z_{SET}-Z_{OBS} has basically positive values.

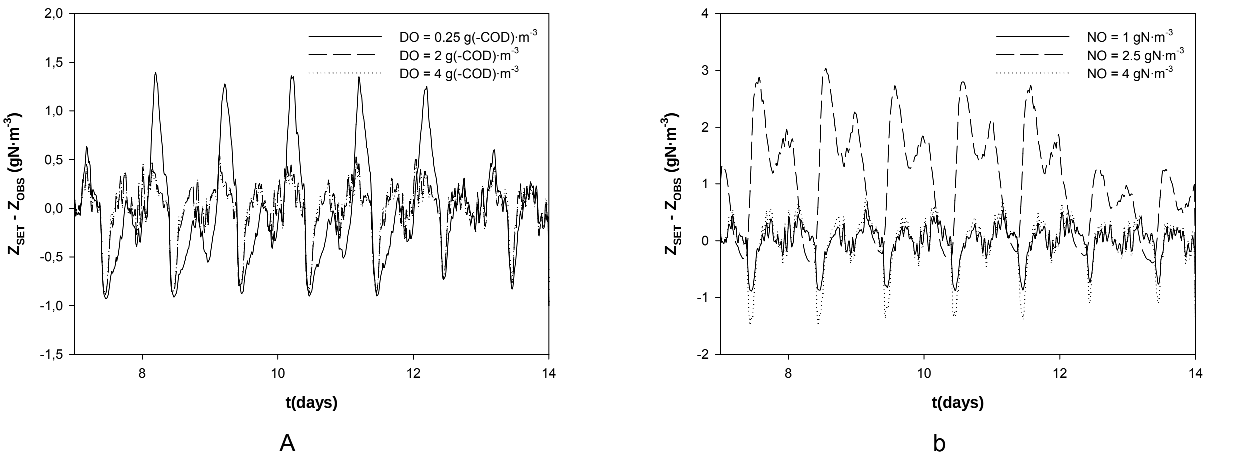


Figure 4.10. Dynamic profiles of the difference between the nitrate in the second anoxic reactor (Z_{OBS}) and the desired set point (Z_{SET}) for different set point combinations a) when the NO set point is constant (NO = 1 g N·m^{-3}) and DO is changed and b) when the DO set point is constant (DO = 2 g (-COD)·m^{-3} and NO is changed

Foaming risk decreases as the concentration of DO in AER3 decreases. Thus, lower aeration in the aerobic section causes a decrease in biomass growth that produces an increase in the F/M ratio (see criteria quantification section, knowledge flow diagram for foaming), which is mainly responsible for the foaming risk.

In **Figure 4.8e** the increase in rising risk between the DO set points of 4 and 0.5 g(-COD)·m^{-3} is shown. This is mainly due to the fact that the higher the DO set point, the higher the removal of the influent organic biodegradable substrate in the aerobic or anoxic zone, thereby preventing its arrival in the secondary settler. Nevertheless, it is important to point out that if the DO set point is lower than 0.5 g (-COD)·m^{-3}, there is a dramatic decrease in the rising risk because the quantity of nitrate produced in the aerobic zone is reduced due to a failure in the plant's overall nitrification capacity.

The last figure (**Figure 4.8f**) highlights the degree of satisfaction of the European Directive for TN. It shows there are lower penalties when DO is low (DO = 0.25 g (-COD)·m^{-3}) and recycle flow high (NO = 4 g N·m^{-3}), because this combination of parameters achieves the best trade-off between the nitrification and the denitrification process.

Results for the remaining criteria are not shown due to lack of space, but the main results are summarized. The plant's adaptation to short term and long term perturbations (X_4) increases as the DO set point increases. In general the DO controller performs well (criterion $X_{6,1}$) except when the set point is high, because it is difficult to reach the desired values using the manipulated variable i.e. the maximum value of the aeration flow rate (K_La) is limited to (300 d^{-1}). The lowest DO concentration in AER3 causes the lowest bulking risk because there is a fall in the F/M1 ratio attributable to a low biomass population in the reaction zone. For this case study X_7, X_8 and X_9 have the same value and are therefore not useful for discriminating between the competing control schemes.

To sum up, an analysis of these results shows that synergies exist in the accomplishment of some objectives, e.g. X_1 and $X_{11,}$ but others are subjected to clear trade offs, e.g. $X_{6\text{-}2}$ with X_1 or $X_{4,}$ and X_5 with X_1.

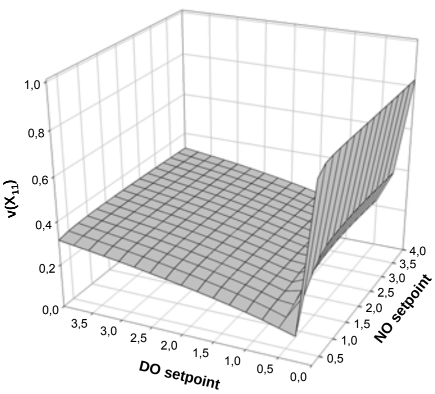
Once the defined criteria are quantified for all the proposed alternatives, the extreme profiles (based on expert judgments) are defined, respectively, as follows:

$$[(x_*) = (x_{1*} = 0\%, x_{2*} = 1\cdot 10^6 €\cdot year^{-1}, x_{4*}= 0, x_{5*} = 0, x_{6,1*} = 1(g(\text{-}COD)\cdot m^{-3})^2\cdot day, x_{6,2*} = 1(gN\cdot m^{-3})^2\cdot day, x_{7,1*} = 100\%, x_{7,2*} = 100\%, x_{7,3*} = 100, x_{8*} = 100\%, x_{9*} = 100\%, x_{10*} = 100\%, x_{11*} =100\%].$$

and

$$[(x^*) = (x_1^* = 100\ \%, x_3^* = 7\cdot 10^{5} €\cdot year^{-1}, x_4^*= 20, x_5^* = 20, x_{6,1}^* = 0\ (g(\text{-}COD)\cdot m^{-3})^2\cdot day, x_{6,2}^* = 0(gN\cdot m^{-3})^2\cdot day\ , x_{7,1}^* = 0\%, x_{7,2}^* = 0\%, x_{7,3}^* = 0\%, x_8^* =0\ \%, x_9^* = 0, x_{10}^* = 0\%, x_{11}^* = 0\%)]$$

A linear model between these extreme values is then adjusted to calculate the intermediate effects (*e.g.* the criterion X_1 has the following value function $v_1(X_1) = 0.01\cdot X_1$) using the same procedure as explained in section 4.2.3.4. **Figure 4.11** shows a representation of the normalized response surfaces for two of the evaluation criteria used in this case study: risk of rising $v(x_{7\text{-}3})$ and time in violation for TN $v(x_{11})$. The most desirable conditions are represented for those values close to 1, but the worst criteria values are closer to 0. These surfaces can be compared to the ones summarized in **Figure 4.8.**



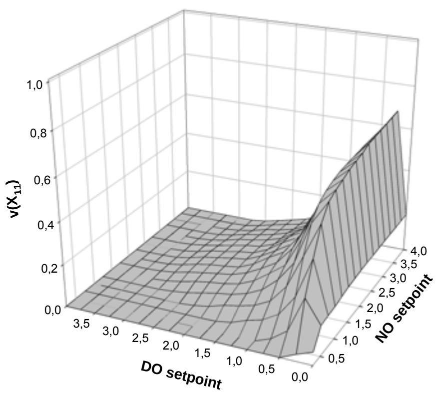
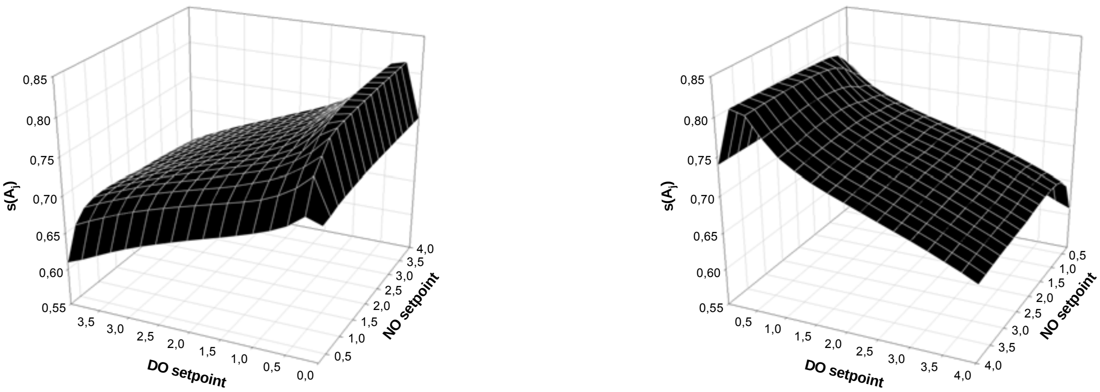


Figure 4.11. Two examples of normalized response surfaces for criteria $X_{7\text{-}3}$ and X_{11} using the methodology described in the present chapter

Finally a new response surface is generated using **equation 4.1**. This *multicriteria* response surface is obtained by adding the normalized value of the single response criteria multiplied by their corresponding weights. **Figure 4.12** represents the degree of satisfaction of the evaluated alternatives according to the relative importance of the control objectives and overall plant performance.



a b

Figure 4.12. Two views of the multicriteria response surfaces generated using equation 4.1 (w_i = 0.25, i = 1 to 4)

4.3.3. *Step 9*. Selection of the best alternative

From an analysis of the results shown in **Figure 4.12** we conclude that the combination of set points that achieves the best level of satisfaction of the control objectives, when all have equal importance, is 0.5 g(-COD)·m^{-3} and 3.25 gN·m^{-3} for DO and NO controllers respectively. The low DO set point is selected mainly due to better denitrification performance, lower operating costs and lower foaming and rising risk. This is in spite of its detrimental effect in terms of plant adaptation to short and long term perturbations (robustness and flexibility), high pumping rates and nitrate control performance.

4.3.4. Sensitivity analysis

As in the first case study, a weight sensitivity analysis is finally performed. Its aim is to show how the selected combination of set points can vary when the relative importance of the control objectives is modified. **Figure 4.13** shows the variations in the DO and NO set points when different combinations of weights are assigned to the defined control strategies.

From the results reported in **Figure 4.13a** it can be seen that high values in w_1 (i.e. *minimize impact on water* is prioritized) favour low aeration flow rates and high pumping rates in the recycling system, thereby improving the denitrification process, operating costs, foaming risk and rising risk as shown in **Figure 4.8a, b, d, e** an **f**. However, as w_2 (*minimize economic costs*) gains in value, this pumping rate is reduced because it leads to higher operating costs (see **Figure 4.8b**). Surprisingly, the DO set point increases slightly. However, this can be explained by the fact that the increase in operating costs is not substantial, and there it causes an improvement in the criteria used to measure the degree of satisfaction of OBJ_3 - e.g. robustness, flexibility and nitrate control performance (see **Figure 4.8c**).

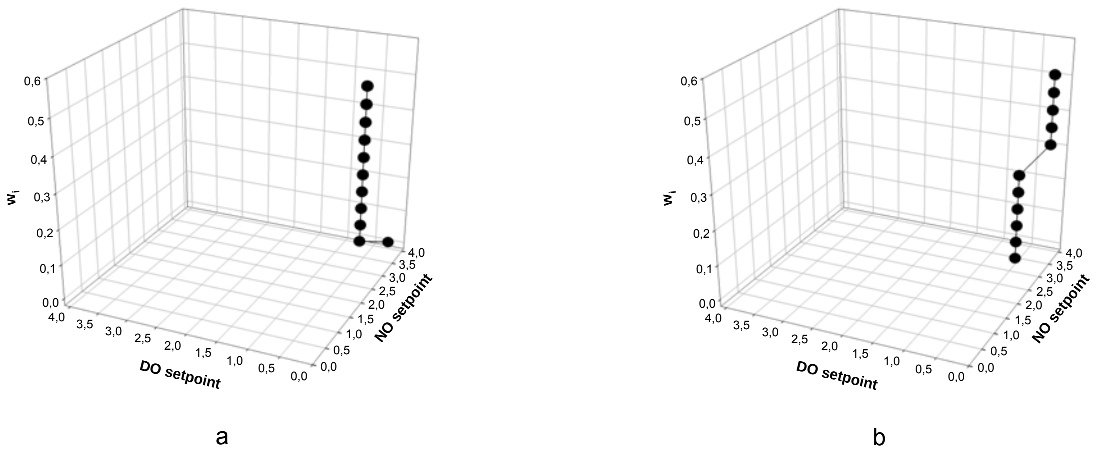


Figure 4.13. Representation of the set point variation when the importance of the control objectives is changed

Otherwise, if OBJ_3 (*maximize technical reliability*) is prioritized at the expense of environmental impact (high values in w_1) higher DO and lower NO set points are recommended. In this way, better adaptation to short and long term perturbations and control performance is ensured. Nevertheless, as soon as the weight of OBJ_1 (*minimize environmental impact*) increases in value, nitrate and oxygen set points increase and decrease respectively because better denitrification efficiency is ensured, as shown in **Figure 4.8a** and **f.**

Nevertheless, it should be mentioned that for all practical purposes the variations recommended by the sensitivity analysis are very small. In other words, although the relative importance of the objectives might change, the combination that ensures the best plant performance always includes low DO and high NO set points

4.4. CONCLUSIONS

This chapter has presented the first block of the conceptual design method for a WWTP presented in this thesis. The block was constructed as a systematic procedure combining the *hierarchical* decision process with *multicriteria* analysis. The *multicriteria* method allows the inclusion of different objectives, e.g. environmental, economic, technical and legal, while the *hierarchical* decision process reduces the design problem to a set of issues that follow a predefined order (reaction, separation and recirculation). This chapter has contributed to solving the problem of the number of evaluations of design alternatives that need to be taken into account by proposing a hierarchy of decisions, and finding a design solution that maximizes the degree of satisfaction of all the objectives considered using *multicriteria* decision analysis.

This procedure allows the integration of different sources of information to quantify the criteria used to evaluate satisfaction of the proposed objectives. These criteria are calculated by standardized indices extracted from the literature using different methodologies (dynamic simulation, model-based cost estimates, knowledge flow diagrams) and integrated into the entire decision procedure.

Different value functions have been proposed as a normalization method for facilitating the comparison of criteria i.e. all of them are quantified in different units. Definitions of the best and the worst situations as extreme points of the evaluation range facilitate the formulation of a mathematical equation to evaluate the intermediate effects.

Finally, a weighted sum is used as an evaluation method to find the most desirable choice among all the competing alternatives on the basis of the defined objectives, their importance and overall process performance. In addition, the sensitivity of the relative importance of the weights is tested, which enables the whole design process to be understood and show, at any given moment, why one alternative is selected and the rest are declined.

The usefulness of this methodology has been tested with two case studies: in the first, the type of biological nitrogen removal process for an existing organic carbon removal and nitrification WWTP is selected. In this case study, postdenitrification is the alternative that is recommended to be implemented. This is mainly due to the good accomplishment of both environmental and legal objectives although the operating costs are high. Thus predenitrification and simultaneous nitrification/denitrification are not selected because their potential advantages are not sufficient to warrant further consideration and more study needs to be devoted to the family of alternatives with postdenitrification. Nevertheless, the sensitivity analysis shows that when OBJ_2 (*minimize economic costs*) gains in value predenitrification become the best alternative in spite of having high construction costs. This is mainly due to the fact that this configuration shows lower operating costs and also a good effluent quality. In the second case study, the combination of DO and NO set points in a nitrogen removal plant is optimized. Low DO and high NO set points, no matter the relative importance of the control objectives, are the recommended combination to ensure a good process performance and a maximum accomplishment of the control objectives

4.5. CRITERIA QUANTIFICATION SECTION (I)

Impact on water is calculated as expressed in **equations A4.1 to A4.4.**

$$X_1 = \frac{IQ - EQ}{IQ} \qquad \text{(A4.1)}$$

Effluent and influent quality index (EQ and IQ) are calculated as shown in **equations A4.3 and A4.4.**

$$EQ = \frac{1}{(t_f - t_0)} \int_{t_0}^{t_f} PU(t) \cdot Q_e(t) \cdot dt \qquad \text{(A4.2)}$$

PU is the result of applying (**equation A4.3**).

$$PU(t) = PU_{TSS}(t) + PU_{COD}(t) + PU_{BOD}(t) + PU_{TKN}(t) + PU_{NO_X}(t) \qquad \text{(A4.3)}$$

The effluent polluting loads PU_K ($kg \cdot day^{-1}$) corresponding to the component k (TSS, COD, BOD_5, TKN and NO_X) are calculated through **equation A4.4.**

$$PU_K = \beta_K C_K \qquad \text{(A4.4)}$$

where β_{TSS} =2, β_{COD} =1, β_{BOD5} =2, β_{TKN} =20, β_{NOx} =20. IQ is calculated in a similar way to the EQ index, replacing the effluent data with the influent data.

Construction costs are quantified by using **equation A4.5** for the costs of the internal recycling system. These costs include the earthwork (COSTE), the pump building (COSTPB), the pumps and driving units (COSTP), and the installation costs (IEC). All these costs are multiplied by a correction factor.

$$COST_{recycle-system} = (COSTE + COSTB + COSTP + IPC)\cdot CF \quad \text{(A4.5)}$$

Several factors are involved in the quantification of mixing systems for the reactors that have to be anoxic. A turbine flocculating device would be used to mix the denitrification zone without introducing oxygen to the wastewater (CSXSA). The costs of the electrical wiring (PMINC), man-hour requirements for installation (IMHA) and finally the crane requirements (CHA) must also be included. All these items are included in **equation A4.6** and multiplied by the number of anoxic reactors (NT) and a correction factor (CF).

$$COST_{mixing-system} = (CSXM + PMINC + IMHA + CHA)\cdot CF \cdot NT \quad \text{(A4.6)}$$

Finally, the cost of the external carbon source feed system is calculated using **equation A4.7**, where A and B are different empirical factors and M is the rate of external carbon source addition ($Kg\cdot day^{-1}$).

$$COST_{feed-system} = A\cdot(M)^B \quad \text{(A4.7)}$$

Operating costs are calculated as shown in **equation A4.8.**

$$X_3 = \alpha_{EQ}\cdot EQ + \alpha_{AE}\cdot AE + \alpha_{PE}\cdot PE + \alpha_{sldg}\cdot P_{sldg} + \alpha_{ME}\cdot ME + \alpha_{CS}\cdot CS \quad \text{(A4.8)}$$

EQ, AE, PE and ME represent the effluent fines, aeration, pumping and mixing energy rates ($kW\cdot h\cdot day^{-1}$) respectively; P_{sldg} is the sludge production rate ($kg\cdot day^{-1}$) and CS is the quantity of chemicals ($m^3\cdot day^{-1}$). AE, PE, ME, P_{sldg}, and CS are calculated by applying **equations A4.9** to **A4.16**. The α_J coefficients in **equation A4.8** are the annual operating cost weight factors. The values used in the simulations reported in this thesis were: α_{sldg} = 50 ($EQ\cdot year^{-1}$)$\cdot$($EQ\cdot day^{-1}$)$^{-1}$, α_{AE} = α_{PE} = α_{ME} = 25 (€$\cdot year^{-1}$)$\cdot$($kW\cdot h\cdot day^{-1}$); α_{sldg} = 75 (€$\cdot year^{-1}$)$\cdot$($kgTSS\cdot day^{-1}$)$^{-1}$. All the α_j values were obtained from the literature (Vanrolleghem and Gillot, 2002), except α_{CS}, which was estimated assuming a cost of 0.3 €$\cdot kg^{-1}$.

Aeration energy (AE) is modelled as presented in **equation A4.9** and based on the aeration consumption of the Degremont DP230 porous disk. However, the calculations have been improved compared to the equation suggested in Copp (2002) by also including the volume of the aeration tanks.

$$AE = \frac{24}{t_f - t_0}\int_{t_0}^{t_f}\sum^{i=n}[c_1\cdot K_L a_t\left(\frac{V_i}{V_{ref}}\right)\cdot(t)^2 + c_2 K_L a_t\left(\frac{V_i}{V_{ref}}\right)\cdot(t)^2]\cdot dt \quad \text{(A4.9)}$$

Pumping energy (PE) is computed as shown in **equation A4.10** and is calculated as the weighted sum of the internal recycling flow (Q_{intr}), external recirculation (Q_r) and waste flow (Q_w).

$$PE = \frac{1}{(t_f - t_0)}\int_{t_0}^{t_f}(PE\_Q_{int}\cdot Q_{int} + PE\_Q_r\cdot Q_r + PE\_Q_w\cdot Q_w)\cdot dt \quad \text{(A4.10)}$$

The suggested values for PE are the following: PE_Q_{intr} = 0.004 $kWh\cdot m^{-3}$, PE_Q_r = 0.008 $kWh\cdot m^{-3}$ and PE_Q_w = 0.05 $kWh\cdot m^{-3}$.

Mixing Energy (ME) is modelled as presented in **equation A4.11**. It is assumed that each individual activated sludge tank requires a mechanical mixing only when K_La is lower than 20 d^{-1}. In other cases aeration is assumed to be enough to maintain the activated sludge in suspension.

$$ME = \frac{24}{(t_f - t_0)} \int_{t_0}^{t_f} \begin{bmatrix} k_L a_i(t) < 20d^{-1} \rightarrow ME_{unit} \cdot V_i \\ k_L a_i(t) > 20d^{-1} \rightarrow 0 \end{bmatrix} \cdot dt \tag{A4.11}$$

Sludge for disposal (P_{sldg}) is modelled as presented in **equation A4.12**, **A4.13**, **A4.14** and **A4.15**.

$$P_{sldg} = \frac{\Delta M(TSS_{SYSTEM}) + M(TSS_W)}{t_f - t_0} \tag{A4.12}$$

$$\Delta M(TSS_{SYSTEM}) = \mathrm{M}(TSS_{SYSTEM})_{t_f} - \mathrm{M}(TSS_{SYSTEM})_{t_0} \tag{A4.13}$$

$$(TSS_{SYSTEM}) = \mathrm{M}(TSS_{reactor}) + \mathrm{M}(TSS_{settler}) \tag{A4.14}$$

$$M(TSS_W) = \int_{t_0}^{t_f} TSS_W \cdot Q_W(t) \cdot dt \tag{A4.15}$$

The amount of chemicals (CS) is modelled as shown in **equation A11**.

$$CS = \frac{COD_s}{(t_f - t_0) \cdot 1000} \int_{t_0}^{t_f} Q_{carb} \cdot dt \tag{A4.16}$$

Robustness is defined as the degree to which the process can handle short term disturbances affecting the dynamics of the process (Grossman and Morari, 1985). The criterion for robustness (X_4) is measured by the operating cost index defined by Vanrolleghem and Gillot (2002), because it combines effluent and operating variables and is quantified as the inverse of the normalized sum of squared sensitivities. This criterion is quantified as shown in **equations A4.17** and **18**. These short term disturbances are: (S_1) storm (of high intensity but a short-lived increase in flow and suspended solids); (S_2) rain (influent flow does not reach the level attained during storm events but high flow is sustained for a longer period of time) as defined by Copp (2002); and (S_3), a 10% increase in nitrogen concentration between the fifth and the seventh day of simulation in the default influent (i.e. a nitrogen shock).

$$S = [S_1, ..., S_p] \text{ with } S_i = \frac{\Delta OCI}{OCI} \quad i = [1,.., p] \tag{A4.17}$$

$$X_4 = \frac{1}{\sqrt{\frac{1}{p}\sum_{i=1}^{p} S_i^{\,2}}} \tag{A4.18}$$

Flexibility is defined as the degree to which process can handle long term changes and return to the steady state (Grossman and Morari, 1985). This long term changes are understood as permanent increases compared to the default conditions in which the plant is designed. The long term changes used in this case study increases of 10 % in the influent organic content, nitrogen and flow although other possibilities are also available e.g. include the effect of temperature changing the kinetic parameters. For these situations, three sensitivities (S_4, S_5 and S_6) are measured for criterion X_3 and quantified following the same procedure as before.

Control performance is approximated according to **equation A4.19** where the controlled variable ($Z_{OBSERVED}$) is either nitrate concentration in the second anoxic tank or the oxygen controller in the third aerobic reactor; the set point ($Z_{SETPOINT}$) is the desired concentration to be achieved by means of the manipulated variable.

$$X_6 = \int_{t_0}^{t_f} (Z_{SETPOINT} - Z_{OBSERVED})^2 \cdot dt \qquad \text{(A4.19)}$$

The percentage of time that the plant is in violation of effluent regulations set by European regulations also has to be reported. Effluent limits are defined in European Directive 91/271 and have the following values: COD= 125 g COD·m^{-3}, BOD_5 = 25 g COD·m^{-3}, TSS = 35 g TSS·m^{-3} and TN = 15 g N·m^{-3}.

4.6. CRITERIA QUANTIFICATION SECTION (II)

Knowledge related to the risk of filamentous bulking proliferation was synthesized into a decision tree with three branches (see **Figure A4.1**). Each branch of the tree evaluates one of the three main causes: low dissolved oxygen concentration (left), nutrient deficiency (middle) and low F/M ratio or substrate limiting conditions (right). The other common causes of filamentous bulking (septic conditions or low pH in the influent) were not considered in the current approach since standard mechanistic models do not include either sulphur or pH modelling. During conditions of low dissolved oxygen (DO) concentration, the growth of filaments is favoured, according to substrate-diffusion and kinetic selection theories (Martins *et al.*, 2004a,b). The left branch of the tree illustrates that the level of occurrence of limiting DO conditions in the biological reactors is related to the current F/M ratio in a non-linear way (Grady *et al.*, 1999). As a result, although DO control is considered standard for most plants, favourable conditions for low DO bulking might arise if the DO set point is not high enough when the WWTP experiences a high F/M ratio.

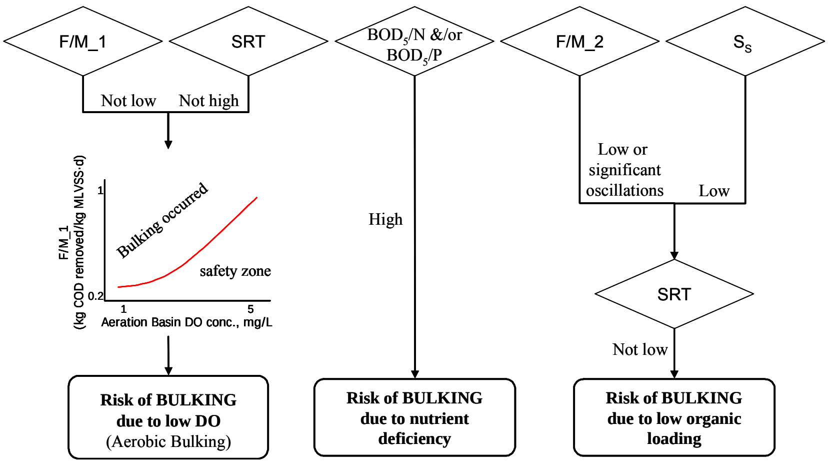


Figure A4.1. Flow diagram developed to evaluate the risk of filamentous bulking.

The branch in the middle evaluates whether nitrogen (N) and/or phosphorus (P) limiting conditions occur. Finally, promoting conditions for the growth of low F/M filamentous bacteria can be caused by both readily biodegradable substrate limiting conditions (S_S) in the bioreactor and by a low or an oscillating influent organic loading rate. Thus, up to seven variables can be used in the knowledge-based flow diagram as symptoms to assess risk of filamentous bulking: SRT, DO, F/M_1 (measured as kg of removed COD per kg biomass and per day), F/M_2 (measured as kg BOD_5 supplied per kg biomass per day), BOD_5/N, BOD_5/P and S_S.

The set of symptoms that was found to be most useful in detecting favourable conditions for filamentous foaming included F/M_2, SRT, DO and the ratio between S_S and slowly biodegradable substrate (X_S) (see **Figure A4.2**). Two of the decision tree's main branches allow operating conditions to be investigated, therefore enhancing the growth of different filamentous microorganisms that would cause biological foaming problems. Nocardioforms and *M. Parvicella*, the most common filamentous organisms causing foaming (Wanner, 1994; Jenkins *et al*., 2003), experience better conditions for growth than floc-forming bacteria when the activated sludge system experiences low F/M ratios or significant oscillations of F/M ratios combined with high SRT. In the case of *M. Parvicella*, which also causes sludge bulking, foam formation is favoured by the two former conditions together with low DO concentrations in the aerobic reactors. The development of biological foams due to growth of type 1863, although less frequent, is also probable if the influent contains a high fraction of readily biodegradable organic matter (RBOM) – i.e. a high S_S/X_S ratio.

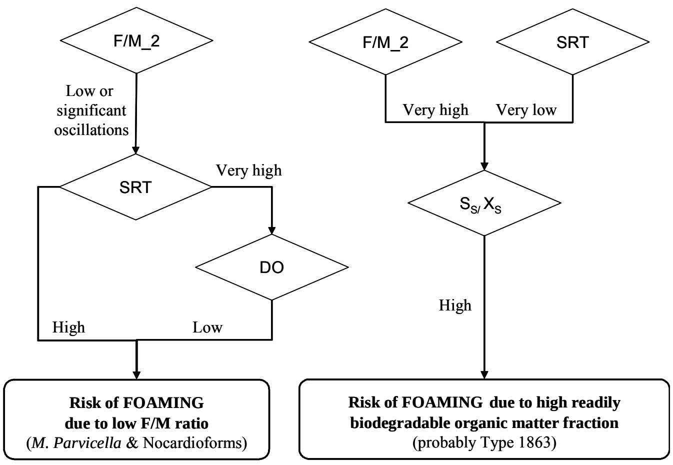


Figure A4.2. Flow diagram developed to evaluate the risk of filamentous bulking.

Figure A4.3 shows the flow diagram developed to estimate the risk of rising sludge in activated sludge systems. According to Henze *et al.* (1993), rising sludge becomes a problem when the nitrate concentration in the secondary clarifier influent is higher than the critical nitrate concentration (8 g N m^{-3} at 15ºC). In this situation, the time required for nitrogen gas production is calculated (based on the denitrification rate and the time delay caused by removal of the remaining oxygen in the bottom of the clarifier), and compared to the sludge residence time in the clarifier (estimated as the amount of sludge in the sludge blanket divided by the Q_r flow rate). The denitrification rate is calculated as in the ASM1 (Henze *et al.*, 2000) but using the active heterotrophic biomass concentration at the bottom of the clarifier. Whenever the nitrate concentration is higher than the critical level, and nitrogen gas production time is lower than or equal to sludge residence time in the secondary settler, then favourable conditions for denitrification are inferred, and consequently the risk of solids separation problems due to rising sludge increases. Fast dissolved oxygen consumption is assumed in the settler and therefore the denitrification rate is always computed assuming no oxygen inhibition (DO = 0 g (-COD)·m^{-3}). Thus, the variables used as symptoms for rising sludge are effluent S_{NO} , Q_r, sludge blanket depth and denitrification rate

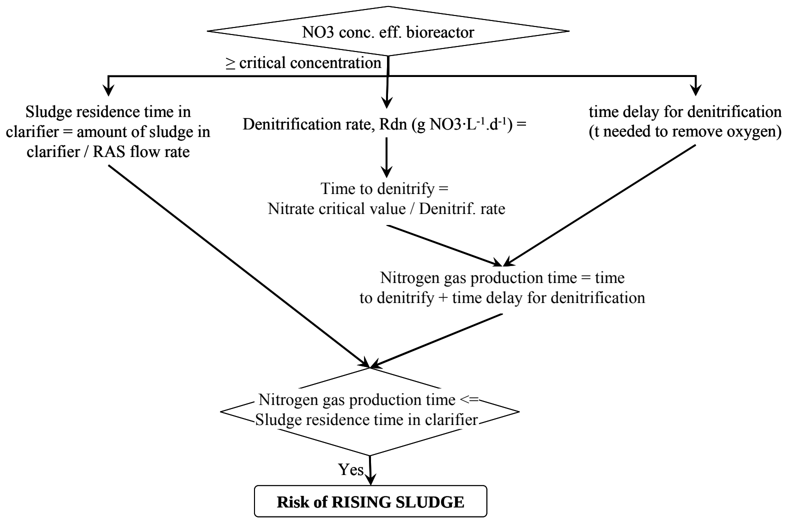


Figure A4.3. Flow diagram developed to evaluate the risk of rising sludge.

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

PhD THESIS

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Flores X., Poch M., Rodríguez-Roda I Bañares-Alcántara R. and Jiménez L. Systematic procedure to handle critical decisions during the conceptual design of activated sludge Systems. Ind. Eng. Chem. Res. 2007. 46(17):5600.

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CHAPTER 5. A SYSTEMATIC PROCEDURE FOR HANDLING *CRITICAL DECISIONS* DURING THE *MULTICRITERIA* EVALUATION OF WASTEWATER TREATMENT PLANT ALTERNATIVES

In this chapter, a new systematic procedure to address *critical decisions* during the design of wastewater treatment plants (WWTPs) is presented. By *critical decisions* we mean those with a great influence on the entire design process (i.e. influencing many other decisions and hence having a significant effect on process structure and operation), and with a set of possible solutions that would result in a similar degree of satisfaction of the design objectives (the most *promising alternatives*).

The proposed approach comprises seven steps organized in two phases: (I) *hierarchical* generation and *multicriteria* evaluation of design alternatives and (II) analysis of *critical decisions.* The evaluation of the design alternatives was described in the previous chapter (*Steps 1* to *3*). The second block consists of a systematic procedure comprising three steps: *Step 4*) preliminary multiobjective optimization where the most *promising alternatives* are compared close to the optimum conditions based on the results of dynamic simulation; *Step 5*) identification of the strong and weak points of each alternative by means of classification trees and the subsequent extraction of rules for each alternative; and *Step 6*) evaluation of the trade-off between the improvement of the criteria identified as weak points of the alternative and the loss of overall process performance through the integrated application of dynamic simulation and qualitative knowledge extracted during the design process.

The usefulness of the whole procedure is demonstrated using a case study where a nitrogen removal plant is redesigned to achieve simultaneous organic carbon, nitrogen and phosphorus removal. The results show that biological nutrient removal results with lower operating costs and a more balanced nitrogen and phosphorus removal although this alternative implies the constructions of additional anaerobic volume. Furthermore, this option undergoes a smaller variation in the overall process performance at the time to improve the criteria identified as a weak. On the other hand, it was discovered the inability of chemical precipitation to achieve good phosphorus removal percentages without decreasing the operating costs and the bad performance in terms of nitrogen removal. Thus, it would make this alternative very expensive to operate if those limitations had to be overcome.

5.1. METHODOLOGY

The second block (analysis of *critical decisions*) follows an evolutionary approach that combines sensitivity analysis, preliminary multiobjective optimization and knowledge extraction to assist the designer during the selection of the best alternative in accordance with the design objectives and process performance (further information about the method presented in this thesis can be found in **Figure 2.1**, **Chapter 2**). It comprises seven steps organized in two phases: (I) *hierarchical* generation and *multicriteria* evaluation of design alternatives and (II) analysis of *critical decisions*. A flowchart that highlights the most important steps in the procedure is shown in **Figure 5.1**.

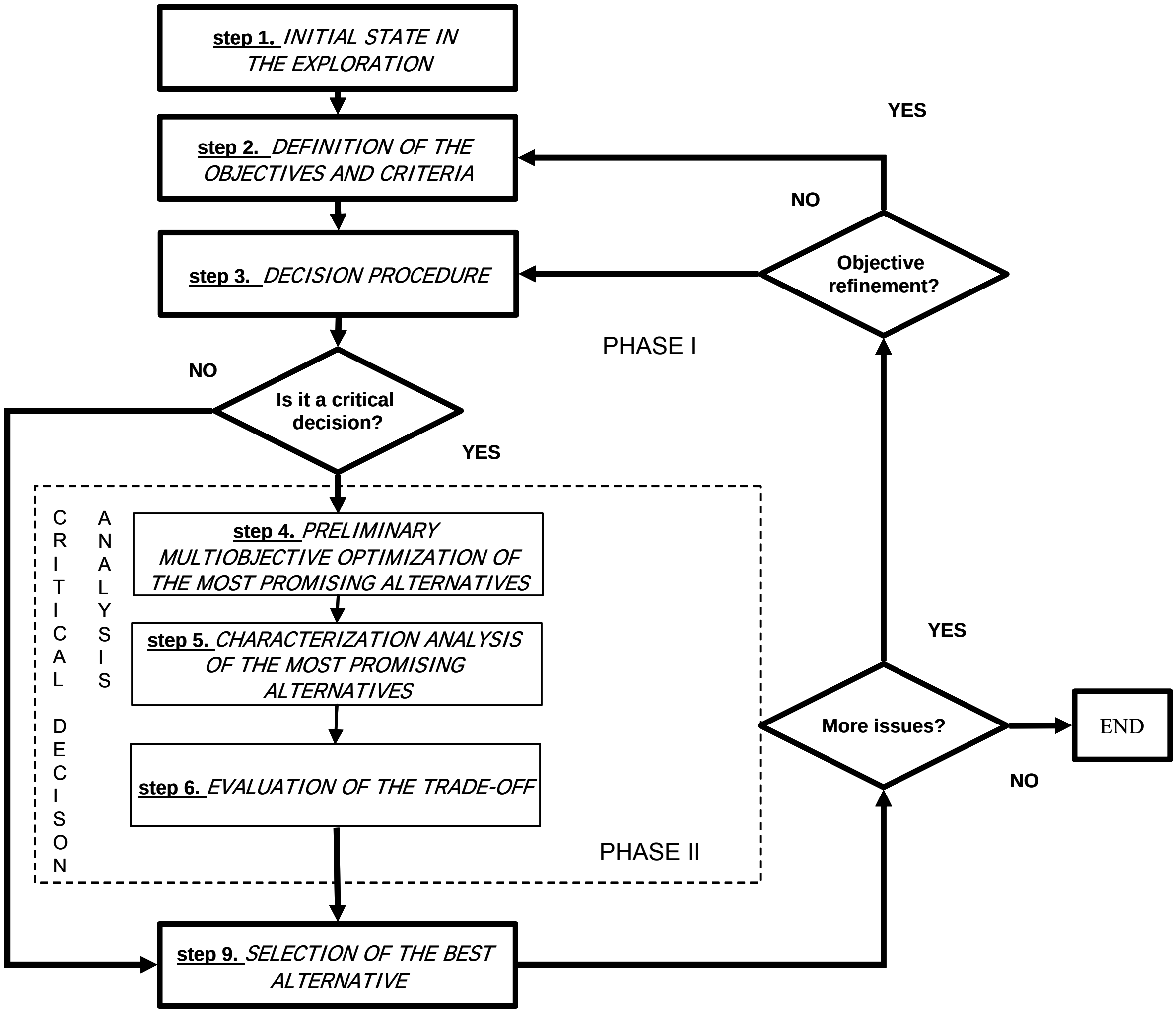


Figure 5.1. Flow diagram of the second block of the conceptual design method (see text for explanations).

Phase I. *Hierarchical* generation and *multicriteria* evaluation of design alternatives

In the first phase (*Steps 1-3*) the design alternatives are evaluated combining the *hierarchical* decision process (Douglas 1988, Smith 2005) with *multicriteria* decision analysis (Vincke, 1992; Belton & Stewart, 2002) techniques.

The design problem is reduced to a set of (Z) issues $[I = \{I_1,..,I_z\}]$ that follow a predefined order: reaction, separation and recycling. Next, the decision procedure involves different tasks such as the generation of the alternatives $[A = \{A_1,..., A_m\}]$, the definition of the objectives $[OBJ = \{OBJ_1,\ldots, OBJ_P\}]$ and the selection of the evaluation criteria $[X = \{X_1,\ldots, X_n\}]$ that are used to measure the degree of satisfaction of the defined objectives. **Table 4.1** summarizes the design objectives, criteria, criteria scales and the sources used to evaluate the different alternatives. The importance of each objective is set by its weight $[w = \{w_1,..., w_p\}]$, distributed among the evaluation criteria [X]. Each alternative under evaluation can be formulated as a vector of scores and represented as an n-dimensional performance score profile $[A_j = (x_{j,i},\ldots, x_{j,n})]$. Value functions [v (X_i)] map the score profiles of all alternatives into a value v$(x_{j,i})$ normalized from 0 to 1. Finally a multiobjective value function is calculated in the form of a weighted sum as stated in **equation 4.1.**

It is important to mention that although we made use of this methodology (*Step*s 1-3) to generate and evaluate the design alternatives, we could have applied other procedures, e.g. those proposed by Uerdingen *et al*. (2003) and Hoffman *et al*. (2003)

Phase II. Analysis of *critical decisions*

The focus of this chapter is on the second phase of the procedure and comprises *Steps 4, 5* and *6.* This second phase is considered only for those issues that are found to be *critical decisions*. By *critical decisions* we mean those with a great influence on the entire design process and with alternatives that satisfy the design objectives to a similar degree. In *Step 4* a preliminary multiobjective optimization is carried out to compare two or more alternatives when each is close to the optimum design conditions. Thus, we propose deferring a numerical optimization until we have selected the most *promising alternatives* and we are certain that we will proceed with the final design, i.e. when we attain a sufficient amount of accuracy to be able to address the next issue in the sequence of decisions, thereby allowing a more unbiased comparison. *Step 4* starts with the identification of those variables *[*$V = \{V_{j,1},..,V_{j,y}\}$*]* for the most *promising alternatives* identified previously (*Step 4.1*). A variable V_f for a given alternative A_j is represented as $V_{j,f}$. In *Step 4.2* the behaviour of the evaluation criteria [X] is investigated by varying by a small percentage (≈ ± 5-10%) the value of the variable being analysed with respect to the initial design conditions (base case). Finally, in *Step 4.3*, these variables are ranked hierarchically according to their impact (see **equation 5.1**) using the rank order parameter presented by Douglas *et al.* (1985).

$$\frac{\partial\, s\,(A_j)}{\partial V_{j,f}}\Delta \mathrm{V}_{\mathrm{j,f}} = \frac{\partial\left(\sum_{i=1}^{n} v(x_{j,i})\cdot w_i\right)}{\partial V_{j,f}}\Delta \mathrm{V}_{\mathrm{j,f}} \qquad \text{eq. 5.1}$$

The sensitivity of the process with respect to a variable V_f is calculated for each alternative $A_{j.,.}$ $\partial\, s\,(A_j) / \partial V_{j,f}$ are the components of the objective function gradient and $\Delta V_{j,f}$ is the scaling factor. The objective function (see **equation 5.1**) is maximized by following an evolutionary approach, i.e. by optimizing, one by one, the selected variables with respect to the design objectives and process performance. The use of local sensitivity values instead of global ones, e.g. Sobol (2000), is justified on two counts: (1) we are interested in studying the sensitivity of a base case design rather than the overall sensitivity of the models used, and (2) we want to avoid excessive computational time during the conceptual design stage. Thus, in our study the calculated optimal solution does not have to coincide with the global optimum.

In order to account for the different emphases that stakeholders place on various design objectives, a sensitivity analysis of their weights is performed in *Step 5*. Thus, the designer is provided with useful information such as: under which conditions each of the alternatives becomes the preferred one, which alternative is the best choice for the widest range of situations, and the identification of each alternative's strong and weak points. A design alternative A_j has a weak point ($x_{j,i*}$) when due to a low score in one or more evaluation criteria it does not sufficiently satisfy a given objective (OBJ_k). Conversely, an alternative has a strong point ($x_{j,i}^*$) when due to a good score in one or more evaluation criteria it satisfies a design objective. The identification of these points is carried out by combining sensitivity analysis and machine learning techniques. A sensitivity analysis of weights allows the study of the variation in the selected alternative when the relative importance of the design objectives within the region defined as feasible is changed. This is done by both recalculating the weighted sum and ranking the alternatives each time (*Step 5.1*). If a given alternative A_j needs a low weight value (w_k) of the objective OBJ_k in order to be selected, the alternative does not sufficiently satisfy OBJ_k, i.e. it has a weak point. Next, all the data generated are processed in *Step 5.2* and qualitative knowledge is extracted by means of classification trees and rules (Quinlan, 1993). This set of rules represents the relationships between the design objectives and the selected alternative and facilitates the interpretation of the multidimensional response surfaces that are generated during analyses. It simplifies the relationships between design objectives and the most *promising alternatives*. Thus, within the limits of the feasible region, it is possible to identify both the strong and weak points for each alternative when the weight of a given objective requires low and high values respectively.

In *Step 6*, there is an evaluation of the trade-off between the improvement of the criteria identified as weak points of the alternative and the loss of overall process performance. This evaluation is carried out combining dynamic simulation and qualitative knowledge. Qualitative knowledge is extracted in *Step 6.1* by classifying the effect of the analysed variables, V_f, on the evaluation criteria, $v(x_{j,i})$, into four different categories according to their trends: directly proportional, indirectly proportional, constant and non-monotonic. Next, the knowledge is codified as IF-THEN rules (*Step 6.2*) of the type "FOR decision I_I IF $V_{j,f}$ increases, THEN $v(x_{j,i})$ decreases". These rules are linked to an inference engine in order to maintain a record of the design decisions [I] together with the design variables [V] and the behaviour of the evaluation criteria [v(X)]. In *Step 6.3*, the rule-based system automatically searches the knowledge base constructed during *Steps 6.1* and *6.2* to propose a set of actions *[Ac = ($Ac_{1,1,1}$,…,$Ac_{m,n,y}$)]* aimed at improving the weak points of each alternative identified in *Step 5*. At the same time, the system alerts the designer to any negative implications in the event of the weak points' possible implementation. Next, this qualitative knowledge is combined with numerical models and the parameter $r_{j,i,f}$ is calculated (**equation 5.2**). This equation represents the rate of improvement in a weakly-satisfied criterion $x_{j,i*}$ in terms of the change in the objective function $s(A_j)$ when one of the decision variables $V_{j,f}$ is modified.

$$r_{j,i,f} = \frac{\left| \dfrac{\partial v(x_{j,i*})}{\partial V_{j,f}} \right|}{\left| \dfrac{\partial s(A_j)}{\partial V_{j,f}} \right|} \qquad \text{Eq. 5.2}$$

The higher the value of $r_{j,i,f}$, the higher the improvement in criterion X with a minimum variation in the overall optimum. The parameter $r_{j,i,f}$ is also a useful tool for guiding the direction of the design of the process because it provides a look-ahead capability and uncovers any hidden limitations in the plant's performance.

Finally, in *Step 9* and based on the information generated during phases I and II, the designer can be more confident of selecting the best alternative from among the most *promising alternatives*. The same procedure is applied to solve each new *critical decision* that arises until the design of the WWTP is completed. Note that objectives are not fixed and can evolve through time, thus allowing a refinement of the initial design objectives as shown in **Figure 5.1**

5.2. CASE STUDY # 3: REDESIGN OF A NITROGEN REMOVAL WWTP TO ACHIEVE SIMULTANEOUS ORGANIC CARBON, NITROGEN AND PHOSPHORUS REMOVAL

The redesign of an activated sludge plant to achieve simultaneous carbon, nitrogen and phosphorus removal is used to illustrate the capabilities of the proposed procedure. Each of the steps in the procedure, together with numerical details, is described and discussed in the following sections.

5.2.1. *Steps 1* & *2*. Initial state in the exploration and definition of design objectives and criteria

The activated sludge plant to be redesigned is the Benchmark Simulation Model plant No. 1 (the schematic representation of the plant can be found in **Chapter 4** (**Figure 4.7**). As previously noted, the benchmark simulation model is a standardized simulation and evaluation example that includes plant layout, simulation models, model parameters and a detailed description of the disturbances to be applied during the testing and evaluation of criteria to check the relative effectiveness of control strategies in activated sludge plants (Copp, 2002). The plant is a predenitrifying system with a modified Ludzack-Ettinger configuration comprising five reactors in series. Tanks 1 (ANOX1) and 2 (ANOX2) are anoxic with a total volume of 2000 m^3, while tanks 3 (AER1), 4 (AER2) and 5 (AER3) are aerobic with a total volume of 3999 m^3. Tanks 5 and 1 are linked by internal recirculation. Finally, there is a secondary settling tank (with a volume of 6000 m^3) and two PI control loops. The first loop controls the dissolved oxygen (DO) in the third aerobic tank (AER3) by the manipulation of the air flow rate (as K_La), and the second loop controls the nitrate level (NO) in the 2^{nd} anoxic tank (ANOX2) by manipulating the internal recycle flow rate (Q_{intr}).

In the aerobic section of the plant the organic matter and ammonia (ammonia is the common form of nitrogen in influent wastewater) is oxidized to carbon dioxide and nitrate. In the anoxic section the nitrate transported by the internal recirculation is reduced to nitrogen. This reduction requires an electron donor, which can be supplied in the form of influent wastewater organic matter, endogenous respiration or an external carbon source.

The average dry weather wastewater to be treated has a flow rate of 18500 $m^3 \cdot day^{-1}$ with an organic, nitrogen and phosphorus load of 7031 kg $COD \cdot day^{-1}$, 971 kg $N \cdot day^{-1}$ and 231 kg $P \cdot day^{-1}$ respectively, and is proposed by Gernaey and Jorgensen (2004). The plant is designed to remove organic carbon and nitrogen, although its denitrification efficiency is very low. Also, since it is located in a sensitive area, it has to remove phosphorus before the water is discharged into the environment. **Figure 5.2** shows both dynamic influent profiles for organic matter, solids and nutrients.

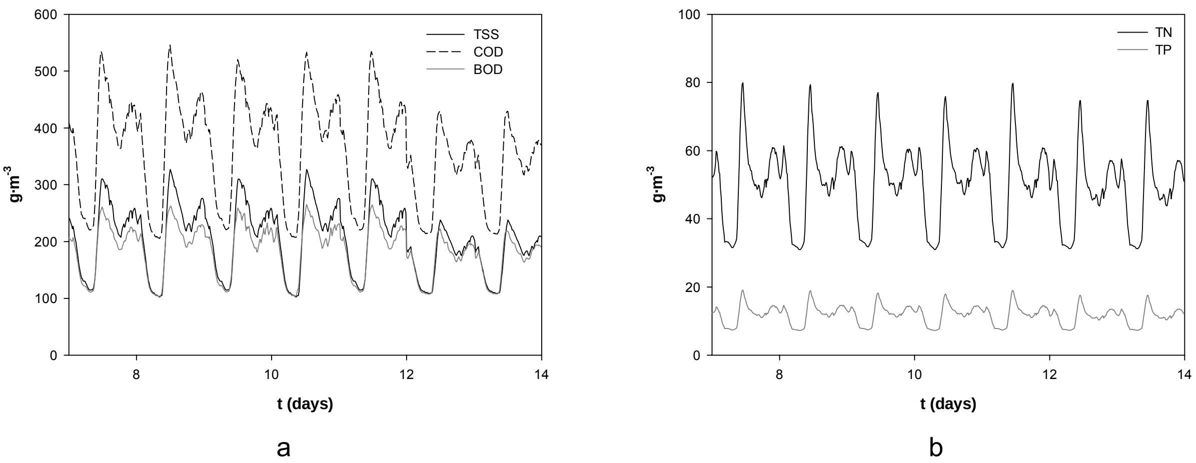


Figure 5.2. Influent wastewater organic matter (COD and BOD_5) and TSS a) and nutrients (N,P) profile.

Finally, the redesign budget is restricted to an investment of $3 \cdot 10^6$ € and operating costs of $1 \cdot 10^6$ €$\cdot$year^{-1} but there is no limitation on land occupation. **Table 4.1** (**Chapter 4**) shows the design objectives and the criteria used to measure their satisfaction. Different weight factors are assigned to each objective by the experts/designer according to relative importance. As weight assessment is not a central issue of this thesis, equal importance for the four design objectives is assumed in the case study; thus, $w_p = 0.25$.

5.2.2. *Step 3*. Decision procedure

The decision procedure starts with the identification of the issues to be resolved. The *hierarchical* decision process determines the direction of the design process by fixing the order of all the issues that arise during redesign, starting with the reaction section. Once all the issues relating to the reactor section are resolved, the design continues with the separation and finally the recirculation sections. *Multicriteria* analysis allows that the simultaneous consideration of several objectives is used as an evaluation method throughout the decision procedure.

5.2.2.1. *Steps 3.1, 3.2 & 3.3*. Identification of the issues to be resolved, generation of the alternatives and selection of criteria

The first issue (I_1, I=1) in the reaction section is the reaction path for phosphorus removal. The removal of phosphorus from wastewater is possible via biological or chemical treatment. In biological phosphorus removal, excess P is incorporated into the cell biomass, which is then removed from the process as a result of sludge wasting. An anaerobic section (without oxygen and nitrates) is needed to promote anaerobic P release and to provide the phosphorus accumulating organisms (PAO) with a competitive advantage over other bacteria. Next, PAO organisms grow using intracellular storage products as a substrate during the anaerobic phase, with oxygen or nitrate as electron acceptors and consuming nitrogen and phosphorus as nutrients (Metcalf and Eddy, 2003). In chemical phosphorus removal, the phosphorus in the influent wastewater is precipitated by the addition of a metal salt, and subsequently removed from the mixed liquor with the sludge in the sedimentation tank (Metcalf and Eddy, 2003).

Three modifications to the original reactor (m = 3) are considered in order to resolve this issue: (A_1) biological phosphorus removal with a preliminary 2000 m^3 anaerobic tank (with a hydraulic residence time of 2.6 hours); (A_2) chemical phosphorus precipitation with iron salts in the third aerobic reactor, with a constant dosage of (Q_{met}) 0.75 $m^3 \cdot day^{-1}$; and (A_3) a hybrid solution with partial biological phosphorus removal (using a 2000 m^3 preliminary anaerobic tank) enhanced with chemical precipitation in the third aerobic reactor (constant dosage of 0.65 $m^3 \cdot day^{-1}$).

In turn, a set of 12 criteria (n = 12) is selected from **Table 4.1** to evaluate the alternatives generated for the first issue (I_1) in the *hierarchy* of decisions: X_1 (impact on water), X_2 (construction costs), X_3 (operating costs), X_4 (robustness), X_5 (flexibility), X_6 (control performance), X_7 (risk of microbiology-related solids separation problems) and X_8 –X_{12} (time in violation).

5.2.2.2. *Step 3.4* Evaluation of the alternatives

In this step, criteria X_1, X_3-X_{12} are quantified by dynamic simulation, while X_2 is evaluated by cost estimations. Simulations are performed using the MatLab-Simulink® environment. Reactors are modelled as a series of continuous stirred tank reactors. The International Water Association activated sludge model number 2d (IWA ASM2d) was chosen as the biological process model (Henze *et al*., 1999). The ASM2d has 19 state variables and describes (bio)chemical phosphorus removal with simultaneous nitrification and denitrification processes in activated sludge systems by means of a set of non-linear differential equations. The double-exponential settling velocity function of Takács *et al*. (1991), based on the solid flux concept, was selected as a fair representation of the settling process, using a 10 layer discretization. Default values at 15°C for kinetic and stoichiometric parameters are used, except for phosphorus precipitation kinetics which are adjusted (Gernaey *et al*., 2002). The settling parameters used are reported by Copp (2002) although the authors are aware that these parameters were initially selected for a classical activated sludge and the floc characteristic may have different characteristics in a chemically precipitated reactor.

Two automatic control loops are included in the plant: (1) a dissolved oxygen control (DO) in the third aerobic reactor manipulating the aeration transfer with a set point of 2 g (-COD)$\cdot m^{-3}$ (Kp = 500 m^3/d/g (-COD)/m^3), Ti = 0.005 d) and (2) an internal recirculation flow control to ensure a nitrate concentration (NO) in the second anoxic reactor of 1 g N$\cdot m^{-3}$ (Kp = 15000 m^3/d/(g N/m^3), Ti = 0.05 d). The DO sensor is assumed to be ideal, with no delay or noise, unlike the NO sensor which has a time delay of 10 minutes, with white, normally distributed and zero mean noise (standard deviation of 0.1 g$\cdot m^{-3}$). Further details abut the controllers can be found in **Table 4.6.**

External recirculation, waste flow and aeration flow in the first (AER1) and second (AER2) aerobic reactors are constant and their respective values are 18446 (Q_r), 385 $m^3 \cdot day^{-1}$(Q_w) and 240 day^{-1} (K_La-3 and K_La-4).

The procedure follows a steady state simulation; this ensures a consistent initial point and eliminates the bias due to the selection of the initial conditions in the dynamic modelling results (Copp, 2002). Even though the length of the influent used to carry out the simulations is of 28 days, only the data generated during the last seven days are used to quantify the criteria.

MatLab-Simulink® is used to calculate construction costs, which are estimated using the CAPDET model (US EPA, 1982). Default parameters for unit costs (excavation, concrete walls, concrete slabs, handrails, etc.), equipment (5 hp vertical mixer) and construction labour rates are used for the cost estimations.

As previously noted, it is important to emphasise that the results of the quantified criteria depend heavily on the model selection. When modelling activated sludge plants, there is a lack of agreement on the best model to apply to a given case. The representation of biomass decay (Gernaey and Jørgensen, 2004), the modelling of phosphorus removal (Gernaey and Jørgensen, 2004; Van Veldhuizen *et al*., 1999; Henze *et al*., 1999; Rieger *et al*., 2001) and the oversimplification of the settling models (i.e. non reactive in most cases, despite the fact that a significant amount of biomass is often stored at the bottom of the secondary clarifier) (Gernaey *et al*., 2006) are issues still under discussion.

Once the criteria are quantified, we obtain the score profile for each design alternative considered. The score profiles are presented in **Table 5.1.** Also note that in this case study X_8, X_9 and X_{10} have the same values, so they are not useful for discriminating between competing alternatives. It must be pointed out that an enhancement of both the analysis and interpretation of the results could be carried out using the *multivariate* based methodology presented in **Chapter 6** of this thesis.

Table 5.1. Score profiles for alternatives generated in the third case study.

OBJ_K	$x_{j,i}$	A_1	A_2	A_3	UNITS
OBJ_1	$x_{j,1}$	82.03	80.88	82.16	%
OBJ_2	$x_{j,2}$	770520	165000	920370	€
	$x_{j,3}$	846000	991300	909960	€·year^{-1}
OBJ_3	$x_{j,4}$	15.92	21.32	16.79	-
	$x_{j,5}$	10.48	15.01	11.72	-
	$x_{j,6-1}$	2.7310^{-6}	0.00025357	$3.11 \cdot 10^{-6}$	(g (-COD)·m^{-3})^2·day
	$x_{j,6-2}$	0.78	0.78	0.71	(g N·m^{-3})^2·day
	$x_{j,7-1}$	84.91	73.85	89.24	%
	$x_{j,7-2}$	48.08	37.48	53.05	%
	$x_{j,7-3}$	64.69	85.00	68.31	%
OBJ_4	$x_{j,8}$	0.00	0.00	0.00	%
	$x_{j,9}$	0.00	0.00	0.00	%
	$x_{j,10}$	0.00	0.00	0.00	%
	$x_{j,11}$	90.18	100.00	89.14	%
	$x_{j,12}$	29.32	0.00	5.65	%

To compare the effects of different variables on the design, the results have to be normalized. Each criterion in the competing alternatives is normalized between 0 and 1 by means of value functions $v(X_i)$. These functions award values of 0 and 1 to the worst and the best situations considered, whilst a mathematical function is proposed to evaluate intermediate effects. The extreme profiles (based on expert judgment) for the criteria used in this case study are summarized in the following lines:

$[(x_{i*}) = (x_{1*}= 0\ \%, x_{2*}= 3\cdot10^6\ €, x_{3*}= 1\cdot10^6 €\cdot year^{-1}, x_{4*}= 0, x_{5*}=0, x_{6\text{-}1*}= 1\ (g(\text{-}COD)\cdot m^{-3})^2\cdot day, x_{6\text{-}2*}=1\ gNm^{-3})^2\cdot day, x_{7\text{-}1*}= 100\ \%, x_{7\text{-}2*}= 100\ \%, x_{7\text{-}3*}= 100\ \%, x_{8*}= 100\ \%, x_{9*}= 100\ \%, x_{10*}= 100\ \%, x_{11*}= 100\ \%, x_{12*}= 100\ \%))\ ]$

and

$[(x_i^*) = (x_1^*= 100\ \%, x_2^*= 0\ €, x_3^*= 7\cdot10^5 €\cdot year^{-1}, x_4^*= 20, x_5^*= 20, x_{6\text{-}1}^*= 0\ (g(\text{-}COD)\cdot m^{-3})^2\cdot day, x_{6\text{-}2}^*=0\ gNm^{-3})^2\cdot day, x_{7\text{-}1}^*= 0\ \%, x_{7\text{-}2}^*= 0\ \%, x_{7\text{-}3}^*= 0\ \%, x_8^*= 0\ \%, x_9^*= 0\ \%, x_{10}^*= 0\ \%, x_{11}^*= 0\ \%, x_{12}^*= 0\ \%))\ ]$

Next, a linear model between these extreme values is applied to calculate the intermediate effects (e.g. for criterion X_1 the value function is: $v(X_1) = 0.01\cdot X_1$).

Finally, a weighted sum (**equation 4.1**) is worked out in order to obtain a single value for all the alternatives, which are then ranked according to the scores obtained, with the final decision resting with the process designer. The results reported in **Table 5.2** lead us to conclude that in accordance with the design objectives, biological phosphorus removal (A_1) with a score of 0.69 and chemical phosphorus precipitation (A_2) with a score of 0.65 are so close together that in practice they can be considered the same, while the alternative A_3 (hybrid system) with a score of 0.63 is marginally rejected. As mentioned above, it is important to note that the scores of the first and second alternatives shown in **Table 5.2** are so similar that in practice they can be considered equivalent. However, the configurations have completely different implications for the resulting plant structure and operation.

Table 5.2. Normalized values, weights and scores obtained for the three generated alternatives.

OBJ_K	$v(x_{j,i})$	A_1	A_2	A_3	w_i
OBJ_1	$v(x_{j,1})$	0.82	0.81	0.82	0.25
OBJ_2	$v(x_{j,2})$	0.23	0.83	0.70	0.075
	$v(x_{j,3})$	0.51	0.03	0.19	0.175
OBJ_3	$v(x_{j,4})$	0.80	1.00	0.84	0.063
	$v(x_{j,5})$	0.55	0.79	0.59	0.063
	$v(x_{j,6\text{-}1})$	1.00	1.00	1.00	0.031
	$V(x_{j,6\text{-}2})$	0.22	0.22	0.29	0.031
	$v(x_{j,7\text{-}1})$	0.15	0.26	0.11	0.021
	$v(x_{j,7\text{-}3})$	0.52	0.63	0.47	0.021
	$v(x_{j,7\text{-}3})$	0.33	0.15	0.32	0.021
OBJ_4	$v(x_{j,8})$	1.00	1.00	1.00	0.05
	$v(x_{j,9})$	1.00	1.00	1.00	0.05
	$v(x_{j,10})$	1.00	1.00	1.00	0.05
	$v(x_{1,11})$	0.10	0.00	0.11	0.05
	$v(x_{j,12})$	0.71	1.00	0.94	0.05
$\sum_{i=1}^{n} v(x_{j,i})\cdot w_i$		**0.69**	**0.65**	**0.63**	**1**

It is important to point out that the criticality of a decision is not "black and white", but it has degrees and it can not be defined as a simple difference between the scores obtained by the generated alternatives. Many times the final decision will rely on the decision maker experience. Alternatives A_1, A_2 and A_3 present similar scores in terms of degree of satisfaction of design objectives, however just biological and chemical phosphorus removal are different enough to make the analysis worthwhile. If alternative A_1 was selected, the next issue to be resolved would include a modification in the location of the anaerobic reactor, and the inclusion (or not) of an additional internal recycle (Metcalf and Eddy, 2003). In contrast, if the alternative selected was A_2, the next issues to be resolved would be related to the dosage point (Metcalf and Eddy, 2003) and the increase in the secondary settling area (Metcalf and Eddy, 2003). Thus, the first issue in the hierarchy is considered a *critical decision* and requires a more detailed analysis to ensure the selection of the best alternative.

5.2.3. *Step 4.* Preliminary multiobjective optimization

5.2.3.1. *Step 4.1*. Selection of the design/operating variables

For the first alternative (A_1), five variables were selected: anaerobic volume ($V_{1,1}$), waste flow ($V_{1,2}$), external recirculation flow ($V_{1,3}$), DO set point ($V_{1,4}$) and NO set point ($V_{1,5}$). For the second alternative (A_2), the variables were: metal flow ($V_{2,1}$), waste flow ($V_{2,2}$), external recirculation flow ($V_{2,3}$), DO set point ($V_{2,4}$) and NO set point ($V_{2,5}$). A sensitivity analysis was carried out for both alternatives to determine the most sensitive parameters.

5.2.3.2. *Step 4.2*. Sensitivity analysis of the design/operating variables

The first variable to analyse for alternative A_1 (biological phosphorus removal) is the anaerobic volume ($V_{1,1}$). As stated previously, this value varies from -10% (1800 m^3) to +10% (2200 m^3) around its base case value (2000 m^3), simulating eight additional scenarios, although only four are shown in **Table 5.3.**

Table 5.3. Sensitivity Analysis and criteria recalculation for alternative A_1 and variable $V_{1,1}$

	$V_{1\text{-}1}$	-10% 1800	-5% 1900	0 2000	+5% 2100	+10% 2200	Units m^3
OBJ_1	$x_{1.1}$	81.43	81.84	82.03	82.00	81.76	%
OBJ_2	$x_{1.2}$	741160	747250	770520	859500	869600	€
	$x_{1.3}$	855000	849000	846000	848000	853000	€·$year^{-1}$
OBJ_3	$x_{1.4}$	17.03	16.49	15.92	15.83	15.65	-
	$x_{1.5}$	11.68	11.17	10.48	9.83	8.77	-
	$x_{1.6\text{-}1}$	$3.77\cdot10^{-6}$	3.2610^{-6}	2.7310^{-6}	2.1510^{-6}	1.6510^{-6}	(g (-COD)·$m^{-3})^2$·d
	$x_{1.6\text{-}2}$	0.88	0.82	0.78	0.75	0.74	(g N·$m^{-3})^2$·d
	$x_{1.7\text{-}1}$	84.49	84.61	84.91	85.37	85.93	%
	$x_{1.7\text{-}2}$	47.56	47.73	48.08	48.56	49.14	%
	$x_{1.7\text{-}3}$	68.44	66.85	64.69	62.08	59.03	%
OBJ_4	$x_{1.8}$	0.00	0.00	0.00	0.00	0.00	%
	$x_{1.9}$	0.00	0.00	0.00	0.00	0.00	%
	$x_{1.10}$	0.00	0.00	0.00	0.00	0.00	%
	$x_{1.11}$	82.89	85.71	90.18	93.90	95.39	%
	$x_{1.12}$	62.65	51.94	29.32	11.61	6.85	%

The representation of the % of variation with respect to the initial value when it is decreased and increased is depicted in **Figure 5.3a** and **b** respectively.

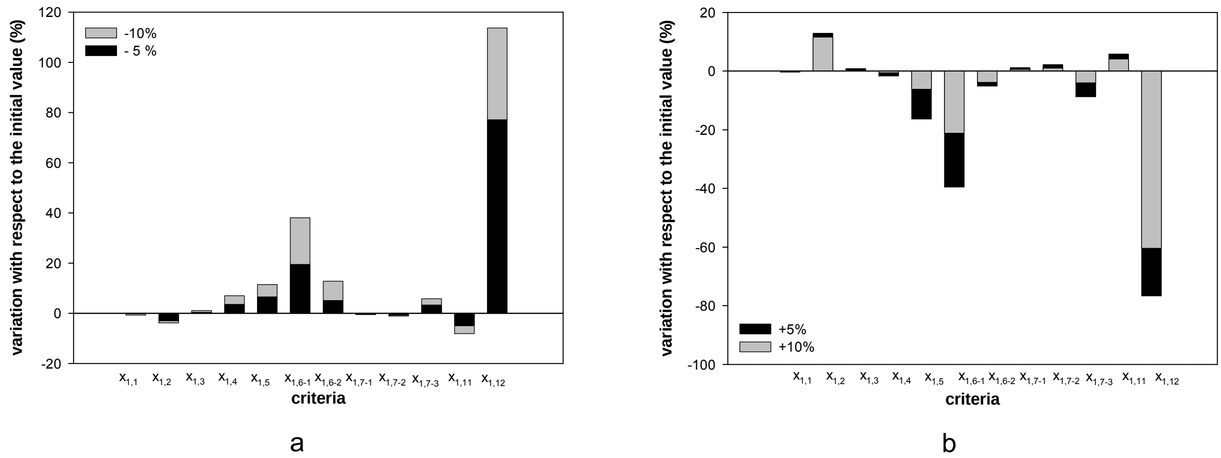


Figure 5.3. Variation of the evaluation criteria ($x_{1,i}$) when the initial value of the anaerobic volume ($V_{1,1}$) is decreased (a) and increased (b) respectively.

From the results generated in the previous analysis, we can conclude that if the volume increases, the construction costs ($x_{1,2}$), bulking risk ($x_{1,7\text{-}2}$) and TIV for TN ($X_{1,11}$) also increase as shown in **Figure 5.3b**. Criterion $x_{1,2}$ increases with volume because a higher volume implies higher earthwork, concrete slab and concrete wall costs (see **equation A5.5**). This volume enlargement implies a proliferation of PAOs, a subsequent increase in biomass and reduction in BOD_5 in the reactor section; this in turn causes a reduction in the F/M ratio and thus an increased risk of bulking, as the knowledge flow diagram in **A4.1** of the previous chapter shows. In addition, an anaerobic volume enlargement implies a decrease in the plant's nitrification capacity, which results in lower production of nitrate nitrogen to be denitrified in the anoxic reactors, and as a consequence a decreased overall nitrogen removal efficiency (see **Figure 5.4**).

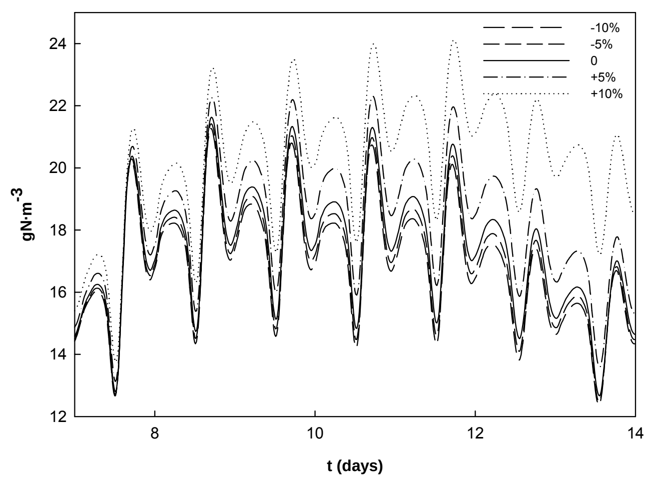


Figure 5.4. Evolution of the total nitrogen concentration in the effluent for the different scenarios: alternative A_1 analysing the variable ($V_{1,1}$).

This decrease in nitrification capacity is attributed to a major decay of autotrophic bacteria due to the additional anaerobic volume. Nevertheless, experimental observations (Siegrist *et al.,* 1999) suggest that the decay rate is electron acceptor dependent and thus different under anaerobic, anoxic and aerobic conditions. As a result, a lower effluent ammonium concentration should be expected. This knowledge is included in more recent activated sludge models e.g. ASM3 (Gujer *et al.,* 1999) and in modifications of the original ASM2d model (Gernaey and Jorgensen, 2004). On the other hand, this volume enlargement causes a reduction in the robustness ($x_{1,4}$), flexibility ($x_{1,5}$), nitrate control performance ($x_{1,6}$), rising risk ($x_{1,7\text{-}3}$) and TIV for TP ($x_{1,12}$) criteria. Surprisingly, this implies a reduction in the ability of the plant to adapt to short term variations, e.g. rain and storm events and nitrogen and phosphorus impacts, and long term variations, e.g. step increase of flow, nitrogen and phosphorus, although one would expect the opposite. This is attributable, as previously noted, to an increased autotrophic decay rate at bigger anaerobic volumes, provoking poorer overall nitrogen removal and a major variation in the effluent quality term used to quantify both robustness and flexibility (Flores *et al*., 2006; Vanrolleghem and Gillot, 2002).

With respect to nitrate control performance, the controller works better with a larger anaerobic reactor because more organic matter is consumed in the anaerobic section for PAOs to form organic cell products. There is also a lower variation in the BOD_5 arriving in the anoxic section, thus facilitating the maintenance of the desired set point and making it easier for the controller to compensate for the situation. The decrease in nitrification capacity caused by the increase in volume of the anaerobic section produces a reduction in the nitrogen (nitrate) that is recycled from the last aerobic reactor to the sedimentation tank, resulting in a decrease in the rising risk. The nitrate in the secondary settler is sent to the first anaerobic reactor via the sludge recycle loop. The presence of lower nitrate concentrations in the anaerobic reactor results in a less pronounced inhibition of the P release, because the organic matter entering the plant is used preferentially for the build-up of cell internal products instead of for denitrification, thus improving the overall phosphorus removal (**Figure 5.5**).

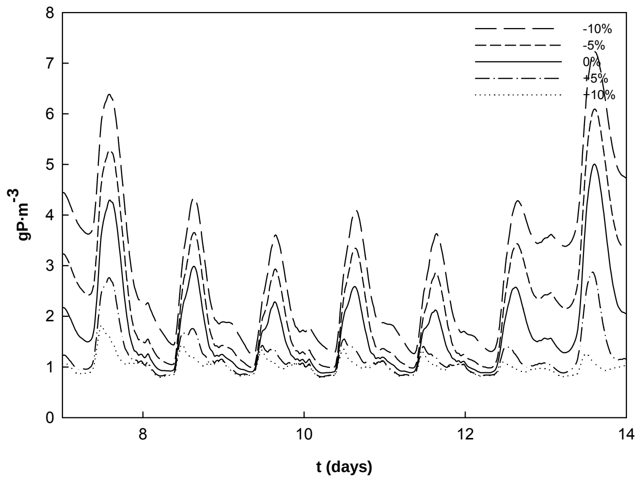
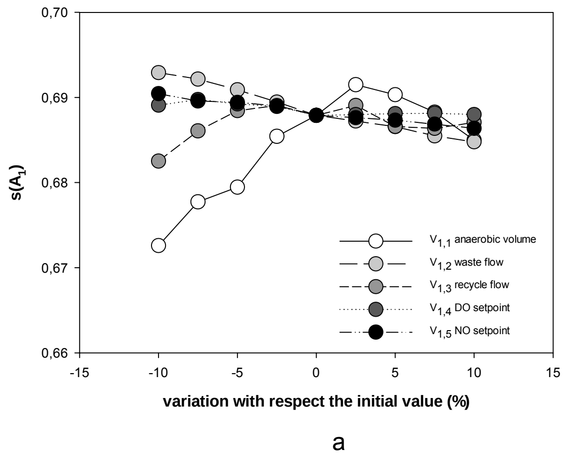


Figure 5.5. Evolution of the total phosphorus concentration in the effluent for the different scenarios: alternative A_1 analysing the variable ($V_{1,1}$).

Criteria $x_{1,1}$ and $x_{1,3}$ have a maximum and a minimum value when the anaerobic volume is 2050 and 2000 m^3 respectively (results not shown). For criterion $x_{1,3}$, there is a higher consumption of electricity due to pumping (PE) and mixing (ME) if the anaerobic volume is increased, but if this volume is reduced there is a higher consumption of electricity due to aeration energy (AE) and an increase in the fines to be paid for the pollutants discharged (EQ). Finally, with respect to criterion $x_{1,1}$, if $V_{1,1}$ is reduced by -10% or increased by +10%, there is either a drop in phosphorus or nitrogen removal, respectively, and a consequent decrease in overall pollution removal efficiency.

Finally, **equation 5.1** is used to determine which variables have more impact on process performance: the higher the improvement in the multiobjective function, the more impact the variable has. These variables, listed in decreasing order of impact, are $V_{1,2}$, $V_{1,1}$, $V_{1,5}$, $V_{1,4}$ and $V_{1,3}$ for alternative A_1 and $V_{2,1}$, $V_{2,4}$,$V_{2,5}$ $V_{2,2}$ and $V_{2,3}$ for alternative A_2. The impact on process performance is calculated by a weighted sum using the same procedure as described in phase I (see **equation 4.1**) with an improvement in the objective function of 0.73%, 0.52%, 0.37%, 0.27%, 0.17% for the first alternative and 1.16%, 0.26%, 0.13%, 0.03% and 0.001% for the second alternative. **Figure 5.6** shows the sensitivity of the objective function for alternative A_1 with respect to the selected variable. In the following step the variables are optimized in the order of their impact.



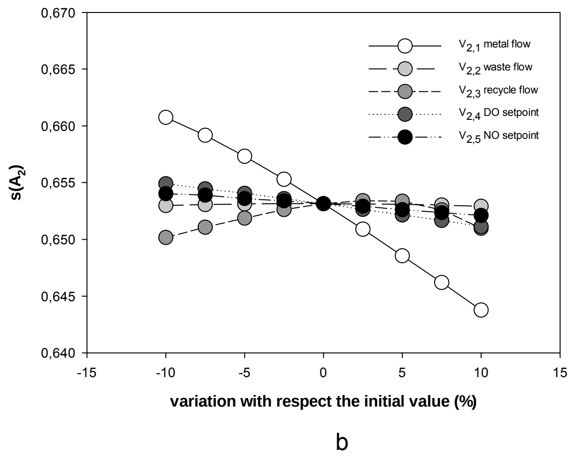


Figure 5.6. Variation of the multiobjective function $s(A_j)$ for the first (a) and the second (b) alternative respectively

5.2.3.3. *Step 4.3*. Optimization of the design/operating variables

As for the sensitivity analysis, the multiobjective function is a weighted sum (**equation 4.1**). The optimized values for each manipulated variable are found through a series of optimization runs at intervals of (± 2.5%) until the optimum is reached. **Table 5.4** is a comparison of the base case values with the optimized variables for the competing alternatives.

As the analysis of all the optimization parameters would require a lengthy discussion, only one variable for alternative A_2 is presented and discussed below.

Variable $V_{2,4}$ (DO set point) is the chosen optimization parameter for alternative A_2 after the second evolution with an accumulative improvement in the multiobjective function of +2.57%. The relative improvements for $V_{2,1}$ and $V_{2,4}$ were +1.35% and +1.20% respectively.

Table 5.4. Optimum values for the most *promising alternatives* (A_1 and A_2).

Design/operating variable	Initial value	Best value	Units
$V_{1,2}$	385	259.87	$m^3 \cdot day^{-1}$
$V_{1,5}$	1	1	$g\ N \cdot m^{-3}$
$V_{1,1}$	2000	2200	m^3
$V_{1,4}$	2	2	$m^3 \cdot day^{-1}$
$V_{1,3}$	18446	18908	$g\ (-COD) \cdot m^{-3}$
$V_{2,1}$	0.75	0.6	$m^3 \cdot day$
$V_{2,5}$	1	0.45	$g\ N \cdot m^{-3}$
$V_{2,2}$	385	385	$m^3 \cdot day^{-1}$
$V_{2,4}$	2	1.2	$g\ (-COD) \cdot m^{-3}$
$V_{2,3}$	18446	18446	$m^3 \cdot day^{-1}$

Figure 5.7 presents the variation in design objectives for alternative A_2 for different values of the analysed variable. In addition, it can be seen how the DO set point in the reactor decreases from a value of 2 to 1.2 g·(-COD) m^{-3}. A reduction in the DO set point implies an improvement in the objective function of +1.19% with respect to the previous evolution, and a total optimization improvement of +3.38%.

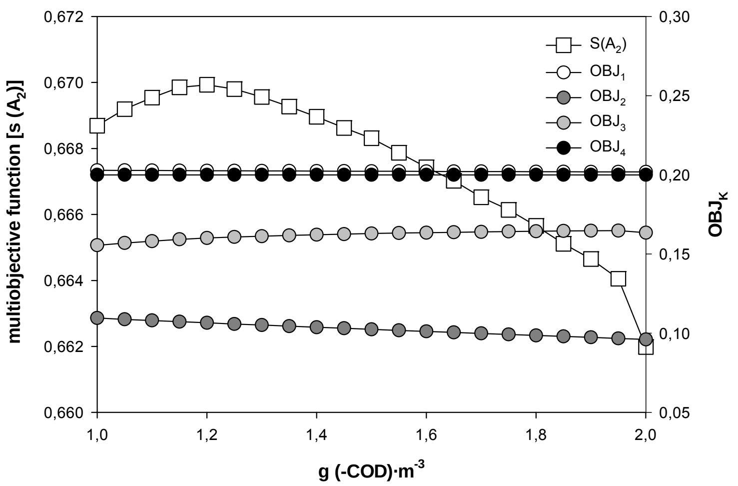


Figure 5.7. Evolution of the different design objectives and the multiobjective function $s(A_2)$.

As expected from the sensitivity analysis, a reduction in the oxygen set point causes an overall reduction in operating costs ($x_{2,3}$) due to aeration energy savings (AE), although pumping energy (PE) is increased (see the decrease in OBJ_2 satisfaction in **Figure 5.7**). The increase in PE can be explained by the reduction of the nitrate concentration in the last aerobic reactor, a consequence of reduced nitrification efficiency. This fact explains the negative effect on $x_{2,1}$ (impact on water) where, as the DO set point increases, the quantity of oxygen that returns with both recirculation and recycling also increases, thereby inhibiting the denitrification process and increasing the risk of rising (see OBJ_1, OBJ_3 and OBJ_4 in **Figure**

5.7). The simulation results show the existence of an interaction between the two control loops: the higher the nitrate concentration in the aerobic reactor, the lower the volume of mixed liquor that has to be pumped via the internal recirculation to maintain the nitrate set point. Also, it is important to mention the failure in plant disturbance rejection, directly correlated with the lowering of control performance. Thus we can conclude that it is more desirable to adopt a set point of 1.2 g (-COD).m^{-3}. The third variable to optimize was $V_{2,5}$ with a gain in the value function of +0,59 % with respect to the previous evolution, while there was no improvement for $V_{2,2}$ and $V_{2,3}$.

The differences between the optimized configurations and the base case are summarized in **Table 5.5**. The objective function increases by +2.75% and +3.18% respectively. For alternative A_1 the most important contribution comes from variable $V_{1,2}$ (+1.57%). In contrast, alternative A_2 shows a higher impact on the value function (+3.18%), mainly due to the optimization of metal flow (V_{2-1}). The new score profiles for alternatives A_1 and A_2 are summarized in **Table 5.5** and can be compared with the originals in **Table 5.2.**

Table 5.5. Score profiles for the most *promising alternatives* once optimized.

OBJ_K	$x_{j,i}$	A_1	A_2	UNITS
OBJ_1	$x_{j,1}$	82.65	80.41	%
OBJ_2	$x_{j,2}$	869600	137860	€
	$x_{j,3}$	823550	962630	€·year^{-1}
OBJ_3	$x_{j,4}$	15.01	20.11	-
	$x_{j,5}$	10.21	13.39	-
	$x_{j,6-1}$	$4.94\cdot10^{-6}$	$1.39\cdot10^{-3}$	(g(-COD)·m^{-3})^2·day
	$x_{j,6-2}$	0.48	0.46	(gN·m^{-3})^2·day
	$x_{j,7-1}$	92.51	74.67	%
	$x_{j,7-2}$	89.63	37.59	%
	$x_{j,7-3}$	75.76	87.71	%
OBJ_4	$x_{j,8}$	0.00	0.00	%
	$x_{j,9}$	0.00	0.00	%
	$x_{j,10}$	0.00	0.00	%
	$x_{j,11}$	71.58	100.00	%
	$x_{j,12}$	20.39	0.00	%

5.2.4. *Step 5*. Characterization analysis of the most *promising alternatives*

In this step a sensitivity analysis with respect to the criteria weights is performed for the four design objectives. Its purpose is to enable understanding of the effect of the stakeholders' preferences with regard to the design space. Thus, the designer is provided with information about the preferred design alternative for the widest range of situations, and at the same time is informed about the strong and weak points of each alternative.

5.2.4.1. *Step 5.1*. Weight sensitivity analysis

The weighted sum is recalculated varying the value of each weight within a feasible range defined as 10% of its initial value (with a 5% interval). Following this procedure the alternatives are ranked again.

5.2.4.2. *Step 5.2*. Classification tree generation and extraction of rules

All the data generated in *Step 5.1* are processed and a set of rules is extracted using classification trees (Quinlan, 1993). The classification tree predicts the value of a discrete dependent variable (in this case the selected alternative) based on the values of a set of independent variables (in this case the values of the evaluation weights, within the limits fixed previously). The classification tree is generated by the algorithm C4.5 (Quinlan, 1993) using the WEKA® software package. All the parameters for the tree induction were left at their default value. **Figure 5.8** shows the representation of the classification tree generated.

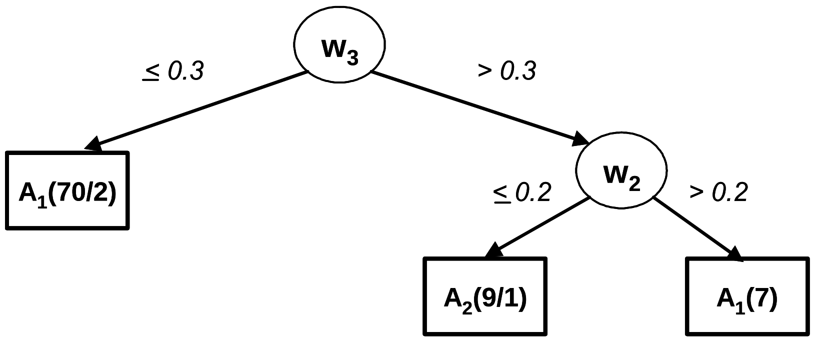


Figure 5.8. Classification tree generated with the data matrix generated during the weight sensitivity analysis.

Thus, a set of four rules is extracted from a data set of 86 samples using four continuous variables (the weights w_1, w_2, w_3 and w_4) that predict if the selected alternative is to be A_1, A_2 or A_3. These rules classify 96.22% of the cases properly, which is a fairly good predictive capability. This set of rules and the correct/incorrect number of classified instances are summarized as follows.

R_1: IF $w_3 \leq 0.30$ THEN the selected alternative would be A_1. [70/2].

R_2: IF $w_3 > 0.30$ and $w_2 \leq 0.2$ THEN the selected alternative would be A_2. [9/1].

R_3: IF $w_3 > 0.30$ and $w_2 > 0.2$ THEN the selected alternative would be A_1. [7].

As can be seen in R_1 and R_3, A_1 is the favoured alternative for the widest range of situations. From rules R_2 and R_3 it can be seen that when OBJ_3 is favoured the selected alternative would be A_2 unless OBJ_2 is prioritized. A_1 would be the selected alternative despite the construction costs (see **Table 5.5**). Moreover, from rule R_1 can be seen that A_1 would be the selected alternative if w_1, w_2 and w_4 had a high value and w_3 a low value because the weight of the objectives is normalized to sum 1 - i.e. the lower the weight of OBJ_3, the higher the weights of both OBJ_1, OBJ_2 and OBJ_4 in order to accomplish $\sum_{k=1}^{P} w_k = \sum_{i=1}^{W} w_i = 1$

These rules can be explained in terms of physical processes and their interaction. For example, alternative A_1 has the lowest operating costs because, as can be seen in the breakdown of the operating costs in **Figure 5.9**, it does not require the purchase of chemical products. Alternative A_2 presents the best technical characteristics and for this reason is selected when OBJ_3 is favoured (see rules R_3). This is mainly due to its low sensitivity to both short and long term perturbations. Sensitivities (S) to different short term (robustness) and long term (flexibility) perturbations are summarized in **Table 5.6**, where it can be seen that A_2 has the best values for most perturbations. This is because A_1 is more sensitive to influent conditions with respect to the removal of N and P (influent BOD_5), and it is subjected to major variations in comparison to A_2, where the removal of P is by precipitation. Moreover, this alternative favours the formation of floc organisms at the expense of filamentous bacteria. This behaviour can be attributed to a lower solids retention time (SRT) and a higher food to microorganism (F/M) ratio for this configuration.

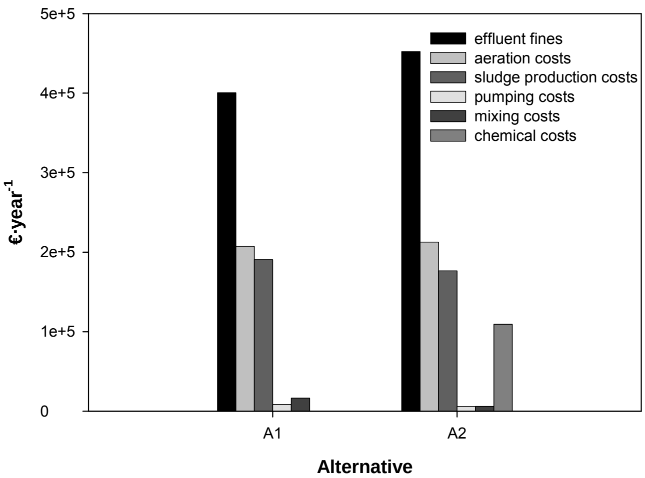


Figure 5.9. Breakdown of the operating costs (X_3) for the most *promising alternatives.*

On the other hand, A_2 achieves a lower overall pollution removal efficiency compared to A_1 as a result of an insufficient anoxic zone and a low biodegradable fraction in the influent organic matter. This inhibits the reduction of the nitrate produced in the aerobic section and, as a consequence, results in partial nitrogen removal. Nevertheless, a good performance in phosphorus removal ($x_{2,12}$ in **Table 5.5**) compensates for the low denitrification rate ($x_{2,11}$ in **Table 5.5**) because both pollutants have equal weights in **equation A.5.3** (criteria quantification section).

Table 5.6. Sensitivities to perturbations (S_i), calculation of the robustness (X_4) and flexibility (X_5) criteria.

	A_1	**A_2**
S_1 (rain event)	0.076899	0.098646
S_2 (storm event)	0.060716	0.087276
S_3 (nitrogen impact event)	0.016911	0.020277
S_4 (phosphorus impact event)	0.001663	0.0017672
$X_4 = \dfrac{1}{\sqrt{\frac{1}{4}\sum_{i=1}^{4} S_i^2}}$	**15.01**	**20.11**
S_5 (step increase in flow)	0.11276	0.15381
S_6 (step increase in nitrogen)	0.061724	0.070503
S_7 (step increase in phosphorus)	0.014208	0.012004
$X_5 = \dfrac{1}{\sqrt{\frac{1}{3}\sum_{i=1}^{3} S_i^2}}$	**10.21**	**13.39**

Thus, we conclude that alternative A_1 had bad scores in plant adaptation to both short and long term perturbations $x_{1,4*}$, $x_{1,5*}$, giving a comparative advantage to A_2 with respect to OBJ_3. This is due to the sensitivity of the efficiency of nitrogen and phosphorus removal to influent organic matter content. In contrast, the weak points identified for A_2 are $x_{2,1*}$ and $x_{2,3*}$ and $x_{2,11*}$ resulting in a poorer satisfaction of OBJ_1, OBJ_2 and OBJ_4 which, in turn, is attributable to the additional costs of metal salt for phosphorus precipitation and an insufficient anoxic zone for nitrogen denitrification.

5.2.5. *Step 6*. Evaluation of trade-offs

The trade-offs between the improvement of the criteria identified as “weak” and the loss of overall process performance are calculated in this step. Information about the trade-off is provided to the designer in two different ways: first, through the parameter $r_{j,i,f}$ that represents the ratio between the improvement of the targeted criterion and the loss in the objective function; and, second, as qualitative information in the form of rules that enable the identification of the causes of the decrease in overall process performance.

5.2.5.1. *Step 6.1* Data handling and knowledge extraction

A new sensitivity analysis at the optimum found in *Step 4* is carried out. The data generated during the new sensitivity analysis is processed to enable qualitative knowledge to be extracted. The objective of this step is to find, for each alternative, the correlations between the five analysed variables and the twelve criteria used. Trends in the evaluation criteria are computed within ±10% of the new base case value found in *Step 4.3*. Finally, these trends are classified in four categories: directly proportional, indirectly proportional, constant and non monotonic. **Table 5.7** summarizes the correlations between the normalized criteria and the variables.

5.2.5.2. *Step 6.2*. Knowledge codification

The knowledge extracted from the data is codified in the form of IF-THEN rules. The set of rules [R = ($R_{1,1,1}$,…,$R_{m,n,y}$)] constitute a knowledge base containing the relationship between the variables that govern the overall process (y = 5) and the twelve evaluation criteria (n = 12) for each alternative considered (m = 2). Finally, these rules are used as an input to an inference engine (in this case we use CLIPS®). As an example, two rules extracted from the data in **Table 5.7** are shown.

$R_{1,11,3,}$: *IF $V_{1,3}$ (recirculation flow) increases THEN TIV TN ($x_{1,11}$) improves.*

$R_{2,3,1,}$: *IF $V_{2,1}$ (metal flow) increases THEN operating costs ($x_{2,3}$) worsen.*

Table 5.7. Relationship between evaluation criteria and analysed variables

Variable	Directly proportional	Indirectly proportional	Constant	No monotonic
$V_{1,1}$	$v(x_{1,6-1})$, $v(x_{1,6-2})$, $v(x_{1,12})$	$v(x_{1,2})$, $v(x_{1,4})$, $v(x_{1,5})$, $v(x_{1,7-1})$, $v(x_{1,7-2})$, $v(x_{1,7-3})$, $v(x_{1,11})$	$v(x_{1,8})$, $v(x_{1,9})$, $v(x_{1,10})$	$v(x_{1,1})$, $v(x_{1,3})$
$V_{1,2}$	$v(x_{1,4})$, $v(x_{1,6-1})$, $v(x_{1,7-1})$, $v(x_{1,7-2})$, $v(x_{1,12})$	$v(x_{1,1})$, $v(x_{1,3})$, $v(x_{1,5})$, $v(x_{1,6-2})$, $v(x_{1,7-3})$, $v(x_{1,11})$	$v(x_{1,2})$, $v(x_{1,8})$, $v(x_{1,9})$, $v(x_{1,10})$	-
$V_{1,3}$	$v(x_{1,3})$, $v(x_{1,4})$, $v(x_{1,5})$, $v(x_{1,6-2})$, $v(x_{1,7-3})$, $v(x_{1,11})$	$v(x_{1,6-1})v(x_{1,7-1})$, $v(x_{1,7-2})$, $v(x_{1,12})$	$v(x_{1,2})$, $v(x_{1,8})$, $v(x_{1,9})$, $v(x_{1,10})$	$v(x_{1,1})$
$V_{1,4}$	$v(x_{1,4})$, $v(x_{1,5})$, $v(x_{1,6-2})$,	$v(x_{1,3})$, $v(x_{1,6-1})$, $v(x_{1,7-1})$,$v(x_{1,7-2})$ $v(x_{1,7-3})$,$v(x_{1,11})$, $v(x_{1,12})$,	$v(x_{1,2})$, $v(x_{1,8})$, $v(x_{1,9})$, $v(x_{1,10})$	$v(x_{1,1})$
$V_{1,5}$	$v(x_{1,1})$, $v(x_{1,3})$, $v(x_{1,5})$, $v(x_{1,7-1})$, $(x_{1,7-3})$, $v(x_{1,11})$	$v(x_{1,4})$, $v(x_{1,6-1})$, $v(x_{1,6-2})$, $v(x_{1,12})$	$v(x_{1,2})$, $v(x_{1,8})$, $v(x_{1,9})$, $v(x_{1,10})$	-
$V_{2,1}$	$v(x_{2,1})$, $v(x_{2,5})$, $(x_{1,6-1})$, $(x_{1,7-1})$, $(x_{1,7-2})$, $v(x_{2,12})$	$v(x_{2,3})$, $v(x_{2,6-2})$, $v(x_{2,7-3})$,	$v(x_{2,2})$, $v(x_{2,4})$, $v(x_{2,8})$, $v(x_{2,9})$, $v(x_{2,10})$, $v(x_{2,11})$,	
$V_{2,2}$	$v(x_{2,7-1})$, $v(x_{2,7-2})$, $v(x_{2,7-3})$, $v(x_{2,12})$	$v(x_{2,1})$, $v(x_{2,3})$, $v(x_{2,6-1})$, $v(x_{2,6-2})$	$v(x_{2,2})$, $v(x_{2,4})$,$v(x_{2,8})$, $v(x_{2,9})$, $v(x_{2,10})$, $v(x_{2,11})$	
$V_{2,3}$	$v(x_{2,1})$, $v(x_{2,3})$, $v(x_{2,4})$, $v(x_{2,7-3})$	$v(x_{2,7-1})$, $v(x_{2,7-2})$, $v(x_{2,12})$	$v(x_{2,2})$, $v(x_{2,8})$, $v(x_{2,9})$, $v(x_{2,10})$, $v(x_{2,11})$	$v(x_{2,5})$, $v(x_{2,6-1})$, $v(x_{2,6-2})$,
$V_{2,4}$	$v(x_{2,4})$, $v(x_{2,5})$, $v(x_{2,6-2})$, $v(x_{2,7-3})$, $v(x_{2,12})$	$v(x_{2,1})$, $v(x_{2,3})$, $v(x_{2,6-1})$, $v(x_{2,7-1})$, $v(x_{2,7-2})$	$v(x_{2,2})$, $v(x_{2,8})$, $v(x_{2,9})$, $v(x_{2,10})$, $v(x_{2,11})$	-
$V_{2,5}$	$v(x_{2,1})$, $v(x_{2,3})$, $v(x_{2,6-1})$, $v(x_{2,7-1})$, $v(x_{2,7-2})$,	$v(x_{2,5})$, $v(x_{2,6-2})$, $v(x_{2,12})$	$v(x_{2,2})$, $v(x_{2,4})$, $v(x_{2,7-1})$, $v(x_{2,8})$, $v(x_{2,9})$, $v(x_{2,10})$, $v(x_{2,11})$	$v(x_{2,5})$,

5.2.5.3. Step 6.3. Knowledge extraction and evaluation of trade-offs

Finally, in *Step 6.3* dynamic simulation is integrated with qualitative knowledge to evaluate the trade-off between the improvement of the weak points for a determined alternative identified in *Step 5* and the loss of overall process performance. Thus, a set of actions that have the potential to improve the weak criteria for A_1 ($x_{1,4*}$ and $x_{1,5*}$) and for A_2 ($x_{2,1*}$ $x_{2,3*}$ and $x_{2,11*}$) are searched for automatically in the knowledge base built into *Steps 6.1* and *6.2* and summarized in **Table 5.7.** Next, optimum sensitivity is calculated, i.e. the rate at which the multiobjective function changes with changes in one of the decision variables. Once the actions are proposed, the adverse effects resulting from the application of those actions are highlighted.

To illustrate these ideas we present an example run of the system. The alternatives under study are alternatives A_1 and A_2, and some of the possible actions aimed at improving the satisfaction of criteria $x_{1,11}$ (TIV-TN) and $x_{2,3}$ (operating costs) are presented and commented on below. The examples are partially edited to shorten the output. The answers given by the user are underlined in italics (*e.g.* <u>*Option A₁*</u>, <u>*TIV-TN*</u>) and the text printed by the system is in Arial bold font.

Which is the alternative that you want to evaluate? <u>*Option A_1*</u>

Which is the criterion that you want to improve? <u>*Robustness*</u>

1. Robustness can be improved by decreasing the NO-set point,

but when the NO-set point is decreased:

The degree of satisfaction of impact on water ($x_{1,1}$) decreases.

The degree of satisfaction of operating costs ($x_{1,3}$) decreases

The degree of satisfaction of flexibility ($x_{1,5}$) decreases

The degree of satisfaction of bulking risk ($x_{1,7-1}$) decreases

The degree of satisfaction of rising risk ($x_{1,7-3}$) decreases

The degree of satisfaction of TIV-TN ($x_{1,11}$) decreases

Alternatively,

2. Robustness can be improved by increasing the recirculation flow

but when the recirculation flow is increased:

The degree of satisfaction of DO control performance ($x_{1,6-1}$) decreases

The degree of satisfaction of bulking risk ($x_{1,7-1}$) decreases

The degree of satisfaction of foaming risk ($x_{1,7-2}$) decreases

The degree of satisfaction of TIV-TP ($x_{1,12}$) decreases

Alternatively,

……

When the recirculation flow is increased, e.g. + 10 %, in alternative A_1 and the proposed scenario is simulated, there is an increase in terms of degree of satisfaction for robustness of 3.6%, i.e. better plant adaptability to short term perturbations. Nevertheless, this increase would suppose an increase in the total suspended solids in the biological reactor and a subsequent decrease in the F/M ratio, thereby increasing the risk of foaming and bulking (see knowledge flow diagram for both bulking and foaming in **Chapter 4**). Also, it is important to point out that this situation implies a higher consumption of organic matter for denitrification with a subsequent restriction of phosphorus release and an overall decrease in phosphorus removal efficiency. All these adverse effects bring about a decrease in the overall process performance of -0.56%. The trade-off between the normalized value of $x_{1,4}$ and the multiobjective function $s(A_1)$ is shown graphically in **Figure 5.10.**

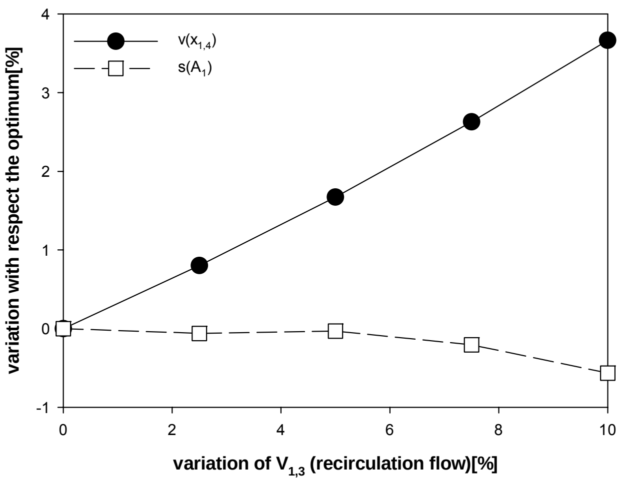


Figure 5.10. Trade-offs between the multiobjective function $s(A_1)$ and the normalized value of criterion robustness $x_{1,4}$.

As another example, take the case of alternative A_2 where the action proposed is aimed at improving the satisfaction of OBJ_2, i.e. reducing operating costs:

Which is the alternative that you want to evaluate? <u>*Option A_2*</u>

Which is the criterion that you want to improve? <u>*Operating costs*</u>

1. Operating costs can be improved by decreasing the waste flow
but when the waste flow is decreased:

The degree of satisfaction of bulking risk ($x_{2,7-1}$) decreases.

The degree of satisfaction of foaming risk ($x_{1,7-2}$) decreases.

The degree of satisfaction of TIV-TP ($x_{2,12}$) decreases

Alternatively,

2. Operating costs can be improved by decreasing the metal flow
but when the metal flow is decreased:

The degree of satisfaction of impact on water ($x_{2,1}$) decreases.

The degree of satisfaction of flexibility ($x_{2,5}$) decreases.

The degree of satisfaction of DO control performance ($x_{2,6-1}$) decreases.

The degree of satisfaction of bulking risk ($x_{2,7-1}$) decreases

The degree of satisfaction of foaming risk ($x_{2,7-2}$) decreases.

The degree of satisfaction of TIV-TP ($x_{2,12}$) decreases.

Alternatively,

……

In this case, there is a dramatic increase in TIV for TP (from 0% to 71% in terms of percentage of time) when metal flow is decreased in alternative A_2. This is due to the fact that phosphorus removal in this plant is carried out by chemical precipitation. If the dosage of iron is reduced, the quantity of phosphorus precipitates is also reduced, thereby increasing the impact on water and reducing overall pollution efficiency. It is important to note that the small reduction in operating costs (-0.09%) can be explained by the rise in effluent fines although the cost associated with the quantity of metal salt decreases. The variation in the normalized value of $x_{2,3}$ and the multiobjective function ($s(A_2)$) is shown in **Figure 5.11.**

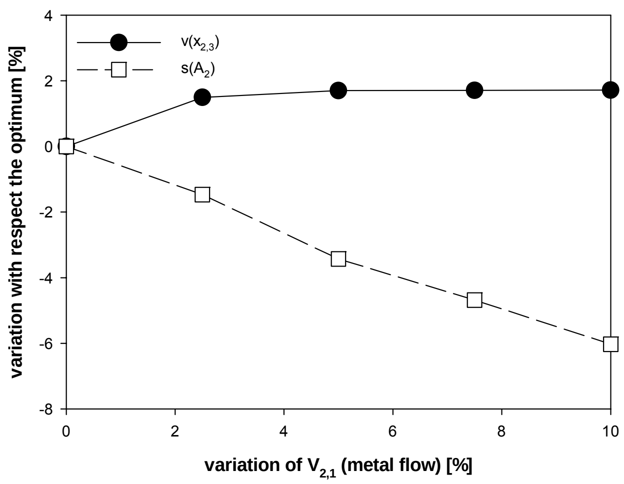


Figure 5.11. Trade-offs between the multiobjective function $s(A_2)$ and the normalized value of criterion robustness $x_{2,3}$.

If the trade-off between criteria improvement and loss in overall process performance is evaluated using **equation 5.2**, we can conclude from these examples that A_1 could be improved with a smaller loss of overall performance. This can be observed in **Figure 5.10** and **Figure 5.11** which show the change in the target criteria and the multiobjective function as a response to the variation in internal recirculation and metal flow respectively. Moreover, we reach the same conclusion if the parameter $r_{j,i,f}$ is calculated for the rest of the weak criteria identified in *Step 5* and all the actions proposed by the system: A_1 undergoes a smaller variation in overall process performance while simultaneously improving all the criteria identified (automatically) as "weak". Hence, this indicates that the objective function for alternative A_1 is less sensitive than for alternative A_2.

Table 5.8. Parameter r (equation 5.2) for the identified weak criteria for each evaluated alternative.

	$r_{1,4}$	$r_{1,5}$	$r_{2,1}$	$r_{2,3}$	$r_{2,11}$
$V_{j,1}$	3.78	7.31	0.68	0.18	-
$V_{j,2}$	21.27	2.99	0.74	1.20	-
$V_{j,3}$	6.49	12.47	0.38	1.9	-
$V_{j,4}$	4.03	8.75	0.80	8.2	-
$V_{j,5}$	19.0	14.31	1.80	0.74	-
$\frac{\sum_{f=1}^{Y} r_{j,i,f}}{Y}$	**10.9**	**9.2**	**0.88**	**2.44**	-

The higher sensitivity of A_2 is mainly due to the fact that high phosphorus removal, one of the plant's strong points, is directly correlated with high operating costs. For this reason there is a large penalty attached to the objective function when metal flow is decreased and there is a consequent reduction in the degree of satisfaction of OBJ_1 and OBJ_4 (see **Figure 5.11**). Furthermore, it is important to note the plant's inability to remove nitrogen. Since nitrogen and phosphorus are equally weighted, the high score of $x_{2,12}$ compensates for the lack of accomplishment of $x_{2,11}$ in OBJ_4. This can be corroborated from the rules extracted in *Step 6.2* and summarized in **Table 5.7,** given there is no possible action that will improve criterion $x_{2,11}$, i.e. the effluent nitrogen concentration is always above the legal limit. The small improvement in criterion $x_{2,1}$ is caused by further phosphorus removal rather than by an improvement in denitrification capacity.

According to these results, improvement to criteria $x_{2,11}$ would require consideration of additional issues (e.g. an additional carbon source, upgrading or adding an anoxic zone). However, this would increase the value of both $x_{2,2}$ and $x_{2,3}$ and worsen the satisfaction of OBJ_2 (a weak point identified in *Step 5* for A_2), as a trade-off for the improvement of $x_{2,11}$.

5.2.6. Step 9. Selection of the best alternative

From all the information generated during the evaluation of the first issue of the reaction section, we conclude that the best alternative is biological phosphorus removal. This implies the construction of additional anaerobic volume, but would bring about a reduction in operating costs, an improvement in both nitrogen and phosphorus removal, and a more balanced accomplishment of European Directive 91/271/ECC.

In addition, even though both alternatives have a similar value after optimization, the improvement in the weak points identified in *Step 5* for alternative A_1 would mean a lower penalty (see **Table 5.8)** in the objective function compared to A_2, with a major increase in the satisfaction of the criteria.

During the evaluation of the trade-off between the improvement of the criteria identified as weak points of the alternative and the loss of overall process performance, a "look ahead" step is performed. As a result of this, the inability of alternative A_2 to achieve good levels of phosphorus removal without reducing operating costs and removing nitrogen (due to inefficient denitrification) is identified, making it necessary to consider more issues in the reaction section in order to remedy this inherent design problem. The ability to predict undesirable process design directions has important implications during the selection of the best alternative.

Finally it is important to mention that all the analyses carried out during this chapter have been based on deterministic rather than stochastic assumptions. *Uncertainty* is a central concept when dealing with natural systems like WWTP's subjected to large and natural variation. The authors are aware of this issue and it is dealt with at length in **Chapter 7** of this thesis.

The design process would continue through evaluation of the remaining issues for the reaction section (e.g. location of the anaerobic reactors), separation section (e.g. increase of the settling area) and, finally, the recirculation section (e.g. additional anoxic to anaerobic recycling).

5.3. CONCLUSIONS

This chapter has addressed the problem of *critical decisions* that arise during the conceptual design of wastewater treatment plants when several design objectives (e.g. environmental, legal, economic and technical) must be taken into account. It has contributed to the solution of this problem by proposing a systematic three-step procedure to support the management of the close interplay between, and the apparent ambiguity emerging from, the *multicriteria* evaluation of competing design alternatives.

The preliminary multiobjective optimization allows comparisons to be made between two or more alternatives when each is close to the optimum design conditions. Thus, we propose deferring a numerical optimization until we have selected the most *promising alternatives* and we are certain that we will proceed with the final design, i.e. when we attain sufficient accuracy to be able to address the next issue in the sequence of decisions, thereby allowing a more unbiased comparison.

The characterization of the alternatives enables an understanding of the design space, so that the designer is aware of the weak and strong points of the most *promising alternatives*. The classification tree and subsequent extraction of rules provides a clear overview of the performance of the competing alternatives. Hence, this evaluation both supports the designer in interpreting the influence of the weights of the design objectives in the final decision, and facilitates data analysis. At the same time, the set of rules shows the preferred alternative for the widest range of situations.

The analysis of the trade-off shows the rate at which overall process performance changes with variations in the design variables (parameter $r_{j,i,f}$). At the same time the system alerts the designer to any negative implications in the event of their possible implementation. All this information has important implications on the selection of design alternatives and provides the designer with valuable information for the reuse of the knowledge generated during the sensitivity analyses. As a result, otherwise hidden limitations in plant performance could very well suggest future desirable (or undesirable) design directions during the plant's retrofit or revamping.

From all the information generated in the previous analyses, the case study showed that the best alternative to achieve simultaneous organic carbon, nitrogen and phosphorus is the construction of an anaerobic tank. Even though implies the construction of an additional unit, it also resulted in a reduction in the operating costs and an improvement of both nitrogen and phosphorus removal. Also, it was possible to discover undesirable directions in the event that chemical precipitation would be the chosen alternative driving to a future configuration with high operating costs and difficulties to remove nitrogen.

Also, there are other advantages in the extraction and maintenance of a record of design knowledge. On the one hand, it is possible to reduce the cognitive load on the designer and enhance his/her understanding thanks to the automatic identification of adverse effects in the event of the implementation of actions with respect to the overall process performance. On the other hand, a wider scope of decision making is made possible by decreasing the number of iterations and enabling the concurrent manipulation of multiple criteria (more than a dozen in the case study presented). The methodology allows the geographical and temporal reuse of knowledge that would otherwise be tacit and of potential use to a single designer only. The procedure has been applied in WWTPs, but could be adapted for other types of (bio)chemical process that environmental/chemical engineers have to address.

5.4. CRITERIA QUANTIFICATION SECTION

Quantification of impact on water is calculated in a similar way to that in Chapter 4

$$X_1 = \frac{IQ - EQ}{IQ} \tag{A5.1}$$

Nevertheless, the load of P must be included and quantified for both effluent and influent quality indexes as shows A 5.2. and A 5.4

$$EQ = \frac{1}{(t_f - t_0)} \int_{t_0}^{t_f} PU(t) \cdot Q_e(t) \cdot dt \tag{A5.2}$$

PU is the result of applying A5.3

$$\begin{aligned} PU(t) = {} & PU_{TSS}(t) + PU_{COD}(t) + PU_{BOD}(t) + PU_{TKN}(t) + PU_{NO_X}(t) + \\ & + PU_{Pinorg}(t) + PU_{Porg}(t) \end{aligned} \tag{A5.3}$$

The effluent polluting loads PU_K ($kg \cdot day^{-1}$) corresponding to the component k (TSS, COD, BOD_5, TKN, NO_X, P_{inorg} and P_{org}) are calculated through A5.4.

$$PU_K = \beta_K C_K \tag{A5.4}$$

Where β_{TSS} =2, β_{COD} =1, β_{BOD5} =2, β_{TKN} =20, β_{NOx} =20, β_{Porg} =20 and β_{Pinorg} =20. As in the previous example IQ is calculated in a similar way to the EQ index, simply replacing the effluent data with the influent data.

The construction cost of an additional anaerobic reactor is quantified in the following way. **Equation A5.5** summarizes all the terms to take into account, where COST_E is the cost of earthwork, COST_CW is the cost of the concrete wall in place, COST_CS is the cost of concrete slab in place, IEC the installed equipment costs, COST_HR the cost of handrails and CF is a correction factor.

$$X_{2-1} = (COST\_E + COST\_CW + COST\_CS + IEC + COST\_HR)\cdot CF \quad \text{(A5.5)}$$

Realisation of the metal dosage system on a WWTP includes installation of one or more storage tanks for chemicals, and pumps combined with a system of pipes to bring the precipitant to the activated sludge tanks. These costs are estimated using an empirical equation that correlates the quantity of metal to be added and the cost of the dosage system.

$$X_{2-2} = A\cdot(M)^B \quad \text{(A5.6)}$$

Operating costs index is quantified in the same way as in Chapter 4,

$$X_3 = \alpha_{EQ}\cdot EQ + \alpha_{AE}\cdot AE + \alpha_{PE}\cdot PE + \alpha_{sldg}\cdot P_{sldg} + \alpha_{ME}\cdot ME + \alpha_{FE}\cdot FE \quad \text{(A5.7)}$$

EQ, AE, PE, ME, P_{sludg} are quantified as described in the criteria quantification section of Chapter 4. Metal consumption is described in **equation A5 8.** The weighing factors are the same α_{sldg} = 50 (EQ·year^{-1})·(EQ·day^{-1})$^{-1}$, α_{AE} = α_{PE} = α_{ME} = 25 (€·year^{-1})·(kW·h·day^{-1}); α_{sldg} = 75 (€·year^{-1})·(kgTSS·day^{-1})$^{-1}$, and α_{FE} that was estimated assuming a cost of 0.523 €·kg^{-1}.

$$FE = \frac{MET_s}{(t_f - t_0)\cdot 1000}\int_{t_0}^{t_f} Q_{met}\cdot dt \quad \text{(A5.8)}$$

Equations for robustness and flexibility can be found in Chapter 4 (**equations A4.17** and **A4.18**). In this case study short term disturbances are: (S_1) storm (of high intensity but short-lived increase in flow and suspended solids) and (S_2) rain (the influent flow does not reach the level attained during storm events but high flow is sustained for a longer period of time) as defined by Gernaey and Jørgensen (2004), and a 10% increase in (S_3) nitrogen and (S_4) phosphorus concentration between the fifth and the seventh day of simulation in the default influent (i.e. a nitrogen and phosphorus shock). A step increase of 10% in the influent organic, nitrogen and phosphorus loads (p=3) are the long term changes used in this case study. Control performance (X_6) and time in violation (X_8 to X_{12}) are also described in Chapter 4.

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Flores X., Comas J., Rodríguez-Roda I., Jiménez L. and Gernaey K.V. Application of multivariate statistical techniques during the multicriteria evaluation of WWTP control strategies at plant wide level. 2007. Wat. Sci. & Tech. 56(6):75.

CHAPTER 6. *MULTIVARIATE* ANALYSIS DURING *MULTICRITERIA* EVALUATION OF WASTEWATER TREATMENT PLANT ALTERNATIVES

The third chapter of this thesis aims to present a *multivariate* based methodology able to mine the *multicriteria* matrixes obtained during the evaluation of conceptual design wastewater treatment plant (WWTP) alternatives. The evaluation of WWTP design alternatives is complex due to the fact that several different objectives, e.g. economic, environmental, technical, and legal, must be taken into account simultaneously. The accomplishment of some of those objectives presents significant synergies but in other cases they are subject to clear trade offs. The result is a hugely complex evaluation matrix consisting of a large number of physico-chemical, operating and technical criteria which are often difficult to interpret, thus making it difficult to draw meaningful conclusions. The absence of efficient tools with which to discover groups of control strategies that perform in a similar way, facilitate interpretation of the complex interactions amongst multiple criteria, and identify the main features of a specific control strategy or group of control strategies, is a significant limitation when evaluating WWTP conceptual design alternatives

In this study, cluster analysis (CA), principal component/factor analysis (PCA/FA) and discriminant analysis (DA) are applied to the matrix data set obtained when several alternatives are evaluated by dynamic simulation. These techniques make it possible i) to determine natural groups or clusters of alternatives with similar behaviour, ii) to find and interpret hidden, casual and/or complex relations in the data set and iii) to identify important discriminant variables within a single or a group of alternatives.

This chapter is organized in the following way: first, a short description of the procedure is provided and, then, its application is illustrated on a case study. The analysis of the results is developed to evaluate 12 control strategies showing the advantages of using *multivariate* statistical techniques when they are compared with traditional evaluation methods. The results show that the nitrate controller manipulating an external carbon source and the TSS controller manipulating the waste flow are the alternatives with a more significant impact on the overall process performance. Also, it was possible to discover direct correlations between the different evaluated criteria such as: better denitrification capacity and lower risk of rising against operating costs, low F/M ratios as the main causes of bulking and foaming or better nitrification capacity with higher aeration energy. Finally it was found that external carbon source, methane production and risk of microbiology-related solids separation problems were the main criteria discriminating amongst the groups of control strategies rendered by cluster analysis

6.1. METHODOLOGY

This section details the approach proposed as a means of exploiting the evaluation matrix data sets obtained during the *multicriteria* evaluation of conceptual design WWTP alternatives. This methodology combines features of the approach presented in **Chapter 4** with new features: i) determination of natural groups or clusters of alternatives that behave similarly, ii) interpretation of hidden, complex and casual relation correlations in the data set and iii) identification of important discriminant criteria within a single or group of alternatives. The interactions between the different procedures developed for this thesis are represented in **Figure 2.1**. As can be seen in **Figure 6.1**, block 3 is directly linked to block 1 to facilitate both analysis and interpretation of the *multicriteria* matrixes obtained during the decision procedure.

The methodology presented in this chapter follows the same pattern as that presented in **Chapter 5**. The first phase: *hierarchical* generation and *multicriteria* evaluation of WWTP alternatives, is followed by the second: *multivariate* analysis. The entire procedure is described in the following section.

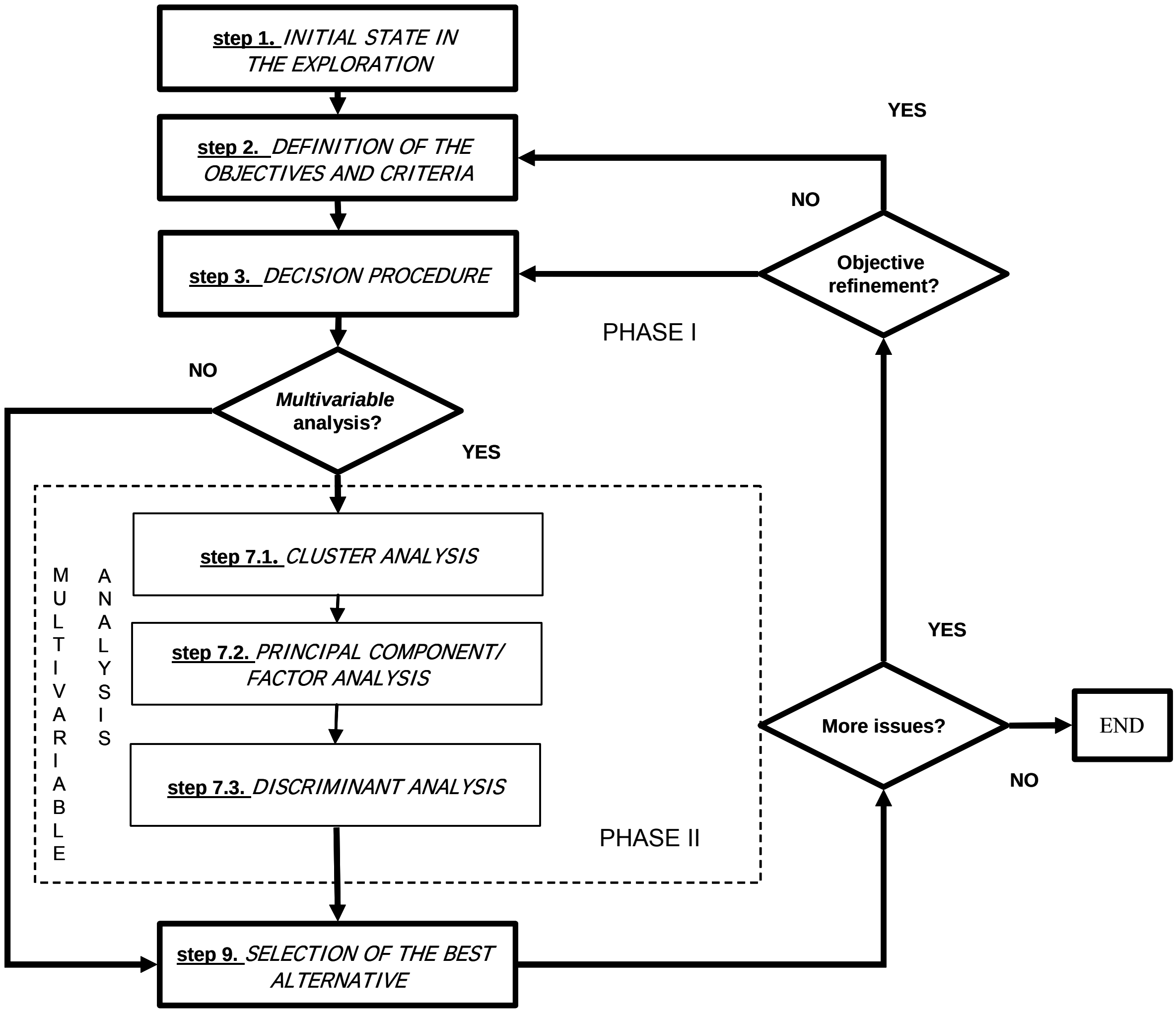


Figure 6.1. Flow diagram of the third block of the conceptual design method (see text for explanation)

Phase I. *Hierarchical* generation and *multicriteria* evaluation of design alternatives

In the first step (*Step 1*) all the information required to carry out the analysis is collected. This involves the description of the WWTP to be studied, the flow rate, the composition and the dynamics of the water to be treated and the applicable legislation. *Step 2* includes definitions of the objectives $[OBJ = \{OBJ_1,..,OBJ_P\}]$ and the evaluation criteria $[X = \{X_1,..,X_W\}]$ used to measure the degree of satisfaction of objectives. In this case there is no assignation of weights because the tool focuses on analysis of the results and no type of decision making is included. In *Step 3* there are a number of tasks: the identification of the issue to be resolved I_1 (*Step 3.1*), the generation of alternative solutions $[A = \{A_1,...,A_m\}]$ (*Step 3.2*), the selection of a subset of criteria $[X = \{X_1,...,X_n\}]$ defined for this issue (*Step 3.3*), evaluation of the alternatives (*Step 3.4*), and finally selection of one of them on the basis of the results obtained by means of the weighted sum (see **equation 4.1**).

Phase II. *Multivariate* analysis during *multicriteria* evaluation of WWTP design alternatives

Multivariate analysis (phase II) of the alternatives is linked to *Step 3* in order to facilitate the interpretation of the *multicriteria* matrixes obtained previously. The block presented in this chapter comprises three steps: *Step 7.1* (cluster analysis), *Step 7.2* (principal component/factor analysis) and *Step 7.3* (discriminant analysis).

Cluster analysis (CA) is an unsupervised pattern recognition technique that uncovers intrinsic structure or underlying behaviour of a data set without making a priori assumptions. Classification of the objects or a system into categories or clusters is based on the nearness or similarity of data points; see, for example, Hair *et al*. (1998). In this paper hierarchical clustering is performed on the data set – after scaling the variables between 0 and 1 – by means of Ward's method, using the Euclidian distance as a measure of similarity. In **equation 6.1** there is a representation of this distance where n is the number of criteria, evaluated from a point $[X = \{X_1,..X_i,..X_n\}]$ to a point $[Y = \{Y_1,..Y_i,..Y_n\}]$.

$$d_n = \left(\sum_{i=1}^{n} \left| X_i - Y_i \right|^2 \right)^{1/2} \qquad \text{(Eq 6.1)}$$

Principal component Analysis (PCA) extracts the eigenvalues and eigenvectors from the covariance matrix of the autoscaled variables $[X = \{X_1,..X_i,..X_n\}]$. The set of $[PC = \{PC_1,..PC_i,..PC_n\}]$ principal components (PCs) are the uncorrelated (orthogonal) variables obtained by multiplying the original correlated variables with the eigenvectors. Each eigenvector consists of a vector of coefficients (loadings) $[a = \{a_1,..a_i,..a_n\}]$ as shown in **equation 6.2**. PCA allows the dimensionality of the original data set to be reduced with a minimum loss of information. Factor analysis (FA) further reduces the contribution of less significant variables obtained from PCA and results in the new groups of variables known as varifactors (VF) extracted through rotating the axis defined by PCA (Vega *et al*., 1998).

$$PC_j = a_{1,j}x_1 + a_{2,j}x_1 + ... + a_{i,j}X_i + ... + a_{n,j}X_n = \sum_{i=1}^{n} a_{i,j}X_i \qquad \text{(Eq 6.2)}$$

Discriminant Analysis (DA) is used to determine the variables which allow discrimination between two or more naturally occurring groups (Johnson and Wichern, 1992). It operates on raw data and the technique constructs a discriminant function $[D = \{D_1,..D_i,..D_z\}]$ for each group (see **equation 6.3**) where j is the number of the function, C_k is the constant inherent to each function, k is the number of parameters used to classify a set of data into a given group, and b_i is the weight coefficient assigned by DA to a given performance evaluation parameter (X_i). In this particular application the number of groups of classes is obtained by CA and the parameters are the evaluation criteria.

$$D_j = C_{i,j} + b_{1,j}X_1 + b_{2,j}X_2 + ... + b_{i,j}X_i + ... + b_{1,j}X_k = \sum_{k=1}^{k} b_{i,j}X_j \qquad \text{(Eq 6.3)}$$

Even though block 3 is linked to block 1 as a part of the whole conceptual design methodology, the third block of this thesis can also be applied to any other methodology to evaluate alternatives e.g. Chen and Shonnard (2004) or Uerdingen *et al*. (2003).

6.2. CASE STUDY # 4: EVALUATION OF WWTP CONTROL STRATEGIES AT PLANT WIDE LEVEL - I

The case study shows the application of the proposed approach to support analysis of the evaluation matrix data set obtained by simulation of several control strategies applied on a plant wide level in a WWTP. It is important to mention that the entire decision procedure is not developed for this case study because the main objective of the chapter is to show the capabilities of the proposed block. Thus part of *Step 3* (criteria normalization, weighted sum) and *Step 9* are omitted.

6.2.1. *Steps 1 & 2*. Initial state in the exploration and definition of the control objectives and criteria.

A preliminary version of the Benchmark Simulation Model N^{O} 2 (BSM2) is the plant wide wastewater treatment plant model under study (see **Figure 6.2**). It is important to state that is not the final version of the BSM2 and further modification has been done by the IWA Task Group (correct code, design volumes and operation settings) when the work was on going.

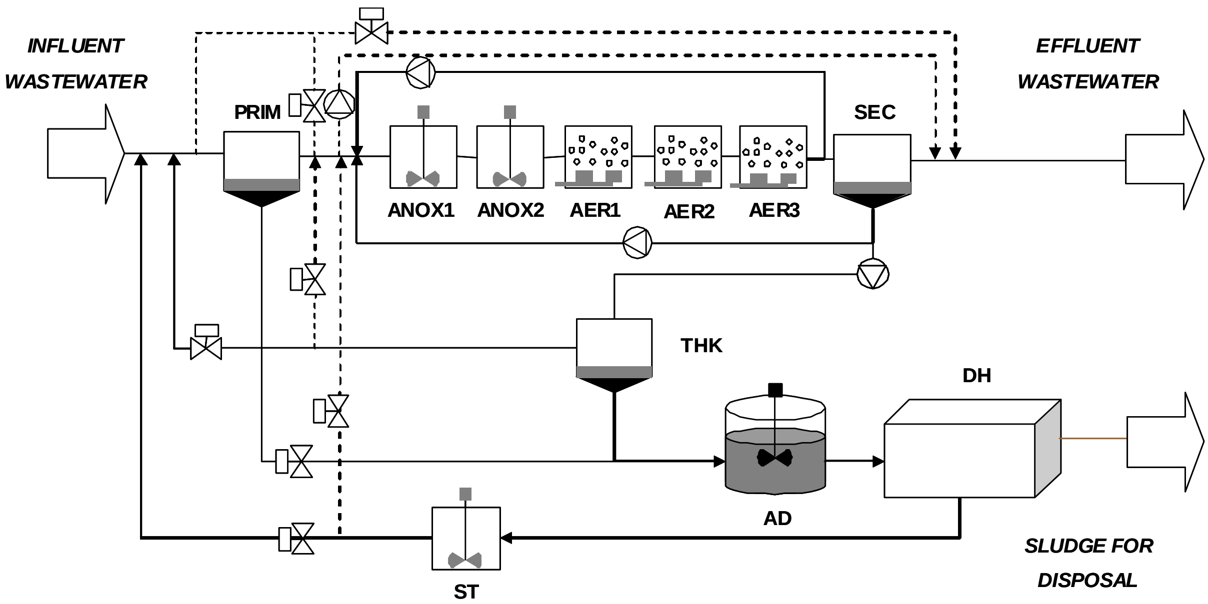


Figure 6.2. Plant layout for the BSM2 (Jeppsson *et al*., 2006)

The predenitrifying activated sludge system – two anoxic reactors (ANOX1 & 2) followed by three aerobic reactors (AER3, 4 & 5) – and the secondary clarifier are identical to those in the Benchmark Simulation Model No 1 (BSM1, Copp, 2002). The plant is designed to remove organic carbon and nitrogen. In the aerobic section of the plant the organic matter and ammonia is oxidized to carbon dioxide and nitrate. In the anoxic section the nitrate transported by the internal recirculation is reduced to nitrogen.

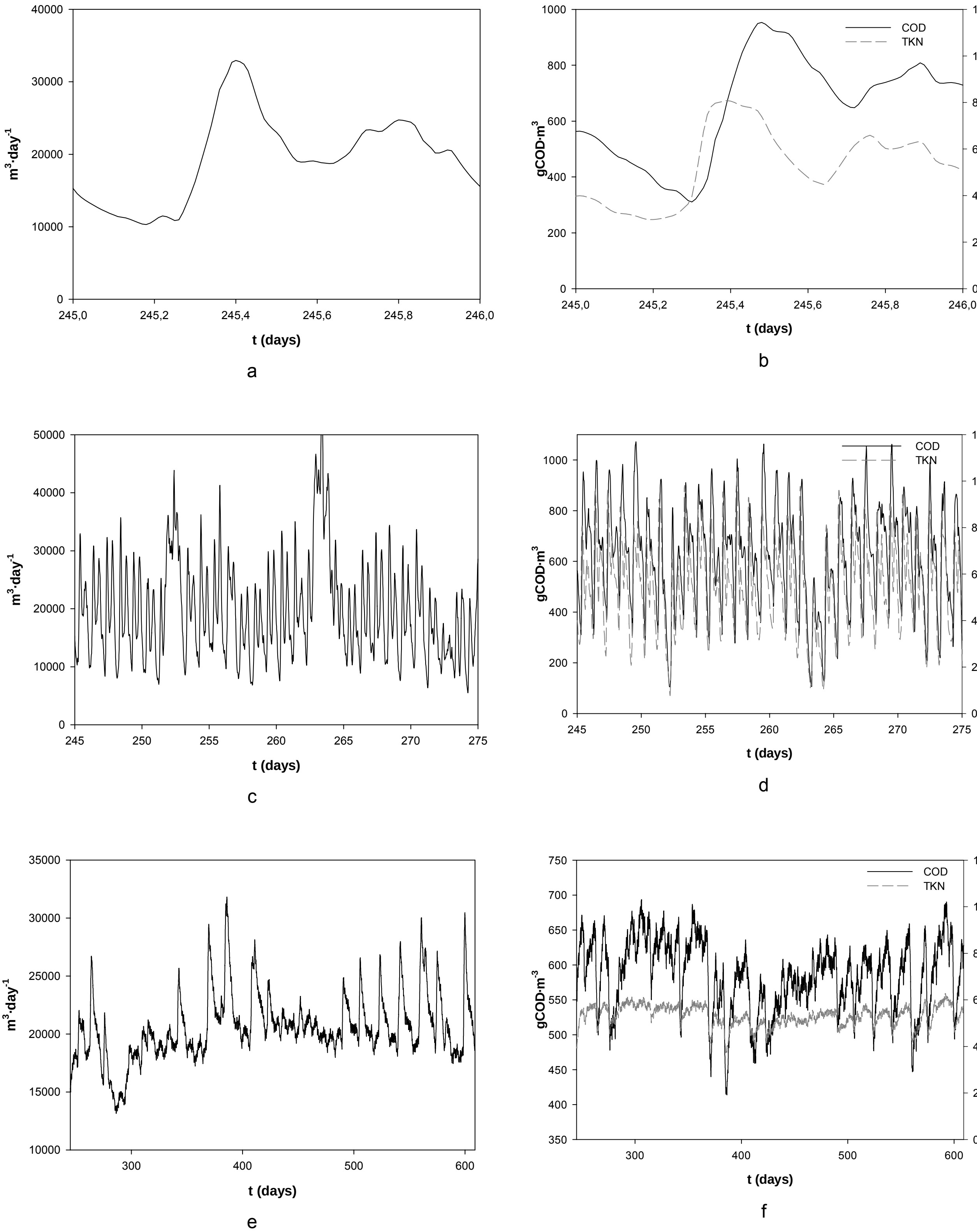


Figure 6.3. Influent wastewater flow (a,c,e) and components (b,d,f) for one day, (a,b) for one month (c,d) and for one year (e,f)

The BSM2 plant also contains a primary clarifier (PRIM), a sludge thickener (THK), an anaerobic digester (AD), a storage tank (ST) and a dewatering unit (DH). In the anaerobic digester the organic biodegradable matter, both soluble and particulate, is converted to methane and carbon dioxide. Since methane is a sparingly soluble gas, most of it is evolved and recovered, thereby removing organic matter from the liquid phase and stabilizing any solids produced in the process.

Plant performance evaluation is based on one year's simulated influent data generated according to the principles outlined in Gernaey *et al*. (2006). It comprises 609 days' dynamic influent data with samples taken every 15 minutes. Typical model file influent phenomena observed in one year in a full scale WWTP were: 1) diurnal variation, 2) a lower average flow rate and pollution concentrations during weekends compared to week days, in an attempt to simulate a WWTP that receives mixed municipal – industrial wastewater, 3) seasonal phenomena reflecting the typical effects of sewer systems and urban drainage, i.e. increased infiltration in winter due to higher infiltration levels, 4) holiday periods during which a lower average wastewater flow rate is maintained for an overall period of several weeks. **Figure 6.3** shows some of the above-mentioned phenomena broken down in terms of both flow rate and organic load in different time scales of one day (**Figure 6.3a** and **b**), one month (**Figure 6.3c** and **d**) and one year (**Figure 6.3e** and **f**). With respect to the one-year temporal series, an exponential 3-day filter has been used to clarify its evolution (further details are given in the criteria quantification section). The average wastewater flow rate to be treated is of 20000 $m^3 \cdot day^{-1}$ (see the complete profile in **Figure 6.3**e) with an organic and nitrogen load of 12200 kg $COD \cdot day^{-1}$ and 1140 kg $N \cdot day^{-1}$ respectively (**Figure 6.3f**).

To quantify the degree of satisfaction of the different control objectives, several criteria are proposed in **Table 4.1**. In this case study, four different objectives are taken into account - *[OBJ₁ = (OBJ₁,..,.OBJ₄)]* (i.e. environmental, economic, technical and legal). In this particular case study, no weights are assigned to the different objectives because a decision making process is not involved.

6.2.2. *Step 3*. Decision procedure.

The analysis of the results starts with the identification of the issue to be resolved. In this case study, the only issue addressed is the analysis of the overall WWTP process performance in terms of maximizing the degree of satisfaction of the objectives described in **Table 4.1**.

Several control strategies (m =11) have been implemented and compared to a default open loop case (A_1). The settings of the open loop case considered in this study were slightly modified compared to the BSM1 (Copp, 2002). The constant waste sludge flow rate (Q_w) was reduced from 385 to 300 $m^3 \cdot day^{-1}$ and the constant oxygen transfer coefficient for the third aerobic reactor was increased from 84 to $240 \cdot day^{-1}$. Values for the other manipulated variables (Q_{intr}= 55.446 $m^3 \cdot day^{-1}$, Q_r= 18.446 $m^3 \cdot day^{-1}$ and Q_{carb}= 0 $m^3 \cdot day^{-1}$) remained at the BSM1 default value. The tested control strategies, summarized in **Table 6.1**, were implemented for the activated sludge reaction section.

Table 6.1. Control strategies evaluated in this case study.

Characteristics	3 DO	Ammonium controller	Q_{intr} controller	Q_{carb} controller	TSS controller	Surmacz controller
Reference	Vanrolleghem and Gillot, 2002	Vrecko *et al.,* 2006	Copp, 2002	Vrecko *et al.,* 2006	Vrecko *et al.*, 2006	Vanrolleghem and Gillot, 2002
Measured variable(s)	S_O in ASU3, 4 & 5	S_{NH} in ASU5	S_{NO} in ASU2	S_{NO} in ASU2	TSS in ASU5	OUR in ASU3
Controlled Variable(s)	S_O in ASU3, 4 & 5	S_O in ASU3, 4 & 5	S_{NO} in ASU2	S_{NO} in ASU2	TSS in ASU5	S_o in ASU3, 4 & 5
Set point/critical value	2, 2 & 2 g (-COD)·m^{-3}	1 g N·m^{-3}	1 g N·m^{-3}	1 g N·m^{-3}	4400 g TSS·m^{-3} (if T< 15^{o}C) 3400 g TSS·m^{-3} (if T> 15^{o}C)	1850 g COD·m^{-3}·d^{-1}
Manipulated variable	K_La	S_O set point in 3 DO strategy	Q_{intr}	Q_{carb}	Q_w	S_O set point in 3 DO strategy
Control algorithm	PI	Cascaded PI	PI	PI	Cascaded PI	ON/OFF cascaded PI
Applied in control strategies (A_j)	A_2, A_3, A_4, A_5, A_6, A_7, A_8, A_9, A_{10}, A_{11} & A_{12}	A_5, A_6, A_7 & A_8	A_3, A_5, A_7, A_9 & A_{11}	A_4, A_6, A_8, A_{10} & A_{12}	A_7, A_8, A_{11}, & A_{12}	A_9, A_{10}, A_{11} & A_{12},

Table 6.1 presents the main features of the different controllers, e.g. manipulated variable, controlled variable and set point. The different combinations of controllers implemented for the various evaluated alternatives are also described. The simulation results (open loop case + 11 control strategies) are the starting point for the work presented in this chapter.

A set of (n=7) criteria (*Step 3.3*) is selected from **Table 4.1** to evaluate the 12 alternatives generated: effluent quality index (X_1), operating costs (X_3), risk of separation problems (X_7) in their three possible forms: bulking ($X_{7\text{-}1}$), foaming ($X_{7\text{-}2}$) and rising ($X_{7\text{-}3}$), and finally the percentage of time that the plant is in violation of legal limits (X_7 – X_{11}). The effluent quality index (EQ) and TIV are calculated in a similar fashion to BSM1 (see Chapter 4). However, the overall risk-of-separation problems index (Comas *et al*., 2006b) and the operating cost index has been modified from the original proposal so that it can be implemented on the BSM2 platform. Further details of these modifications can be found in the criteria quantification section. Furthermore, in order to enhance understanding of the entire evaluation process, sub criteria are included in the analysis thereby making it possible to know what the main causes are of any deviation in the calculated criteria for each implemented control strategy (see **Table 6 2**).

All the criteria are quantified by dynamic simulation using the Matlab-Simulink© environment in *Step 3.4*. The primary clarification is based on Otterpohl and Freund (1992) and Otterpohl *et al*. (1994). The International Water Association Activated Sludge Model number 1 (ASM1) is chosen as a biological process model for the reactor (Henze *et al.*, 2000) while the double exponential settling velocity model of Takács *et al*. (1991) based on the solid flux concept, was selected as a fair representation of the settling process with a ten layer discretization. Both gravity thickening and dewatering units are ideal, continuous models with no biological activity and 98% solids removal efficiency respectively. The anaerobic digester is based on the

International Water Association Anaerobic Digestion Model No 1 (Batstone *et al*., 2002). Finally, the recent work of Nopens *et al*. (2008) has been used for the interfaces between the AD and AS models. A full description of the models can be found in **Chapter 3**.

Table 6 2. Objectives, criteria and sub criteria used during the analysis

OBJECTIVE (OBJ_k)	CRITERION (X_i)		CALCULATED FROM
OBJ_1: minimize environmental impact	X_1 : effluent quality index		X_{1-1}: TKN X_{1-2}: TN X_{1-3}: COD X_{1-4}: BOD_5 X_{1-5}: TSS
OBJ_2: minimize economic cost	X_3 : operating costs		X_{3-1} : sludge production (SP) X_{3-2} : aeration energy (AE) X_{3-3} : pumping energy (PE) X_{3-4} : carbon source (CS) X_{3-5} : mixing energy (ME) X_{3-6} : heating energy (HE) X_{3-7} : methane production (MP)
OBJ_2: maximize technical reliability	X_7: risk of microbiology-related solids separation problems	X_{7-1}: bulking	$X_{7-1,1}$: low C/N ratio $X_{7-1,2}$: low DO bulking risk $X_{7-1,3}$: low F/M bulking risk
		X_{7-2}: foaming risk	$X_{7-2,1}$: low FM foaming risk $X_{7-2,2}$: high S_s/X_s foaming risk
		X_{7-3}: rising risk	-
OBJ_4: meet the European directive	X_8 : TIV (time in violation) COD		-
	X_9 : TIV BOD_5		-
	X_{10} : TIV TSS		-
	X_{11} : TIV TN		-

The DO, T and TSS sensors were assumed to be ideal, without noise or delay. The nitrate (S_{NO}) and ammonium (S_{NH}) nitrogen sensors had a time delay of 10 minutes, with zero mean white noise (standard deviation of 0.1 $gN \cdot m^{-3}$). Finally the OUR sensor was assumed to be a batch type sensor with a time delay of 30 minutes (batch operation of the measurement), and with zero mean white noise (standard deviation of 50 $gCOD \cdot m^{-3}$). All the dynamic simulations (609 days) were preceded by a steady state simulation (200 days). This insures a consistent starting point and eliminates bias due to the selection of initial conditions in dynamic modelling results. Only the data generated during the last 365 days of the simulation were used for plant performance evaluation. The values for all the evaluation criteria used in this case study are summarized in **Table 6.3.**

Figure 6.4 represents the behaviour of the different controllers. In **Figure 6.4a** there is a snapshot of the DO profile (S_o) in the last aerated reactor (AER3) with and without a controller. As can be seen from the dotted line representing the evolution of S_o in that reactor, aeration intensity (K_La = 240 $days^{-1}$) is not adequate during daytime and is excessive at night. **Figure 6.4b** and **c** show the evolution of nitrate nitrogen (S_{NO}) with and without controller in ANOX2 and AER3 respectively, with manipulation of either the internal recycle (Q_{intr}) or the external carbon source (Q_{carb}). **Figure 6.4d** shows the ammonium nitrogen (S_{NH}) in the third aerobic reactor (AER3) with and without a controller. As happens with the DO controller, the aeration set point (DO = 2 $g(-COD) \cdot m^{-3}$) is not adequate and needs to be changed according to the nitrogen load.

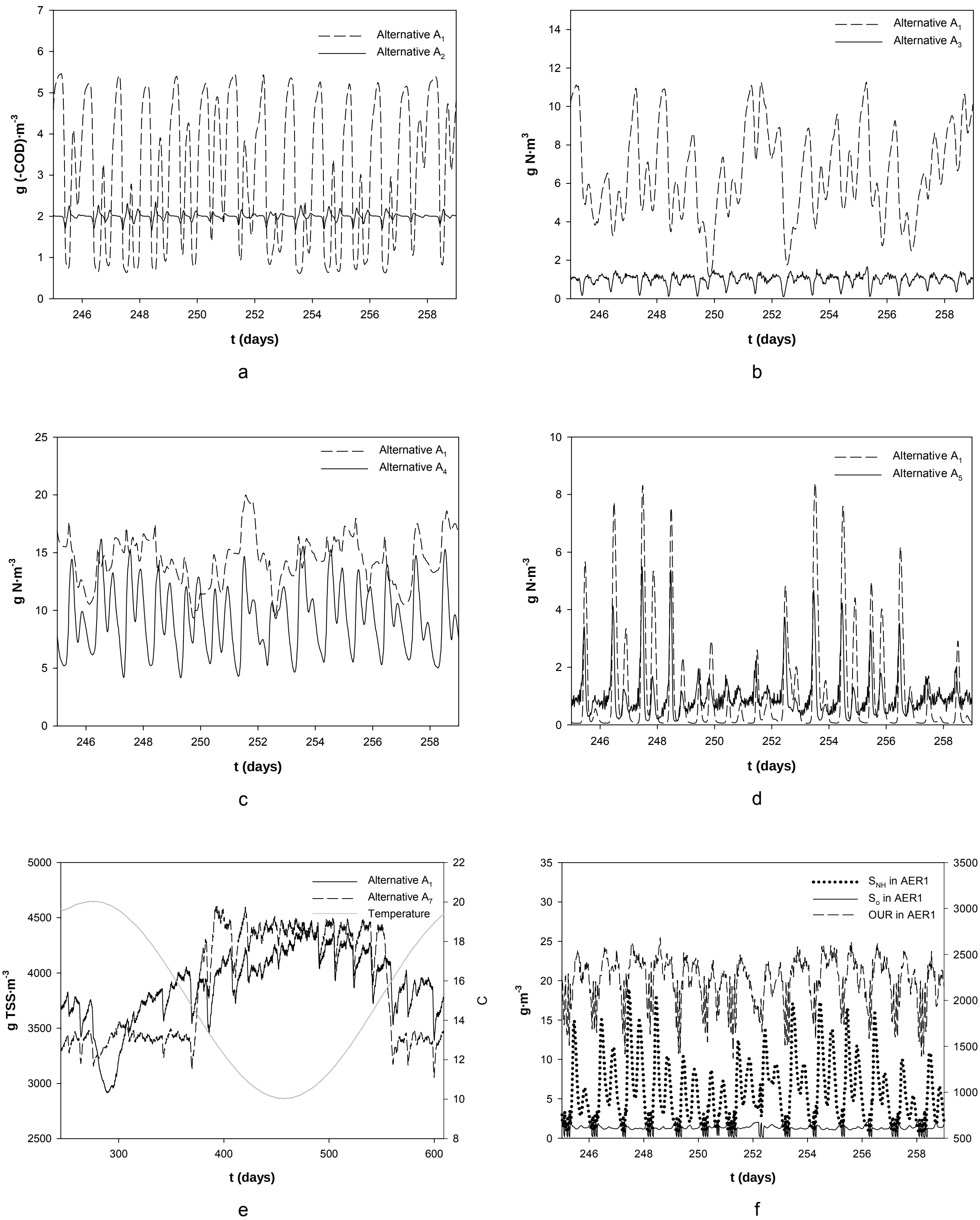


Figure 6.4. Behaviour of the different controllers studied: (a) S_o controller, (b) S_{NO} controller by means of the manipulation of $Q_{intr,}$ (c) S_{NO} controller by means of manipulation of Q_{carb}, (d) S_{NH} controller, (e) TSS controller and f) OUR controller

Table 6.3. Values of the evaluation criteria for the 12 tested control strategies

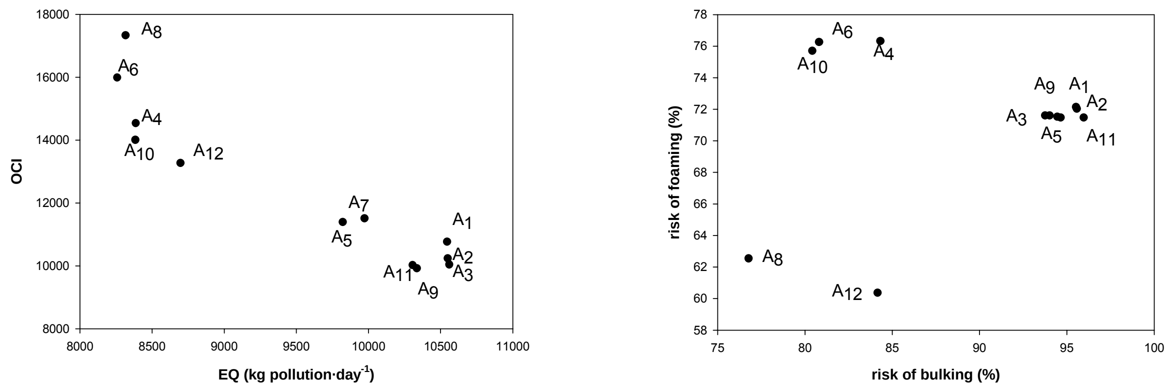
	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8	A_9	A_{10}	A_{11}	A_{12}
$X_{1\text{-}1}$	6.42	6.55	6.92	7.22	5.84	6.57	5.49	7.36	7.19	7.48	6.50	9.08
$X_{1\text{-}2}$	21.12	21.13	21.15	15.50	19.36	14.85	19.69	15.65	20.61	15.52	20.50	16.58
$X_{1\text{-}3}$	50.24	50.24	50.22	53.01	50.26	55.39	50.51	50.60	50.25	52.82	50.51	50.65
$X_{1\text{-}4}$	3.21	3.21	3.21	3.75	3.22	4.14	3.27	3.54	3.22	3.71	3.27	3.49
$X_{1\text{-}5}$	15.90	15.90	15.90	17.95	15.92	19.72	16.11	16.11	15.90	17.78	16.10	16.10
X_1	10545.00	10549.00	10560.00	8386.70	9822.10	8258.00	9972.60	8317.00	10335.00	8384.20	10306.00	8696.90
$X_{3\text{-}1}$	2654.50	2654.30	2650.90	2818.40	2653.50	2799.40	2656.40	2922.30	2650.60	2806.20	2654.10	2856.80
$X_{3\text{-}2}$	8548.40	8020.60	7985.20	8540.90	9321.20	10152.00	9446.90	10851.00	7849.00	8319.10	7958.80	7770.80
$X_{3\text{-}3}$	397.70	397.70	245.43	397.99	256.44	397.97	248.10	402.58	253.20	397.97	244.98	401.58
$X_{3\text{-}4}$	0.00	0.00	0.00	1193.80	0.00	1157.80	0.00	1342.50	0.00	1094.30	0.00	1028.30
$X_{3\text{-}5}$	648.00	648.00	648.00	648.00	648.00	648.00	648.00	648.00	655.18	653.85	654.46	655.58
$X_{3\text{-}6}$	4253.00	4252.60	4251.30	4355.20	4252.90	4353.40	4253.50	4453.20	4251.10	4348.80	4251.60	4398.10
$X_{3\text{-}7}$	1131.60	1131.60	1131.40	1180.70	1132.00	1180.10	1133.20	1227.10	1131.40	1177.20	1132.40	1202.20
X_3	10768.00	10240.00	10043.00	14539.00	11394.00	15989.00	11513.00	17333.00	9921.10	14009.00	10026.00	13270.00
$X_{7\text{-}1,1}$	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
$X_{7\text{-}1,2}$	31.74	16.64	18.45	15.43	21.54	19.48	20.86	17.01	19.42	16.95	18.26	19.43
$X_{7\text{-}1,3}$	74.30	74.29	74.25	77.46	74.20	77.65	77.80	65.80	74.10	76.92	77.76	67.62
$X_{7\text{-}1}$	78.42	75.91	76.20	78.70	76.38	79.34	80.47	68.31	76.33	78.47	79.76	70.51
$X_{7\text{-}2,1}$	70.90	70.90	70.97	75.76	70.98	75.63	71.24	59.06	70.88	75.20	71.29	61.50
$X_{7\text{-}2,2}$	1.01	1.01	1.09	1.24	1.07	1.38	2.29	7.52	1.09	1.12	2.36	6.23
$X_{7\text{-}2}$	71.47	71.47	71.61	76.32	71.61	76.26	72.03	60.37	71.53	75.70	72.14	62.55
$X_{7\text{-}3}$	94.64	95.97	93.75	84.32	94.01	80.81	95.57	84.16	94.46	80.42	95.52	76.78
X_8	0.00	0.00	0.00	0.28	0.00	0.56	0.00	0.00	0.00	0.26	0.00	0.00
X_9	0.01	0.01	0.01	1.70	0.01	2.08	0.60	0.60	0.01	1.57	0.59	0.59
X_{10}	0.00	0.00	0.00	0.54	0.00	0.92	0.03	0.05	0.00	0.52	0.03	0.05
X_{11}	80.56	86.20	85.29	27.97	63.53	22.61	68.10	29.95	77.60	29.12	77.39	38.59

The work of Sumarcz-Gorska, which suggested stopping aeration as soon the respiration rate (OUR) dropped below a certain threshold, was the inspiration behind this controller; if the respiration rate is sufficiently low, aeration is switched off in the three aerated reactors (AER1-2 & 3) and denitrification can take place as shown in **Figure 6.4e**. Finally **Fgiure 6.4f** shows the change in the TSS set point when the temperature changes in order to keep the biomass active during winter periods

It is important to mention that the results obtained by this analysis depend greatly on both the selection of models and the evaluation criteria. In this case study the recommended models are those proposed by the IWA task group on benchmarking WWTP control strategies. The results of the analysis would be completely different if different model-types or numbers of criteria were used.

6.2.3 *Step 7. Multivariate* analyses

The behaviour of the proposed controllers is evaluated by simulation using the previously mentioned set of evaluation criteria. The correlation between effluent quality (X_1) and operating costs (X_2) indexes is shown in **Figure 6.5a**. At the same time, this plot differentiates strategies with (A_4, A_6, A_8, A_{10} and A_{12}) and without (A_1, A_2, A_3, A_5, A_7, A_9 and A_{11}) an external carbon source addition, according to their environmental and economic values. **Figure 6.5b** correlates the overall risk of bulking ($X_{7\text{-}1}$) and foaming ($X_{7\text{-}2}$) and groups strategies: 1) with both TSS controller and external carbon source (A_8 and A_{12}), 2) with external carbon source but without TSS controller (A_4, A_6 and A_{10}), and 3) the rest of the strategies (A_2, A_3, A_6 and A_9). This approach proposed by Gernaey *et al.*, 2007 approach gives a quick but only partial overview of controller performance. First and foremost the relationships between the control strategies discovered in each plot are based only on a single pair of criteria. Secondly, this approach is not capable of finding the main features amongst multiple criteria. Finally, it is not possible to know if the criteria used to find a relationship are really discriminant or not with respect to the rest of the criteria. Therefore, other tools are necessary to carry out further complex evaluations to deal with both complexity and ambiguity amongst those indices during *multicriteria* evaluation. Thus, the evaluation matrix (data for 26 evaluation criteria collected for 12 control strategies) is subjected to the *multivariate* statistical techniques previously described to explore the behaviour of the control strategies tested on a plant-wide level.



a b

Figure 6.5. Representation of two pairs of evaluation criteria for all the evaluated strategies

6.2.3.1. *Step 7.1* Cluster Analysis (CA)

CA rendered a dendrogram where all the implemented control strategies are grouped into two main statistically significant clusters (results not shown). The first (strategies A_1, A_2, A_3, A_5, A_7, A_9 and A_{11}) and the second cluster (strategies A_4, A_6, A_8, A_{10} and A_{12}) correspond to strategies without and with exogenous carbon source addition respectively. If these clusters are further classified, four groups of control strategies can be found. Thus, the first cluster is divided into a subgroup containing strategies A_1, A_2, A_3, A_5, A_9 and a second subgroup containing strategies A_7 and A_{11} (**Figure 6.6a**). The second cluster is subdivided into a subgroup with strategies A_4, A_6, A_{10} (cluster 4.3) and another subgroup containing strategies A_8 and A_{12} (**Figure 6.6b**). The clustering indicates that there are four main types of control strategies, where the presence or absence of external carbon source addition control and/or a TSS controller are the key elements creating the differences between the clusters.

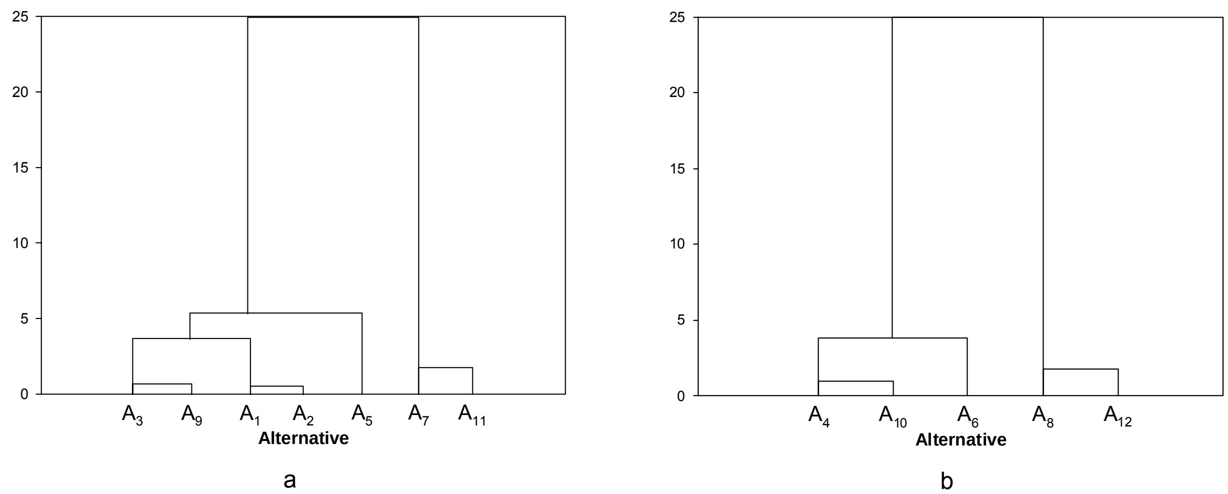


Figure 6.6. Dendrogram showing clustering of the implemented control strategies in the WWTP studied for the first (a) and the second (b) group of control strategies

6.2.3.2. *Step 7.2*. Principal component/factor analysis (PCA/FA)

PCA/FA is applied to the autoscaled simulation output to compare the evaluation criteria between the implemented control strategies and to identify the most influential factors. PCA of the entire data set resulted in five PCs with eigenvalues >1. A varimax rotation of the PCs to five different VFs explained about 94.70% of the total variance.

The values of the PCs are further cleaned up using this technique; in VFs, original variables contribute more clearly (see **Table 6.4)**. The factor loadings are classified as "*strong*", "*moderate*" and "*weak*", corresponding to absolute loading values of > 0.70, 0.70-0.5 and <0.5 (Liu *et al.*, 2003).

Table 6.4. Loadings of the evaluation criteria on the first rotated PC for the complete data set. The variable $X_{7\text{-}1,1}$ is excluded from this analysis because it exhibits a constant value (i.e. zero variance).

OBJ	X_i	Description	VF1	VF2	VF3	VF4
OBJ_1	$X_{1\text{-}1}$	TKN	0.41	-0.53	***-0.71***	0.05
	$X_{1\text{-}2}$	Total nitrogen concentration	***-0.96***	0.18	-0.03	0.14
	$X_{1\text{-}3}$	COD	***0.88***	0.44	0.08	-0.01
	$X_{1\text{-}4}$	BOD_5	***0.97***	0.16	0.06	-0.04
	$X_{1\text{-}5}$	TSS	***0.87***	0.46	0.09	-0.02
	X_1	Effluent quality index	***-0.94***	0.23	-0.02	0.15
OBJ_2	$X_{3\text{-}1}$	Sludge production	***0.83***	-0.54	-0.04	-0.07
	$X_{3\text{-}2}$	Aeration energy	0.42	-0.25	***0.84***	-0.07
	$X_{3\text{-}3}$	Pumping energy	0.69	-0.25	-0.07	0.50
	$X_{3\text{-}4}$	External carbon source	***0.94***	-0.32	-0.04	-0.07
	$X_{3\text{-}5}$	Mixing energy	-0.01	-0.11	***-0.85***	-0.21
	$X_{3\text{-}6}$	Heating energy	***0.79***	-0.60	-0.01	-0.07
	$X_{3\text{-}7}$	Methane production	***0.79***	-0.60	-0.02	-0.08
	X_3	Operating cost index (OCI)	***0.89***	-0.35	0.29	-0.06
OBJ_3	$X_{7\text{-}1,2}$	low DO bulking risk	-0.34	0.07	0.18	***0.81***
	$X_{7\text{-}1,3}$	low F/M bulking risk	-0.02	***0.97***	0.06	-0.12
	$X_{7\text{-}1}$	Overall risk of bulking	-0.09	***0.95***	0.08	0.02
	$X_{7\text{-}2,1}$	Low F/M foaming risk	0.11	***0.98***	0.01	0.00
	$X_{7\text{-}2,2}$	High S_s/X_s foaming risk	0.24	*-0.92*	0.01	-0.14
	$X_{7\text{-}2}$	Overall risk of foaming	0.12	***0.98***	0.01	-0.01
	$X_{7\text{-}3}$	Rising risk	***-0.89***	0.30	0.28	-0.02
OBJ_4	X_8	TIV COD	***0.84***	0.49	0.09	0.02
	X_9	TIV BOD_5	***0.88***	0.46	0.06	-0.01
	X_{10}	TIV TSS	***0.92***	0.32	0.01	-0.16
	X_{11}	TIV TN	***-0.95***	0.18	-0.04	0.12

VF1, which explains 51.76% of the total variance, has strong (in bold) positive loadings for $X_{1\text{-}3}$, $X_{1\text{-}4}$, $X_{1\text{-}5}$, $X_{3\text{-}1}$, $X_{3\text{-}4}$, $X_{3\text{-}6}$, $X_{3\text{-}7}$, X_3, $X_{7\text{-}3}$, X_8, X_9 and X_{10} and strong negative loading for $X_{1\text{-}2}$, X_1, $X_{7\text{-}3}$ and X_{11}. This VF correlates operating costs and denitrification efficiency. It is important to emphasize that the periodic addition of an external carbon source ($X_{3\text{-}4}$) implies a subsequent increase in sludge production ($X_{3\text{-}1}$) and thus also an increase in methane ($X_{3\text{-}7}$) and heating energy ($X_{3\text{-}6}$) production, resulting from sludge digestion. As a result, there is an improvement in the denitrification rates, reducing the total effluent nitrogen ($X_{1\text{-}2}$), the percentage of time that the TN is in violation (X_{11}) and the overall effluent quality index (X_1), but leading to poorer organic carbon removal efficiency (see the strong positive loading in $X_{1\text{-}3}$, $X_{1\text{-}4}$, $X_{1\text{-}5}$, X_8, X_9, X_{10}) and high operating costs (X_3) as a trade off. Also, the increase in the denitrification rate caused by the addition of an external carbon source causes a reduction in the amount of nitrate nitrogen that is transported from the last aerobic reactor to the sedimentation tank, thereby reducing the risk of rising sludge ($X_{7\text{-}3}$). VF2, which explains 29.81% of the total variance, presents strong positive loadings for $X_{7\text{-}1,3}$, $X_{7\text{-}2,1}$, $X_{7\text{-}1}$ and $X_{7\text{-}2}$. This VF highlights the fact that low F/M ratios are the main cause of foaming and bulking. VF3, explaining 8.70% of the total variance, has a strong positive loading for $X_{3\text{-}2}$, and a strong negative loading for $X_{1\text{-}1}$ and $X_{3\text{-}5}$. This correlation is mainly due to improvement in the nitrification process when the airflow in the aerobic zone increases. It is important to point out how the mixing energy ($X_{3\text{-}5}$) increases when the air flow to the aerobic section is switched off in order to maintain completely mixed conditions for the biomass. Finally VF4, which explains 4.4% of the total variance, presents only strong positive correlation with DO bulking problems ($X_{7-1,2}$).

Once the principal components are identified and labelled, the scores obtained by the implemented control strategies can be calculated as a linear combination of the original variables. The representation of the scores is depicted in **Figure 6.7**.

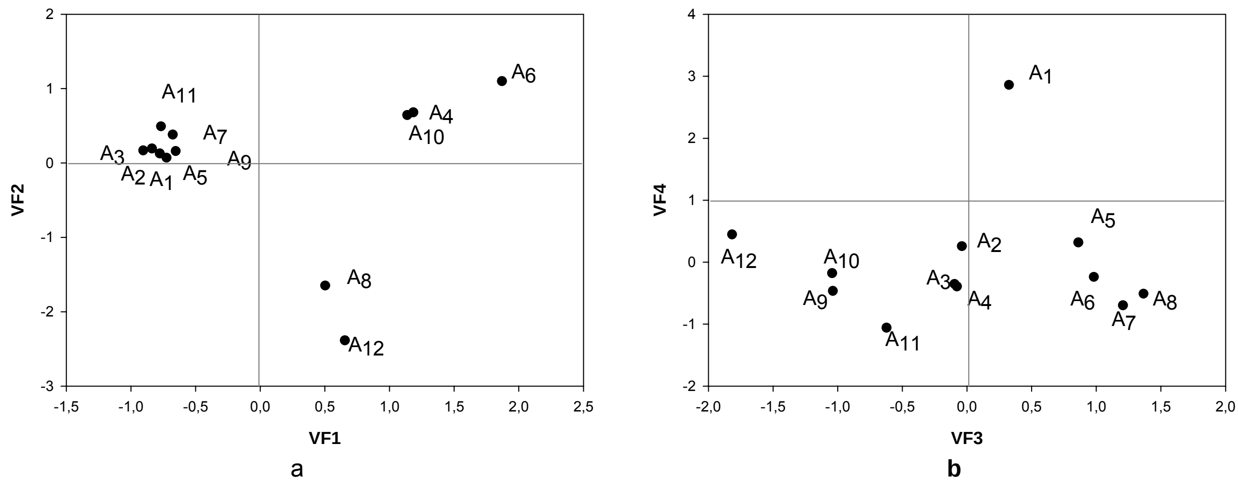


Figure 6.7. Principal component scores for the implemented control strategies for principal component 1 and 2 (a) and for principal component 3 and 4 (b)

As expected, the results of PCA/FA are in good agreement with the CA. Control strategies with an external carbon addition (clusters 4.3 and 4.4) present positive scores in VF1, and are characterized by high operating costs and a low effluent nitrate concentration (see **Figure 6.7a**). Cluster 4.4 presents low scores in the varifactor VF2 associated with bulking and foaming problems. This is attributable to a higher F/M ratio due to the addition of an external carbon source and a reduction in the biomass in the reactor during summer, a direct consequence of the TSS controller. Strategies A_4, A_6 and A_{10} (strategies with external carbon addition and without a TSS controller) got high scores in VF2 because there is not such a reduction of biomass and the TSS values are high during the whole year. VF3 separates the strategies with an oxygen cascade controller (A_5, A_6, A_7 and A_8) from the strategies with an OUR controller (A_9, A_{10}, A_{11} and A_{12}) – **Figure 6.7b** – because these scenarios typically have a rather high aeration air flow rate in order to reduce the ammonium concentration. Otherwise, the control strategies with an ON/OFF cascaded PI controller got high values in VF3 mainly due to lower aeration costs and higher mixing energy consumption. Finally, the occasional deficit of DO and the high F/M ratios (results not shown) in the default open loop control strategies (A_1) causes high values in VF4 (DO bulking risk).

6.2.3.3. *Step 7.3.* Discriminant Analysis (DA)

Finally, discriminant analysis (DA) is performed to divide the original data set into the four groups obtained by CA - control strategies with and without an external carbon source and control strategies with and without TSS controller. The control strategy is the grouping variable, while all the evaluation criteria are the independent variables. DA is performed using all the evaluation criteria except X_{11}, rendering the corresponding classification matrixes (CM) and assigning 100% of the cases correctly. The step-wise DA shows that the criteria $X_{3\text{-}4}$, $X_{3\text{-}7}$, $X_{7,1\text{-}3}$, $X_{7,2\text{-}1}$, $X_{7\text{-}3}$ and $X_{7,1}$ are the discriminant parameters.

The correct grouping pattern of DA coincides with the clusters obtained in CA. Both CA and DA predict important differences in water quality, operating costs and plant performance due to the impact of external carbon addition and TSS control. The discriminant functions are listed in **Table 6.5.**

Table 6.5. Classification functions (see Eq. 6.3.) for discriminant analysis of the implemented WWTP control

	Description	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$
$X_{3\text{-}4}$	External carbon source	-0.261	-0.142	0.0005
$X_{3\text{-}7}$	Methane production	0.891	1.358	0.057
$X_{7\text{-}1,3}$	Low F/M bulking risk	-2.878	-6.719	7.245
$X_{7\text{-}2,1}$	Low F/M foaming risk	26.929	-6.915	0.810
$X_{7\text{-}3}$	Rising risk	2.591	0.239	-0.089
$X_{7\text{-}1}$	Overall risk or bulking	12.138	16.441	-4.225
$C_{i.k}$	Constant	-4652.75	-6455.57	-479.65

Figure 6.8 represents the scores of each control strategy to a determined discriminant function (Dk). D1 presents the highest discriminant ability (84.5%) separating cluster 4.1 and 4.2 from cluster 4.3 and 4.4. This is mainly due to the effect of the external carbon source controller in overall plant performance (see **Figure 6.8a**). The TSS controller in the last aerated reactor explains the separation of clusters 4.1 and 4.3 from clusters 4.2 and cluster 4.4 by D2 as shown in **Figure 6.8a**. Function D2 has a lower discriminant power than D1 (14.7% of the total variance). Finally, D3, with the least explanation of the total variance (0.8%), discriminates clusters 4.1 and 4.4 from clusters 4.2 and 4.3 (see **Figure 6.8b**).

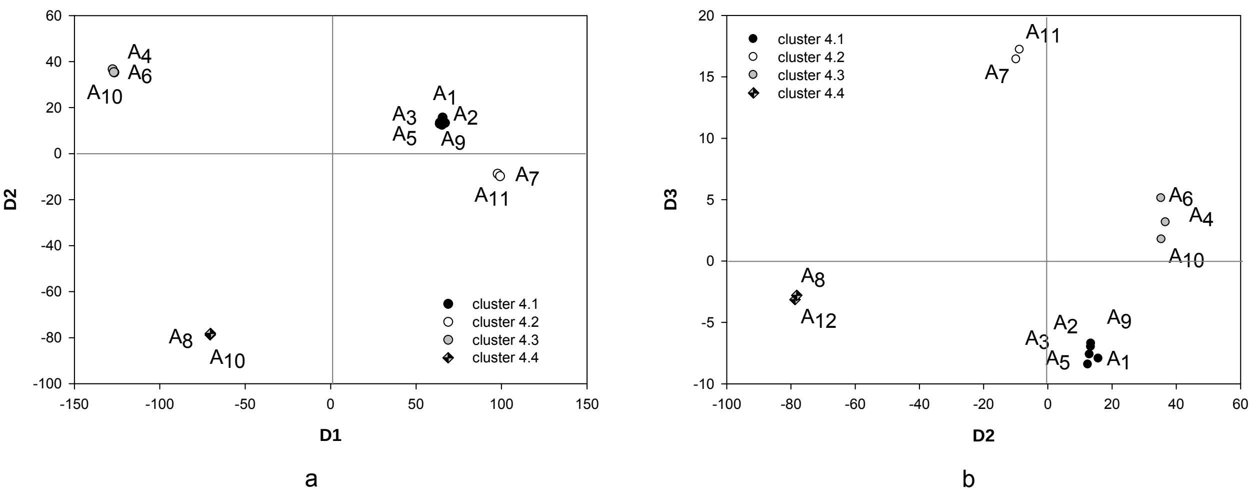


Figure 6.8. Classification functions (see Eq. 6.3.) for discriminant analysis of the implemented WWTP control

Finally, it is important to mention that the tool developed is an excellent complement to the rest of the techniques developed in this thesis. The *multivariate* statistical analysis carried out can be also applied when evaluating *critical decisions* (further details in **Chapter 5)** or during *uncertainty* analysis (**Chapter 7**).

6.3. CONCLUSIONS

This chapter has contributed to improve the *multicriteria* evaluation of WWTPs using a methodology based on *multivariate* statistical techniques, i.e. cluster analysis (CA), principal component/factor analysis (PCA/FA) and discriminant analysis (DA).

Cluster analysis (CA) proved to be a useful tool offering reliable classification of groups of control strategies according to their behaviour. CA performs this function well, rendering four groups of similar control strategies and identifying similar patterns in the control strategies with and without external carbon addition and/or TSS controller.

Principal component analysis/factor analysis (PCA/FA) showed the main correlations between the evaluation criteria and the control strategies influencing those criteria. The five PCs identified were responsible for 94.7% of the total variability (compared to 26 original variables). As a result, various synergies were identified, e.g. better denitrification capacity with lower risk of rising and low F/M ratios as main causes of foaming and bulking. Tradeoffs were also identified, e.g. better nitrification capacity with higher aeration energy. In addition, with the results of the factorial scores, it proved possible to identify the similarities between the implemented control strategies and the PCs extracted in the first part of the analysis.

Finally, discriminant analysis (DA) showed that only six parameters are useful for discriminating within the classes obtained by CA. Three discriminant functions were obtained, allowing 100% correct assignation and resulting in considerable data reduction. The representation of the discriminant scores allowed the important features amongst the discriminant variables and the group of classified control strategies to be found.

To summarize, this study has shown how the combination of these *multivariate* statistical techniques serves as an excellent exploratory tool for both the analysis and interpretation of complex *multicriteria* data sets. As a result, there is a significant improvement in the accessibility of information needed for effective evaluation of control strategies. There is also a reduction in the cognitive load on the decision maker, yielding more knowledge than current evaluation methods and enhancing understanding of the whole evaluation process.

6.4. CRITERIA QUANTIFICATION SECTION (I).

Impact on water is calculated using the same means as used in other chapters in this thesis, i.e. as a weighted averaged sum of relevant effluent concentrations. The difference in this case is the evaluation period $t_f - t_0$, which has been extended from one week to one year (365 days).

$$EQ = \frac{1}{(t_f - t_0)} \int_{t_0}^{t_f} PU(t) \cdot Q_e(t) \cdot dt \qquad \text{(A6.1)}$$

PU is the result of applying **A6.2.**

$$PU(t) = PU_{TSS}(t) + PU_{COD}(t) + PU_{BOD}(t) + PU_{TKN}(t) + PU_{NO_X}(t) \qquad \text{(A6.2)}$$

The effluent polluting loads PU_K (kg·day^{-1}) corresponding to the component k (TSS, COD, BOD_5, TKN and NO_X) are calculated through **A6.3**

$$PU_K = \beta_K C_K \qquad \text{(A6.3)}$$

where $\beta_{TSS} = 2$, $\beta_{COD} = 1$, $\beta_{BOD5} = 2$, $\beta_{TKN} = 20$ *and* $\beta_{NOx} = 20$. *IQ* is calculated in a similar way to the *EQ* index, simply replacing the effluent data with the influent data.

The estimation of the operating costs at plant wide level is calculated as a weighted sum of different costs (Vrecko *et al.*, 2006) as stated in **equation A6.4**

$$X_3 = AE + PE + 3 \cdot SP + 3 \cdot EC + ME - 6MP + \max(0, HE^{net}) \qquad \text{(A6.4)}$$

where *AE* is aeration energy, *PE* is pumping energy, *SP* is sludge production for disposal, *EC* is external carbon addition, *ME* is mixing energy, *MP* stands for methane production and HE^{net} is the heating energy needed to increase the temperature of the sludge in the anaerobic digester. Compared to the previous chapters, the weight for the *SP* has been reduced to 3. This is because the cost of sludge treatment disposal is now estimated to be considerably lower compared to the values suggested for BSM1 since large parts of the sludge treatment are now part of the whole plant. The value of the weight of *MP* is set to 6, which implies that around 43% of the theoretical energy content of the methane can provide electricity for the gas motor. Most of the remaining energy (50%) is assumed to be available for heating the influent sludge in the digester and about 7% is lost.

Aeration energy (*AE*), calculated in terms of kW·h·day^{-1}, is modelled as presented in **equation A6.5** and is based on the aeration consumption of the Degremont DP230 porous disk. However an improvement in the calculations has been made on the equation suggested in Copp (2002) by also including the volume of the aeration tanks

$$AE = \frac{24}{t_f - t_0} \int_{t_0}^{t_f} \sum^{i=n} [c_1 \cdot K_L a_t \left(\frac{V_i}{V_{ref}} \right) \cdot (t)^2 + c_2 K_L a_t \left(\frac{V_i}{V_{ref}} \right) \cdot (t)^2] \cdot dt \qquad \text{(A6.5)}$$

where K_La is the oxygen transfer rate (d^{-1}) in the individual tank, V_i is the individual tank volume (m^3) and V_{ref} is 1333 m^{-3}. In this way, aeration energy can be calculated using different volumes than the ones proposed by the BSM1 configuration. Again, the main difference lies in the evaluation period $t_f - t_0$, which has been extended from one week to one year (365 days).

Pumping energy (*PE*) is calculated using the approach presented in the criteria quantification section in **Chapter 4**. However, this time the pumping requirements of the additional units are included in the index, as shown in **equation A6.6.** The additional flows are: Q_{pr} primary clarifier underflow rate, thickener unit underflow Q_{tu} and dewatering unit overflow rate Q_{do}:

$$PE = \frac{1}{(t_f - t_0)} \int_{t_0}^{t_f} \begin{pmatrix} PE\_Q_{\text{int}} \cdot Q_{\text{int}} + PE\_Q_r \cdot Q_r + PE\_Q_w \cdot Q_w + \\ PE\_Q_{pr} \cdot Q_{pr} + PE\_Q_{tu} \cdot Q_{tu} + PE\_{}_{do} \cdot Q_{do} \end{pmatrix} \cdot dt \qquad \text{(A6.6)}$$

The suggested values for *PE* are the following: $PE\_Q_{intr} = 0.004\ kWh\cdot m^{-3}$, $PE\_Q_r = 0.008\ kWh\cdot m^{-3}$, $PE\_Q_w = 0.05\ kWh\cdot m^{-3}$, $PE\_Q_{pr} = 0.075\ kWh\cdot m^{-3}$, PE_Q_{tu}: $0.060\ kWh\cdot m^{-3}$ and PE_Q_{do}: $0.004\ kWh\cdot m^{-3}$.

Sludge production for disposal (*SP*) is calculated based on the amount of solids that are accumulated in the plant and from the solids that are removed from the plant as dewatered sludge. The equation to calculate sludge production in the whole WWTP is stated in **A6.7**

$$SP = \frac{1}{(t_f - t_o)}\left(M_{TSS}(t_f) - M(t_o) + \int_{t_0}^{t_f} TSS_{du}(t)\cdot Q_{du}(t)\cdot dt \right) \quad \text{(A6.7)}$$

where $Q_{du}(t)$ is the dewatering unit underflow flow rate and TSS_{du} represents the total solids concentration in the underflow of the dewatering unit. M_{TSS} (see **equation A6.8**) represents the total suspended solid mass present in the individual unit processes:

$$M_{TSS}(t) = M_{TSS,as}(t) + M_{TSS,s}(t) + M_{TSS,p}(t) + M_{TSS,ad}(t) + M_{TSS,ss}(t) \quad \text{(A6.8)}$$

In which

$$M_{TSS,as}(t) = \sum_{i=1}^{5} TSS_i(t)\cdot V_i \quad \text{(A6.9)}$$

$$M_{TSS,s}(t) = \sum_{i=1}^{10} TSS_j(t)\cdot z_j \cdot A \quad \text{(A6.10)}$$

$$M_{TSS,p}(t) = TSS_p(t)\cdot V_p \quad \text{(A6.11)}$$

$$M_{TSS,ad}(t) = TSS_{ad}(t)\cdot V_{ad} \quad \text{(A6.12)}$$

$$M_{TSS,ss}(t) = TSS_{ss}(t)\cdot V_{ss} \quad \text{(A6.13)}$$

In the above equations, V_i,, V_p, V_{ad} and V_{ss} represent the volume of the activated sludge tank i (m^3), the primary clarifier, the anaerobic digester and the sludge storage tank respectively: z_j is the height of a layer in the secondary settler (m), whereas *A* equals the total area of the settler (m^2). It is important to notice that total solids concentration in the anaerobic digester (TSS_{ad}) is calculated in a simple way by using the ASM1 states generated as the output of the ADM1/ASM1 interface. The problem of defining a new TS value based on ADM1 state variables is thereby avoided and TSS throughout the BSM2 is based on ASM1 state variables.

The amount of chemicals (CS) is modelled as presented in **A6.14.**

$$CS = \frac{COD_s}{(t_f - t_0)\cdot 1000}\int_{t_0}^{t_f} Q_{carb}\cdot dt \quad \text{(A6.14)}$$

where COD_s is the carbon source concentration ($4\cdot 10^5$ g COD·m^{-3}) and Q_{carb} is the external carbon flow rate.

Mixing energy (ME) combines the energy used for mixing the activated sludge tanks (ME_{as}) and the energy used for mixing the anaerobic digester (ME_{ad})

$$ME = ME_{as} + ME_{ad} \quad \text{(A6.15)}$$

Mixing energy in the activated sludge units is calculated as described in Chapter 4, which implies that each individual activated sludge tank requires a mechanical mixing only when K_La is lower than 20 d^{-1}. In other cases the aeration is assumed to be enough to maintain the activated sludge in suspension.

$$ME_{unit,as} = \frac{24}{(t_f - t_0)} \int_{t_0}^{t_f} \begin{bmatrix} k_L a_i(t) < 20d^{-1} \rightarrow ME_{unit} \cdot V_i \\ k_L a_i(t) > 20d^{-1} \rightarrow 0 \end{bmatrix} \cdot dt \qquad \text{(A6.16)}$$

It is assumed that the anaerobic digester is mixed constantly, so the mixing energy can be calculated simply as:

$$ME = 24 \cdot ME_{unit,ad} \cdot V_{ad} \qquad \text{(A6.17)}$$

where $ME_{unit.as}$ and $ME_{unit.ad}$ is the mixing energy consumption for the activated sludge and anaerobic digester respectively, with a value of 0.005 kW·m^{-3}.

Methane production (MP) in the anaerobic digester represents an economic benefit and can be included in the cost index as a negative cost. An average value of the quantity of methane produced per day can be derived from **equation A6.18.**

$$CS = \frac{p_{atm} \cdot 16}{T \cdot R \cdot Temp_{op}} \int_{t_0}^{t_f} \frac{1}{p_{gas,tot}(t)} \cdot p_{gas,CH4}(t) \cdot Q_{gas}(t) \cdot d(t) \qquad \text{(A6.18)}$$

where $p_{gas.CH4}$ (bar) is the pressure of the methane gas produced in the head space, R is the universal gas constant (8.3145·10^{-2} bar·m^{-3}·kmol^{-1}·K^{-1}), $Temp_{op}$ is the operating temperature of the anaerobic digester (308.15 K), $p_{gas.tot}$ (bar) is the total gas pressure in the head space, p_{atm} (bar) is the atmospheric pressure (1.013bar) and Q_{gas} (m^3·day^{-1}) is the normalized gas flow rate produced (at p_{atm}). The number 16 represents the atomic weight of methane and $t_f - t_0$ is the total evaluation period.

The term heating energy (*HE)*, defined as max (*0, HE^{net}*), takes into account the energy demand for heating the anaerobic digester, which is met by the heat generated by the gas motor assumed to be used for the electrical production of biogas, at least if the anaerobic digester is operating efficiently. Assuming that 1 kg CH_4 produces 7 kWh of heat from the gas motor, the net heating demand will be as expressed in **equation A6.19**

$$HE^{net} = \max(0, HE - 7 \cdot MP) \qquad \text{(A6.19)}$$

A correction needs to be made as the term can never be negative. Therefore, any surplus heat that may be produced during the generation of electricity that is not used for heating the anaerobic digester is not evaluated elsewhere.

The energy needed to heat the flow of sludge fed to the anaerobic digester is calculated as the average energy input needed to heat the inlet sludge flow to the anaerobic digester until it reaches the desired temperature in the anaerobic digester.

$$HE = \frac{24}{86400 \cdot (t_f - t_0)} \int_{t_0}^{t_f} \rho_{H20} \cdot c_{H20} \cdot (Temp_{op} - Temp_{ad,in}(t)) \cdot Q_{ad}(t) \cdot dt \qquad \text{(A6.20)}$$

where ρ_{H20} is the water density (1000 kg·m^{-3}), c_{H20} is the specific heat capacity of water (4.1816 kJ·kg^{-1}), $Temp_{op}$ is the operating temperature of the anaerobic digester (35^{o}C or 308.15K), $Temp_{ad.in}$ is temperature of the anaerobic digester influent (expressed in the same units as $Temp_{op}$) and Q_{ad} is the flow rate to the anaerobic digester (m^3·day^{-1}). It is assumed that the sludge is heated with a constant heat, and reaches the desired temperature within the hydraulic retention time. Heat losses to the surroundings via the digester walls are ignored in the calculation.

The percentages of time when the effluent violates legal limits also have to be reported. The effluent limits in this case are defined as follows: TN < 18 g N·m^{-3}, COD < 100 g COD·m^{-3}, BOD_5 < 10 g·m^{-3} and TSS < 30 g TSS·m^{-3}.

6.5. CRITERIA QUANTIFICATION SECTION (II)

For long simulation periods, the result of the risk of separation problems model is smoothed by means of an exponential filter with a time constant related to the dynamics of each specific problem. The filter can be written as shown in **equation A6.21**

$$y_{filtered}(t) = \alpha \cdot y_{filtered}(t-1) + (1-\alpha) \cdot y(t) \quad \text{(A6.21)}$$

where $y_{filtered}$ represents the filtered data, y is the raw data and α is calculated according to:

$$\alpha = 1 - \frac{1}{t_k * \left(\frac{1440}{sample} \right)} \quad \text{(A6.22)}$$

where t_k represents the time constant in days and *sample* is the sampling interval in minutes. Applying the filter, with a time interval of two hours for rising sludge and three days for filamentous bulking and foaming problems facilitates visualization and interpretation of the risk assessment results

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

PhD THESIS

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CHAPTER 7: *MULTICRITERIA* EVALUATION OF WASTEWATER TREATMENT PLANTS ALTERNATIVES UNDER *UNCERTAINTY*

The objective of this chapter is to develop a systematic procedure to support *multicriteria* evaluation of wastewater treatment plant (WWTP) alternatives under *uncertainty*. Although WWTPs are relatively well characterized processes, some of the model parameters used to carry out the evaluation of the alternatives can present *uncertainty* e.g. influent fractions of the wastewater arriving to the treatment plant and the effect of either toxics compounds or temperature on the kinetic and stoichiometric parameters affecting the resulting rank of preferences. The chapter consists of two sections. Firstly, there is the evaluation of the different WWTP alternatives using *multicriteria* decision analysis setting the model parameters at their default value following the same approach as developed in Chapter 4. In the second section, the *uncertainty* in model parameters is introduced i.e. input *uncertainty*, characterising it by means of probability distributions based on the available process knowledge. Then, input *uncertainty* is sampled using the Latin Hypercube sampling method and Monte Carlo simulations are run to see how those input uncertainties are propagated through the model and affect the different outcomes.

This procedure brings several benefits such as: i) the quantification of the variation of the overall degree of satisfaction of the design objectives for the generated WWTP alternatives, ii) the identification of that environmental, legal, economic and technical objectives to the existing variance and finally iii) the analysis of the influence of the relative importance of the design objectives during the selection of alternatives.

The chapter is organized in the following way. First there is a description of the developed methodology. Next, using a modified version of the IWA Benchmark Simulation Model No 2 as a case study, the proposed systematic procedure shows the variation in the decision making when the *uncertainty* in the ASM1 model parameters is either included or not during the evaluation of WWTP control strategies. The results show that the control strategies with an external carbon source addition reduce the output *uncertainty* in the criteria used to quantify the degree of satisfaction of environmental, technical and legal objectives, but increasing the economical costs and their variability as a trade-off. Also, it is shown how a preliminary selected alternative with cascade ammonium controller becomes less desirable when input *uncertainty* is included, while simpler alternatives are evaluated to have a higher chance of being successful. The chapter ends with a sensitivity analysis where it is shown how a control strategy becomes more or less favoured depending on the prioritization of objectives.

7.1. METHODOLOGY

The fourth block (*Uncertainty* Analysis) follows an evolutionary approach that combines dynamic simulation, random number generation, descriptive statistics and *multicriteria* decision analysis to assist the decision maker during the selection of the best alternative in accordance with the defined objectives, input *uncertainty* and the WWTP process performance. It comprises different steps organized in two phases: (I) *hierarchical* generation and *multicriteria* evaluation of the design alternatives and (ii) *uncertainty* analysis. A flowchart that highlights the most important steps in the procedure is shown in **Figure 7.1**

In the first phase, a reference case is presented, by evaluating and comparing several WWTP alternatives based on the traditional method, i.e. by using the default (deterministic) values of model parameters (see **Chapter 4** for further deatails). Secondly (Phase II), the WWTP alternatives are compared while considering *uncertainty* in the model parameters. Subsequent sections describe these steps in more detail

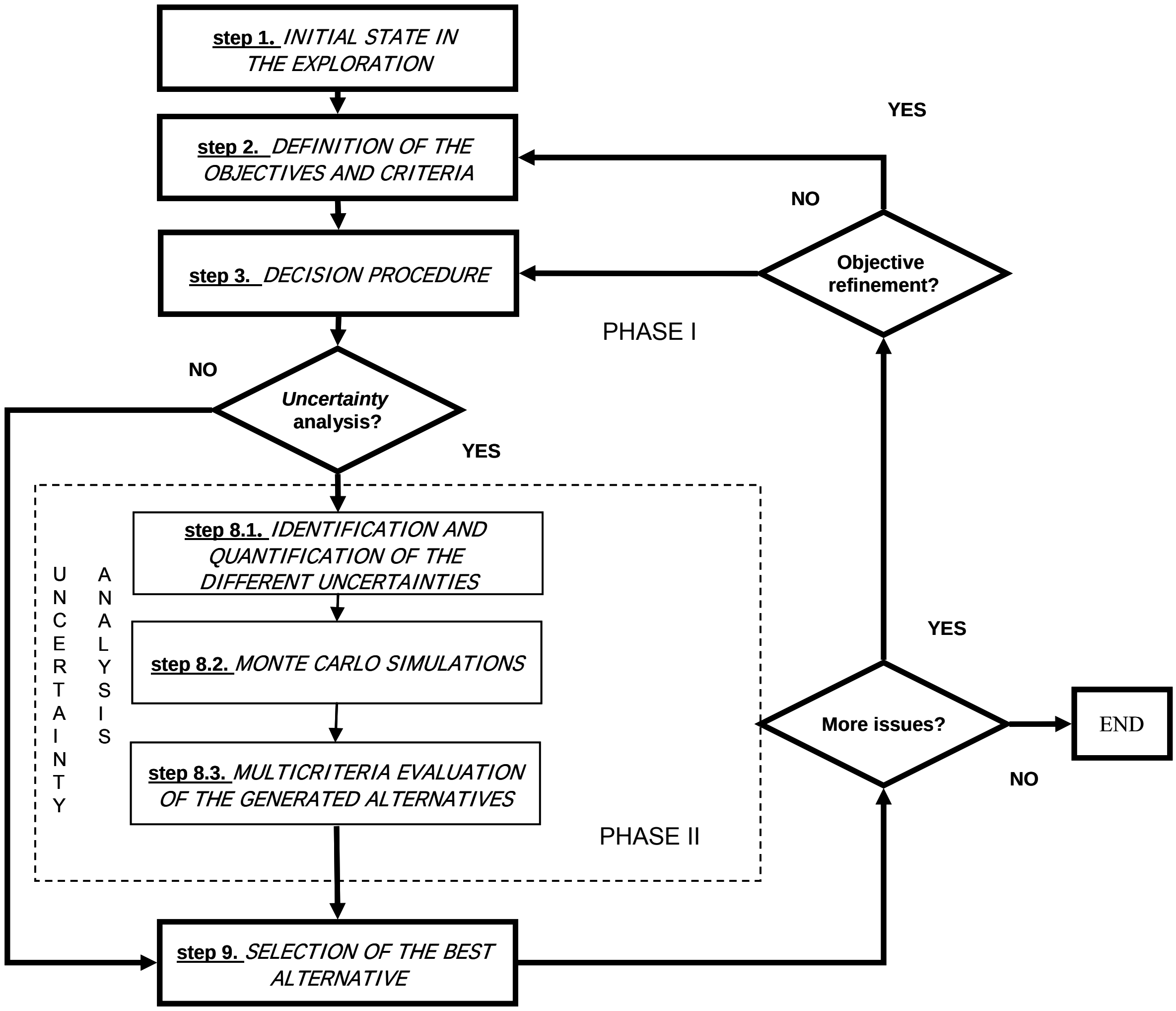


Figure 7.1. Flow diagram of the conceptual design methodology

Phase I. *Hierarchical* generation and *multicriteria* evaluation of design alternatives (*multicriteria* evaluation of WWTP alternatives without *uncertainty*)

Step 1, 2 & 3 have the same function as already presented in the previous chapters. In the first step (*Step 1*) there is a collection of all the information required to carry out the analysis. It involves the description of the WWTP to be studied, the flow rate, the composition and the dynamics of the wastewater to be treated, the applicable legislation. *Step 2* includes the definition of the objectives $[OBJ = \{OBJ_1,..,OBJ_P\}]$ and the evaluation criteria $[X = \{X_1,..,X_W\}]$ used to measure the degree of satisfaction of objectives$[w= \{w_1,..,w_p\}]$. In step 3 there are a number of tasks such as: the identification of the issue to be solved I_1 (*Step 3.1*), the generation of the alternatives $[A = \{A_1,...,A_m\}]$ (*Step 3.2*); the selection of a subset of criteria $[X = \{X_1,...,X_n\}]$ defined for this issue (*Step 3.3*) and evaluation of the alternatives (*Step 3.4*) to finally select one with the results obtained by the weighted sum (see **equation 4.1**)

It is important to emphasize – similarly to several other chapter in the thesis – that although this methodology was used (*Steps 1-3*) to generate and evaluate the design alternatives, other procedures could also be applied for the generation and evaluation of design alternatives e.g. those proposed by Kim and Smith (2004) or Shonnard and Hiew (2000).

Phase II. *Multicriteria* evaluation of WWTP alternatives under *uncertainty*

The focus of this chapter is on the second phase of the procedure and comprises *Steps 8.1, 8.2* and *8.3*. The second phase of the proposed procedure is considered for those decisions that require to be evaluated under *uncertainty* or simply when the robustness of a decision needs to be tested. *Step 8.1* starts with the identification of the types of model parameter *uncertainty* that are to be studied $[H = \{H_1\ldots, H_H\}]$. The different types of uncertainties considered using the proposed methodology are represented as H and specified by subscript h, with H the total number of uncertainties taken into account. Next, for each H_h a number of *uncertainty* parameters are identified $[U = \{U_1\ldots, U_U\}]$ and quantified by means probability distribution functions $[D = \{D_1\ldots, D_U\}]$ based on the available process knowledge. Next , in *Step 8.2* the WWTP model is then coupled to a Monte Carlo engine that randomly samples parameters from the selected parameter distributions, thus solving the model and quantifying the evaluation criteria for each parameter sample (Mckay *et al*., 1979; Iman *et al*., 1981). Finally in *Step 8.3*, the new probability functions generated during this iterative process can be aggreated using the metrics defined in the previous chapter (**equation 4.1**) quantifying the variation in the overall degree of satisfaction of the design objectives for the generated WWTP alternatives and identifying the contributions of the different objectives to the existing variance

Summarizing, based on the information generated during phase I and II, the decision maker is more confident in *Step 9* when selecting the most desirable option amongst the generated alternatives. It is important to highlight that the quantification of this *uncertainty* with the developed tool will not eliminate *uncertainty*. Rather, by quantifying it, a better knowledge can be developed on how the overall process performance may vary. Therefore, more informed and rational decisions about selection of one or another option can be made. The same procedure is applied to solve each issue generated trough the proposed procedure that merits *uncertainty* analysis until the conceptual design of the WWTP is completed

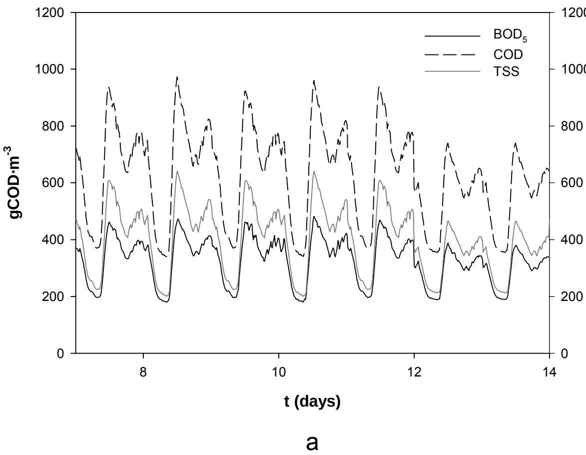
7.2. CASE STUDY # 5: EVALUATION OF WWTP CONTROL STRATEGIES AT PLANT WIDE LEVEL - II

The implementation and evaluation of control strategies in order to improve the organic carbon and nitrogen removal and their evaluation at the plant wide level is used to illustrate the capabilities of the proposed procedure. Each of the steps in the procedure, together with the numerical details, is described and discussed in detail in the following sections

7.2.1. *Step 1 & 2*. Initial state in the exploration and definition of the control objectives and criteria

The different control strategies are implemented in the activated sludge bioreactor of the Benchmark Simulation Model N^o 2 plant (see schematic representation of the whole WWTP in **Figure 6.1**). The predenitrifying activated sludge unit has a modified Ludzack-Ettinger configuration with five reactors in series. Tanks 1 (ANOX1) and 2 (ANOX2) are anoxic with a total volume of 2000 m^3, while tanks 3 (AER1), 4 (AER2) and 5 (AER3) are aerobic with a total volume of 3999 m^3. The secondary settler presents a surface area of 1500 m^2 with a total volume of 6000 m^3 The BSM2 plant further contains a primary clarifier (PRIM), a sludge thickener (THK), an anaerobic digester (AD), a storage tank (ST) and a dewatering unit (DH). Further details about the plant layout can be found in **Chapter 6.**

Plant performance evaluation has been reduced from one year simulation to one week in order to reduce the computational burden of the whole study. The default dry weather wastewater to be treated has a flow rate of 18500 m^3·day^{-1} with an organic and nitrogen load of 12228 kg COD·day^{-1} and 1025.20 kg N·day^{-1} respectively. The wastewater influent is the same as for the Benchmark Simulation Model N^o 1, but increasing the particulate concentration of organic matter and nitrogen in order to take into account the effect of the primary clarifier. **Figure 7.2** shows both dynamic influent profiles for organic matter and nutrients



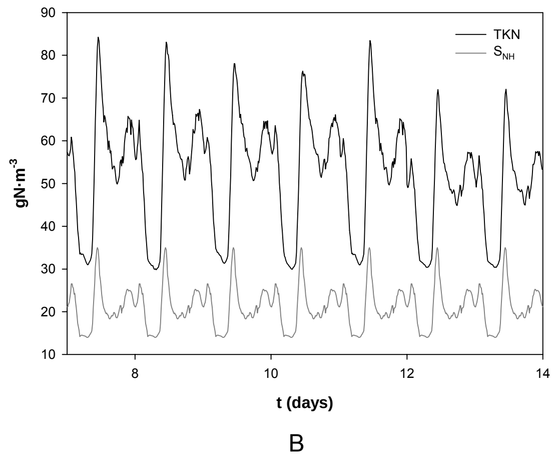


Figure 7.2. Influent wastewater a) organic matter (TSS, COD and BOD$_5$) and b) nitrogen (TKN and ammonium) profile

Finally, the operating cost budget is restricted to 15000. **Table 4.1** (**Chapter 4**) shows the objectives and the set of criteria used to quantify their degree of satisfaction. Different weights are assigned to each objective in order to assign their relative importance. Nevertheless, as weight assignment is not the topic of the thesis, equal importance is considered for the different objectives, thus w_p = 0.25.

7.2.2. *Step 3*. Decision procedure

The improvement of the overall biological nitrogen removal by means of different control strategies is the analyzed issue (I_I= 1) in this case study. All the biological nitrogen removal processes include an aerobic zone in which biological nitrification occurs i.e. ammonium oxidation to nitrate. Some anoxic volume or time must be foreseen to provide biological denitrification to complete the objective of the total nitrogen removal where the produced nitrate is reduced to nitrogen gas. This nitrate reduction requires an electron donor, which can be supplied in form of the influent wastewater, by endogenous respiration or by addition of an external carbon source.

Five modifications of the original reactor (m=5) are considered to solve this issue by means of the implementation of the combination of the controllers. The main features of the different combinations of controllers used to improve the overall plant performance are summarized in **Table 7.1.** Also, in **Figure 6.4** (**Chapter 6**) the dynamic behavior of some of these controllers can be seen.

Table 7.1. Main features of the controllers to be evaluated by the proposed procedure

Oxygen controller in the aerated section		
Controller type	PI with anti-windup	
Proportional gain	100	$m^3(g\ (-COD))^{-1}\cdot d^{-1}$
Integral time constant (Ti)	0.01	d
Anti wind up constant (Tt)	0.01	d
Controller variable	S_o in AER1, 2 & 3	
Set point	2	$g\ (-COD)\cdot m^{-3}$
Manipulated variable	K_La	d^{-1}
Max deviation of MV	300	d^{-1}
Implemented in alternatives	A_2, A_3, A_4, A_5 and A_6	
Nitrate controller in the anoxic section		
Controller type	PI with anti-windup	
Proportional gain	10000	$m^3(g\ N)^{-1}\cdot d^{-1}$
Integral time constant (Ti)	0.04	d
Anti wind up constant (Tt)	0.04	d
Controller variable	S_{NO} in ANOX2	
Set point	1	$g\ N\cdot m^{-3}$
Manipulated variable	Q_{intr}	$m^3\cdot d^{-1}$
Max deviation of MV	92336	$m^3\cdot d^{-1}$
Implemented in alternatives	A_3 and A_5	
Nitrate controller in the anoxic section		
Controller type	PI with anti-windup	
Proportional gain	-1	$m^3(g\ N)^{-1}\cdot d^{-1}$
Integral time constant (Ti)	0.1	d
Anti wind up constant (Tt)	0.1	d
Controller variable	S_{NO} in ANOX2	
Set point	1	$g\ N\cdot m^{-3}$
Manipulated variable	Q_{carb}	$m^3\cdot d^{-1}$
Max deviation of MV	5	$m^3\cdot d^{-1}$
Implemented in alternatives	A_4 and A_6	
Ammonium controller in the aerated section		
Controller type	Cascaded PI	
Proportional gain	-1	$m^3(g\ N)^{-1}\cdot d^{-1}$
Integral time constant (Ti)	0.2	d
Anti wind up constant (Tt)	0.2	d
Controller variable	S_{NH} in AER3	
Set point	1	$g\ N\cdot m^{-3}$
Manipulated variable	S_o set point in AER3,4 & 5	$m^3\cdot d^{-1}$
Max deviation of MV	0-5	$g(-COD)\cdot m^{-3}$
Implemented in alternatives	A_5 and A_6	

In turn, a set of 7 (n) criteria selected from **Table 4.1** are used to evaluate the alternatives generated for this issue: X_1 (impact on water), X_2 (operating costs), risk of microbiology-related solids separation problems (X_7) and X_8 –X_{11} (time in violation). As happened in the previous case study, in order to enhance the comprehension of the whole evaluation process subcriteria are included in the analysis in such a way as summarized in **Table 6.2.** in **Chapter 6**. Moreover it is important to point out that the objective of this case study is to evaluate the overall performance of the presented controller rather than the start-up. For this reason construction costs are excluded from the analysis

All the criteria are quantified by dynamic simulation in a Matlab-Simulink© environment. The primary clarification is based on Ottherpohl and Freund (1992) and Otterpohl *et al*. (1994). The IWA Activated Sludge Model number 1 (ASM1) is chosen as a biological process model for the reactor (Henze *et al*., 2000) while the double exponential settling velocity of Takács *et al*. (1991) based on the solid flux concept, was selected as a fair representation of the settling process with a ten layer discretization. Both gravity thickening and dewatering units are ideal and continuous models with no biological activity and 98 % of solids removal efficiency respectively. The anaerobic digester is based on the International water Association Anaerobic Digestion Model No 1 (Batstone *et al*., 2002). Finally the recent work of Nopens *et al*. (2008) has been used for the interfaces between the AD and AS models.

The DO sensor is assumed to be ideal without noise or delay. The nitrate (S_{NO}) and ammonium (S_{NH}) nitrogen sensors had a time delay of 10 minutes, with zero mean white noise (standard deviation of 0.1 g $N{\cdot}m^{-3}$). All the dynamic simulations follow a steady state simulation; this ensures a consistent starting point and eliminates bias due to the selection of the initial conditions in the dynamic modelling results (Copp, 2002). Even though the length of the dynamic influent time series used as WWTP input to carry out the simulations is 28 days, only the data generated during the last seven days are used to quantify the criteria. As mentioned several times already in the thesis, it is important to remark that the result of the case study highly depends on the model selection. Selection of different models to represent the processes taking place in the WWTP under study can lead to different conclusions.

Table 7.2. Score profiles for the six evaluated alternatives without *uncertainty*

	A_1	A_2	A_3	A_4	A_5	A_6	Units
X_1	8114.10	7770.90	7784.70	5879.90	7108.70	5824.90	g pollution·m^{-3}
X_3	10682	9853	9787	13551	9187	12746	-
X_{7-1}	78.89	78.00	78.08	80.79	77.93	80.33	%
X_{7-2}	77.94	77.94	77.75	81.94	77.73	81.05	%
X_{7-3}	86.32	94.37	91.01	91.25	97.67	85.05	%
X_8	0.00	0.00	0.00	0.00	0.00	0.00	%
X_9	0.00	0.00	0.00	0.00	0.00	0.00	%
X_{10}	0.00	0.00	0.00	0.00	0.00	0.00	%
X_{11}	44.79	15.18	18.01	0.00	6.85	0.00	%

To compare the effects of the different criteria during the evaluation procedure, it is necessary to map these score profiles into normalized values because all those criteria are measured in different units. Value functions award values from 0 to 1 to the worst and the best situation considered respectively, whilst a mathematical function is proposed to evaluate the intermediate effects. The extreme profiles (based on expert judgment) are summarized in the following lines

$$[(x_{i*}) = (x_{1*}= 60935 \text{ kg pollution}\cdot\text{day}^{-1}, x_{3*}= 15000, x_{7\text{-}1*}= 100\ \%, x_{7\text{-}2*}= 100\ \%, x_{7\text{-}3*}= 100\ \%, x_{8*}= 100\ \%, x_{9*}= 100\ \%, x_{10*}= 100\ \%, x_{11*}= 100\ \%)]$$

and

$$[(x_i^{*}) = (x_1^{*}= 0 \text{ kg pollution}\cdot\text{day}^{-1}, x_3^{*}= 7500, x_{7\text{-}1}^{*}= 0\ \%, x_{7\text{-}2}^{*}= 0\ \%, x_{7\text{-}3}^{*}= 0\ \%, x_8^{*}= 0\ \%, x_9^{*}= 0\ \%, x_{10}^{*}= 0\ \%, x_{11}^{*}= 0\ \%)]$$

A linear model was applied between these extreme values to calculate the intermediate effects (e.g. for criterion X_2 the value function is $v(X_2) = - 0.000113\cdot X_2 +2$). Finally, a multi-objective function calculated as a weighted sum (**equation 4.1**) was applied in order to obtain a single value for all the alternatives which were then ranked according to the scores obtained, with the final decision as to which alternative is best in fulfilling the evaluation criteria resting on the decision maker. As weight assessment is not a central topic in this paper, equal importance for all the objectives is assumed (w_p = 0.25). The results of the weighted sum lead us to the following conclusion: in accordance with the control objectives, alternative A_5 with a score $S(A_5)$ of 0.75 is the selected option, while A_1, A_2, A_3, A_4 and A_6 with a score in the weighted sum of 0.68, 0.72, 0.72, 0.63 and 0.66 respectively are rejected.

Despite the fact that this control strategy has a higher risk of rising, alternative A_5 is the most favourable mainly because this alternative showed the lowest scores in OBJ_2 (*minimize economical costs*). The latter result is basically attributed to an efficient use of the aeration energy in this control strategy, providing just the sufficient quantity of oxygen to maintain a reasonable effluent ammonium concentration. Also, it is important to mention that alternative A_5 performed well in both environmental (OBJ_1) and legal (OBJ_4) objectives, because this control strategy improves the overall nitrification efficiency.

7.2.3. *Step 8. Uncertainty* analysis of WWTP alternatives

7.2.3.1. Step 8.1. Identification and quantification of the input *uncertainty* of the ASM model.

In this section, the same control strategies presented in **Table 7.1** were evaluated, but now incorporating *uncertainty* in the ASM parameters (H_h = 1). The main objective was to investigate the influence of those input uncertainties on the model predictions, and to evaluate whether the ranking of the alternatives found for the deterministic approach (see previous section) was influenced by including the effect of *uncertainty* in the analysis. This section of the chapter provides details of the procedure followed to evaluate the WWTP control strategies under *uncertainty*: first, the quantification of the input *uncertainty* of the ASM model parameters is presented; then the set-up of the Monte Carlo simulations is explained, and finally *multicriteria* evaluation of the simulation results is presented and discussed in detail.

Even though the BSM2 contains several submodels as explained above, the scope of the work was entirely focused on the ASM parameters, i.e. *uncertainty* in the settler and anaerobic digester model parameters was not considered. To carry out this analysis, the *uncertainty* associated to the ASM parameters *[U = U_1,…,U_u,…U_{32}]* was characterized by a set of probability distributions *[D = D_1,…,D_u,…D_{32}]*. These distributions were assumed to characterize a degree of belief with respect to where the appropriate values for the elements of [U] are located for use in the simulation of the BSM2. When used in this manner, these distributions are providing a quantitative representation of what is referred as subjective or epistemic *uncertainty* (Helton and Davis, 2003).

Table 7.3. Parameter distributions used for the Monte Carlo simulations including default parameter values and assigned parameter class and variation range for class 1 and 2 parameters

Uncertainty parameter ($U_{p,\ K\&S}$)	Symbol	Default value	Class	range	Units
autotrophic yield	Y_H	0.67	1	0.067	g COD·(g N)$^{-1}$
heterotrophic yield	Y_A	0.24	1	0.024	g COD·(g COD)$^{-1}$
fraction of biomass to particulate products	f_P	0.08	1	0.008	Dimensionless
fraction of nitrogen in biomass	i_{XB}	0.08	1	0.008	g N (g COD)$^{-1}$ in biomass
fraction of nitrogen in particulate products	i_{XP}	0.06	1	0.006	g N(g COD)$^{-1}$ in X_P
conversion from COD to particulates	X_{I2TSS}	0.75	1	0.075	g TSS.(g COD)$^{-1}$
conversion from COD to particulates	X_{S2TSS}	0.75	1	0.075	g TSS.(g COD)$^{-1}$
conversion from COD to particulates	X_{BH2TSS}	0.75	1	0.075	g TSS.(g COD)$^{-1}$
conversion from COD to particulates	X_{BA2TSS}	0.75	1	0.075	g TSS.(g COD)$^{-1}$
conversion from COD to particulates	X_{U2TSS}	0.75	1	0.075	g TSS.(g COD)$^{-1}$
maximum specific heterotrophic growth rate	μ_H	4.00	2	2.00	d^{-1}
half saturation (hetero. growth)	K_S	10.00	2	5.00	g COD.m^{-3}
half saturation (hetero. oxygen)	K_{OH}	0.20	2	0.10	g COD.m^{-3}
half saturation (nitrate)	K_{NO}	0.50	2	0.25	g N.m^{-3}
heterotrophic specific decay rate	b_H	0.30	2	0.15	d^{-1}
maximum specific autotrophic growth rate	μ_A	0.50	2	0.25	d^{-1}
half saturation (auto. growth)	K_{NH}	1.00	2	0.50	g N.m^{-3}
half saturation (auto. oxygen)	K_{OA}	0.40	2	0.20	g COD.m^{-3}
autotrophic specific decay rate	b_A	0.05	2	0.02	d^{-1}
anoxic growth rate correction factor	η_g	0.80	2	0.40	dimensionless
ammonification rate	k_a	0.05	2	0.02	m^3(g COD.d)$^{-1}$
maximum specific hydrolysis rate	k_h	3.00	2	1.50	g X_S(g X_{BH} COD·d)$^{-1}$
half saturation (hydrolysis)	K_X	0.10	2	0.05	g X_S(g X_{BH} COD)$^{-1}$
anoxic hydrolysis rate correction factor	n_{yh}	0.80	2	0.40	Dimensionless

In this case study those distributions were developed through interpretation of available process knowledge. Three *uncertainty* classes were distinguished *[C = C_1, C_2, C_3]* to allow presentation of the parameter *uncertainty* in a structured way, and each *uncertainty* parameter U_y was assigned to a certain class C_c depending on the extent of knowledge available in the literature about this specific parameter value. The first class was assigned to low *uncertainty* and included mostly stoichiometric parameters. In this class (C_1), the parameters were assumed to have a 5 % upper and lower bound around their default values [U_1,…, U_{10}]. The second class (C_2), corresponded to medium *uncertainty* and involved kinetic parameters such as the maximum specific growth rate and the affinity constants [U_{11},…, U_{24}]. In this class, 25 % upper and lower bounds around the default values were assumed. For simplification, all the kinetic and stoichiometric parameters were supposed to be independent although the authors are aware of possible correlations amongst several parameters e.g. the maximum specific growth rate and the half saturation constants. **Table 7.3** summarizes these parameters, the classes to which they belong and the range of evaluated parameters.

Finally, the third class of *uncertainty* (C_3) corresponded to high *uncertainty* and included the influent fraction related parameters, assuming upper and lower bounds equal to 50 % of the default parameter values. **Figure 7.3** represents how the *uncertainty* in the influent fractions is handled in this case study. Several class 3 *uncertainty* factors were applied to the default stoichiometric coefficients used to calculate the different ASM1 influent state variables – such as the soluble readily biodegradable substrate (S_S) or the particulate biodegradable substrate (X_S) concentration – from the influent COD load, resulting in a range of influents to be applied in the simulations [U_{25},…,U_{28}]. A similar method was applied to influent nitrogen [U_{29},…,U_{32}], where the fraction coming from particulate products and biomass was removed first, to finally obtain the inorganic (ammonium, S_{NH}) and organic influent nitrogen compound concentrations (either soluble or particulate, S_{ND} or X_{ND}).

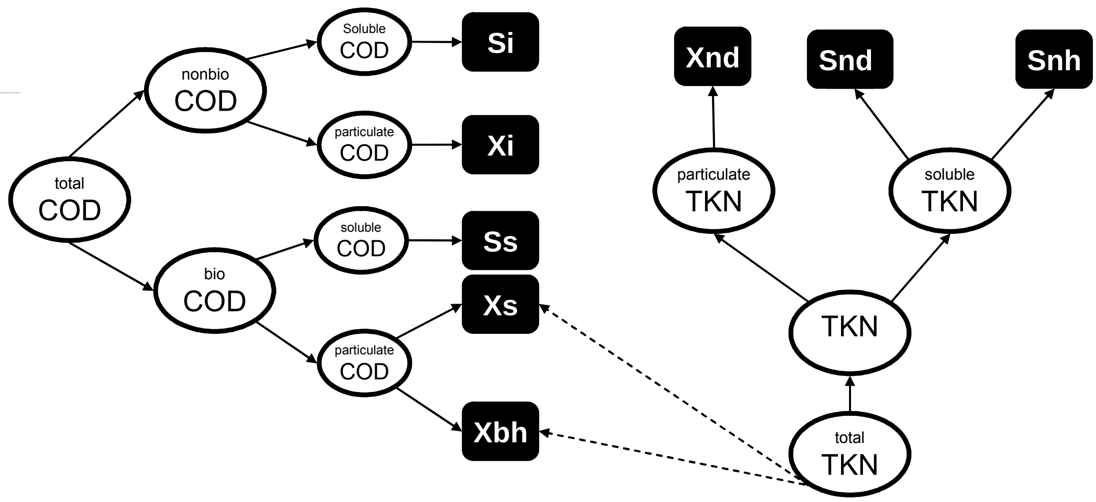


Figure 7.3. Illustration of the influent fractionation procedure and the assumed parameters in the fractionation

In order to maintain the COD and N mass balances the *uncertainty* in the different fractions is obtained in a hierarchical fashion as shows **Figure 7.3**. Thus, for example first of all is calculated the *uncertainty* in the non-biodegradable fraction of COD using a C_3 *uncertainty* factor, while the biodegradable fraction is determined as the difference between 1 and the non-biodegradable fraction. Next, once the non-biodegradable fraction is determined, the *uncertainty* is then about the soluble and particulate fraction. Again, a C_3 *uncertainty* factor is used to determine one i.e. soluble (S_i) while the other i.e particulate (X_i) is quantified as the difference between the total non-biodegradable fraction and the soluble fraction. A similar procedure is used for the biodegradable fraction and its respectively state variables such as S_S (soluble organic fraction), X_S (organic particulate fraction) and heterotrophic biomass (X_{BH}). In **Table 7.4** are represented the stoichiometric factors and their *uncertainty* used to obtain the different influent fractions

Table 7.4. Mean values of the dynamic stoichiometric factor and their *uncertainty* used to calculate the different influent fractions

Uncertainty parameter ($U_{p, K\&S}$)	Symbol	Default value	Max-Min	Units
Fraction of soluble inorganic in COD	α_{SI}	0,09	0,17	$gS_i \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of particulate inorganic in COD	α_{XI}	0,18	0,22	$gX_i \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of soluble organics in COD	α_{SS}	0,12	0,20	$gS_S \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of particulate organics in COD	α_{XS}	0,53	0,33	$gX_S \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of heterotrophic biomass in COD	α_{XBH}	0,07	0,11	$gX_{XB} \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of ammonium in TKN	α_{SNH}	0,65	0,31	$gS_{NH} \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of organic soluble in TKN	α_{SND}	0,14	0,17	$gS_{ND} \cdot m^{-3} \cdot gCOD \cdot m^{-3}$
Fraction of organic particulate in TKN	α_{XND}	0,21	0,21	$gX_{ND} \cdot m^{-3} \cdot gCOD \cdot m^{-3}$

It is important to point out that despite the apparent advantages of a formal assessment of *uncertainty*, one should be aware that the conclusions arising from this case study considering *uncertainty* can always only be as good as the underlying assumptions. Thus, the results of the *uncertainty* analysis will to a large extent depend on the characteristics of the defined distributions, similar to the base case performance where the obtained results will depend on the model selection, as indicated earlier

7.2.3.2. Step 8.2. Monte Carlo Simulations

The input *uncertainty* space is sampled using the Latin Hypercube method (McKay *et al.*, 1979; Iman *et al.,* 1981). In this study, 1000 samples $[U_{u,y} = U_{1,1},\ldots,U_{1,y},\ldots U_{1,1000}]$ are generated to make sure that the input *uncertainty* space is covered uniformly. Each Latin Hypercube sample contains one randomly selected value $U_{u,y}$ from each of the previously defined probability distributions D_u. The Monte Carlo simulations are performed by evaluating the BSM model for each one of the generated Latin Hypercube samples, solving the entire model and quantifying the defined criteria [X] for each tested alternative [A]. The solution of the model for each parameter combination results in a distribution of possible values for the desired performance criteria, whose distributions reflect the possible variation of the performance criteria taking into account the input *uncertainty*. Both interpretation and representation of the results of the Monte Carlo simulations is subsequently carried out using descriptive statistical techniques such as multiple box plots, error bar charts, three dimensional representations of the inter-quartile range, etc. The following paragraphs focus on the interpretation of the simulation results, describing how the defined uncertainties are propagated trough the model and affect the different outcomes for each evaluated alternative.

ENVIRONMENTAL OBJECTIVES (OBJ_1)

According to the previous section, a single criterion (X_1) is used to quantify the degree of satisfaction of objective OBJ_1 (*minimize environmental impact*). **Figure 7.4** shows the results of the Monte Carlo simulations in a box plot fashion (Hair *et al.*, 1998). The different box plots illustrate that there is a clear pattern: all the control strategies including an external carbon source addition (A_4 and A_6) result in lower values in both average effluent quality index terms and in effluent quality index variability, i.e the range between the first and the third quartile is smaller compared to the other control strategies.

This differentiation between the control strategies can be explained by the lack of soluble biodegradable carbon in the influent and the low hydraulic retention time in the biological reactor, resulting in poor denitrification rates as long as no external carbon source is dosed. The external carbon source addition results as an extra electron donor enhancing the total nitrogen removal by improving the reduction of the produced nitrate to nitrogen gas and decreasing the impact of the nitrate term in the effluent quality index. Also, this input increases the robustness of the denitrification because this process now no longer depends on the organic substrate contents in the influent. Instead, the controller is now supplying the necessary biodegradable carbon to maintain the nitrate concentration in the second anoxic reactor (ANOX2) at the desired set point.

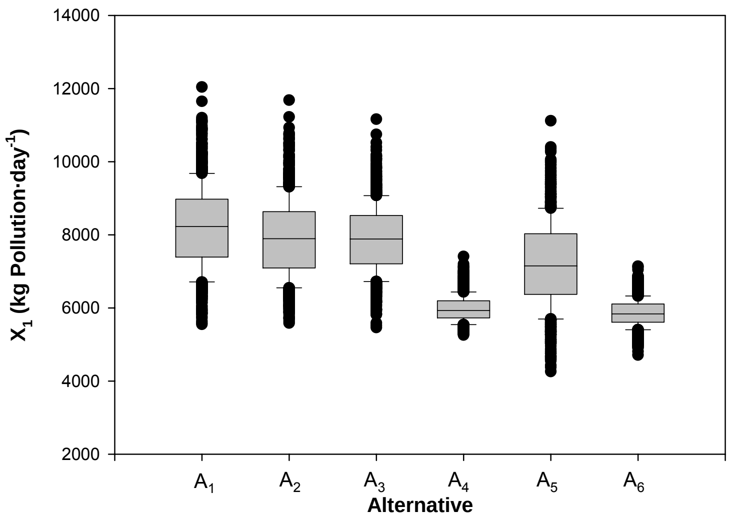


Figure 7.4. Effluent quality index (X_1) variation using a multiple box plot representation.

It is also important to point out the effect of the S_{NH} cascade controller in the propagation of the *uncertainty* when it is compared to other control strategies, e.g. the open loop controller (A_1) and the DO controller (A_2, A_3 and A_4). The S_{NH} controller with its DO set point that varies as a function of the ammonium concentration in the last aerated tank improves the nitrification efficiency of the whole plant and reduces its variability. A constant aeration flow rate or dissolved oxygen set point results in situations where there is either lack of or excess of dissolved oxygen to nitrify all the ammonium entering the plant.

The improvement of the aeration system obtained by introducing the cascade controller reduces the percentage of time when the aeration flow is not adequate e.g. due to differences of the influent load during daytime and night, thus reducing the overall variability of effluent total Kjeldahl nitrogen (TKN) as shown in the frequency histograms of **Figure 7.5.** Nevertheless, **Figure 7.4** reveals that alternative A_5 is the alternative with a larger variation in terms of effluent quality index mainly due to an increase of the *uncertainty* in the denitrification efficiency. This plot elucidates the trade-off that has to be made between improving of nitrification efficiency on the one hand and the overall effluent quality index variation on the other hand.

Regarding the rest of the controllers (A_1, A_2 and A_3), it is just worth mentioning that these do not have a clear effect in both effluent quality and effluent variability reduction. Alternatives A_2 and A_3 result in a slight improvement of the degree of satisfaction of objective OBJ_1, reducing also its variation to a limited extent.

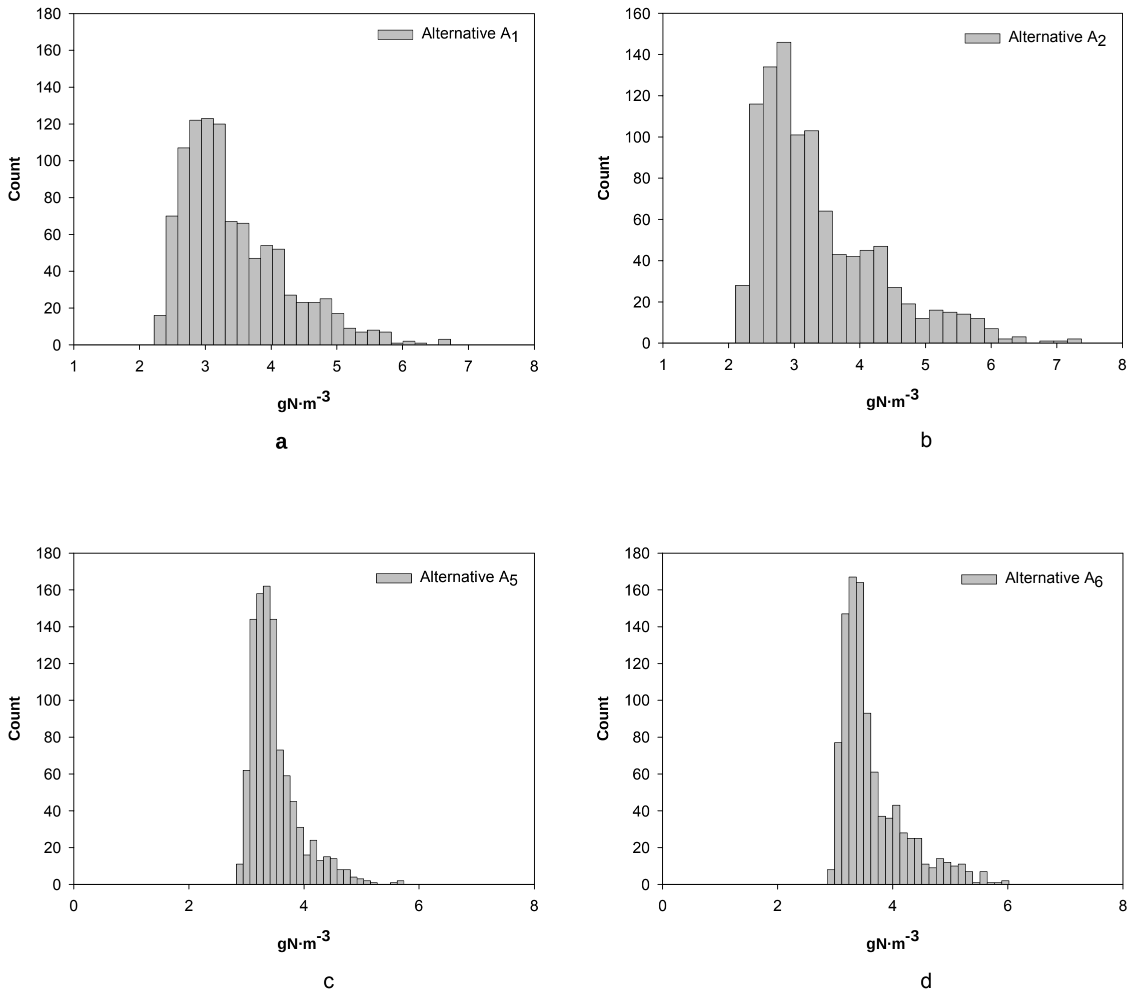


Figure 7.5. Histograms of the effluent TKN variation when alternative A_1 (a), A_2 (b), A_5 (c) and A_6 (d) are evaluated under ASM parameter uncertainty

ECONOMIC OBJECTIVES (OBJ_2)

The plant operating costs (X_2) are used to evaluate the degree of satisfaction of OBJ_2 (*minimize economic costs*). In **Table 7.5** the mean and the standard deviation of the breakdown of the operating costs used to evaluate the economic feasibility of the controllers can be found

Table 7.5.. Mean and standard deviation of the operating costs breackdown for the different generated alternatives under uncertainty

		A_1	A_2	A_3	A_4	A_5	A_6	units
$x_{j,3-1}$	MEAN	2652.56	2654.65	2653.00	2825.55	2653.88	2816.98	$kgTSS \cdot day^{-1}$
	ST.DEV	336.15	336.36	336.12	371.70	336.11	383.29	$kgTSS \cdot day^{-1}$
$x_{j,3-2}$	MEAN	8548.40	7685.97	7751.88	8164.18	7699.25	8547.70	$Kw.h \cdot day^{-1}$
	ST.DEV	0.00	622.03	638.14	670.05	1710.82	2138.73	$Kw.h \cdot day^{-1}$
$x_{j,3-3}$	MEAN	396.47	396.47	250.24	396.71	282.03	396.64	$Kw.h \cdot day^{-1}$
	ST.DEV	0.11	0.11	42.25	0.13	68.33	0.15	$Kw.h \cdot day^{-1}$
$x_{j,3-4}$	MEAN	0.00	0.00	0.00	997.43	0.00	827.00	$kgCOD \cdot day^{-1}$
	ST.DEV	0.00	0.00	0.00	345.35	0.00	478.75	$kgCOD \cdot day^{-1}$
$x_{j,3-5}$	MEAN	648.00	648.00	648.00	648.00	648.00	648.00	$Kw.h \cdot day^{-1}$
	ST.DEV	0.00	0.00	0.00	0.00	0.00	0.00	$Kw.h \cdot day^{-1}$
$x_{j,3-6}$	MEAN	3854.48	3854.72	3854.27	3940.95	3854.49	3916.35	$Kw.h \cdot day^{-1}$
	ST.DEV	41.79	41.79	41.70	48.59	41.65	55.11	$Kw.h \cdot day^{-1}$
$x_{j,3-7}$	MEAN	1659.76	1659.55	1659.39	1715.41	1659.66	1702.79	$m^3CH_4 \cdot day^{-1}$
	ST.DEV	140.84	140.77	140.75	144.89	140.79	144.54	$m^3CH_4 \cdot day^{-1}$
$x_{j,3}$	MEAN	10682.08	9824.52	9740.82	13563.42	9721.67	13468.58	-
	ST.DEV	1490.13	1087.08	1083.81	1724.57	1999.21	3801.00	-

The values in **Table 7.5** again demonstrate a clear difference between the control strategies with and without external carbon source addition. The periodic purchase of an external carbon source (X_{3-4}) implies a subsequent increase of both quantity and variation of the sludge production (X_{3-1}), aeration energy (X_{3-2}), heating energy (X_{3-6}) and the overall operating cost index (X_3) although it should be mentioned that there also is an increase of the methane production (X_{3-7}). The inclusion of carbon source dosage in the control strategy does not have any effect on mixing energy (X_{3-5}) and pumping energy (X_{3-3}), when comparing A_4 and A_6 with A_1. Hence, it can be concluded that the addition of external carbon source reduces the impact on water (X_1) and its variability as a trade-off to an increase of the operating costs (X_3) and their variability.

Alternatives with a DO controller (A_2, A_3, A_4, A_5 and A_6) are characterized by having a larger variation in the aeration costs (see values of $X_{j,3-2}$) when they are compared to the plant running in open loop regime (A_1). The effect of the cascade-ammonium controller can be noticed clearly from the results of **Table 7.** in both alternatives A_5 and A_6: a large variation in operating costs can be observed mainly due to variation in the aeration energy cost (see values of $X_{5,3-2}$ and $X_{6,3-2}$). This fact is attributable to the dynamics of the cascade controller which introduces a variable DO set point instead of the permanent DO set point (2 g(-COD)·m^{-3}) that is applied for the alternatives A_2, A_3 and A_4.

Control strategies A_3 and A_5 have lower average values and higher variability in pumping energy (X_{2-3}) because the controller manipulates the internal recycle in order to maintain the nitrate concentration in ANOX2 to the desired set point (1 g N·m^{-3}).

TECHNICAL OBJECTIVES (OBJ_3)

The risk of occurrence of separation problems (X_7) is used to evaluate the technical reliability (OBJ_3) of the proposed control strategies. As mentioned earlier the risk of microbiology-related solids separation problems is evaluated by determining the operating conditions that potentially can drive the plant to bulking (X_{7-1}), foaming (X_{7-2}) and rising sludge (X_{7-3}). The variation of those indexes is represented in a three dimensional representation in terms of inter-quartile range. At first sight, the results of this figure lead to the following conclusions: Alternatives A_4 and A_6 are clearly different from the rest of the evaluated alternatives. In terms of reduction of the rising risk variability, alternatives with an external carbon source controller present the lowest variability because this type of controller results in a rather low and constant effluent nitrate level, where the presence of high nitrate levels in the settler – and thus the effluent – is the main factor contributing to the occurrence of rising sludge (Comas *et al.*, 2006b).

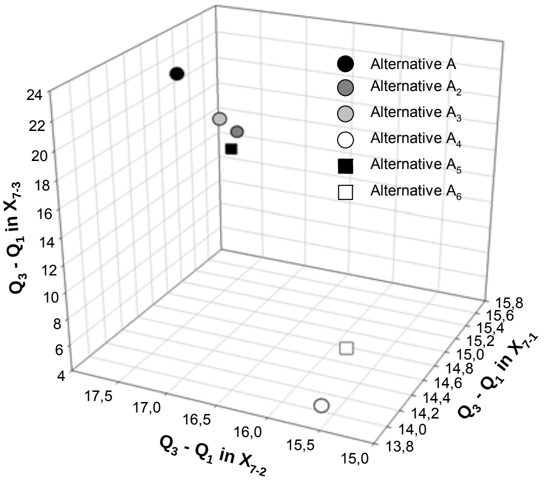


Figure 7.6. Risk of separation problems (X_3), 3-d representation of the inter quartile rang (Q_3 –Q_1) for all the evaluated control strategies under uncertainty

It is important to also highlight the low variation in terms of bulking and foaming risk from one alternative to another. Only the controllers with an external carbon source addition result in a marginal reduction in $X_{7\text{-}1}$ and $X_{7\text{-}2}$ because the food to microorganisms ratio (Comas *et al*., 2006) is more constant for such a scenario due to the external carbon source addition, which will in fact do nothing else than compensate for low influent concentrations of readily biodegradable substrate, for example during night time. On the other hand, again, the external carbon source increases the concentration of solids in the reactor, thus reducing the food to microorganisms ratio and increasing the risk of bulking and foaming.

LEGAL OBJECTIVES (OBJ_4)

Finally, the percentage of time that the plant is in violation of the legal effluent discharge limits for the different pollutants (X_8 – X_{11}) forms the set of criteria to evaluate the accomplishment of OBJ_4 (*comply with the limits set by the law)*. For this case study criteria X_8, X_9 and X_{10} are always below the limits without any variation, and as a consequence they are not useful in discriminating between the competing alternatives. Control strategies A_4 and A_6 are characterized by high denitrification rates because the external carbon source enhances the nitrate reduction to nitrogen gas, and as a consequence the effluent nitrate concentration is continuously below the limits and without variation as shown in **Figure 7.7**.

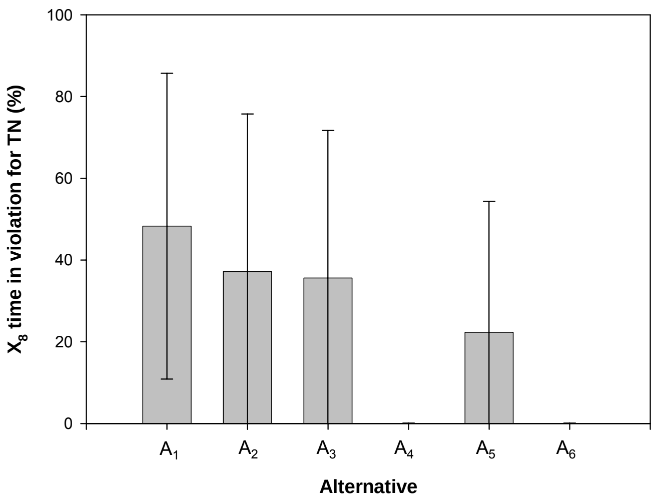


Figure 7.7. Error bar chart of criterion X_{11} (TIV-TN) for the generated control strategies under uncertainty

This fact can be observed in **Figure 7.8** also, where the simulated dynamic TN effluent profile corresponding to the 5 and 95% percentiles are shown for alternatives A_2, A_3, A_4 and A_6 respectively. With respect to the rest of the controllers it can in general be concluded that as long as the level of plant instrumentation increases (more on-line sensors and control) the percentage of the time that the plant is in violation and its *uncertainty* will decrease

7.2.3.3. *Step 8.3. Multicriteria* evaluation of the generated WWTP alternatives

The multi-objective function defined in the previous section (**equation 4.1**) is used as a metric to quantify the overall degree of satisfaction of the control objectives for the different generated alternatives. This metric is calculated for all 1000 simulations that were performed for each alternative, where each simulation is based on one of the parameter combinations resulting from the Latin Hypercube Sampling method described in the previous section. In this case, the most desirable alternative has the highest mean and lowest standard deviation in terms of the multi-objective function. A practical way to see this relationship is by using the coefficient of variation (see **Table 7.6**).

Table 7.6. Mean, standard deviation and coefficient of variation of the multiobjective function for the different control strategies under uncertainty

$S(A_j)$	Alternative A_1	Alternative A_2	Alternative A_3	Alternative A_4	Alternative A_5	Alternative A_6
MEAN	0.68	0.71	0.72	0.63	0.71	0.64
ST.DEV	0.04	0.03	0.02	0.04	0.06	0.10
CV	17.00	24.73	36.00	15.75	11.83	6.40

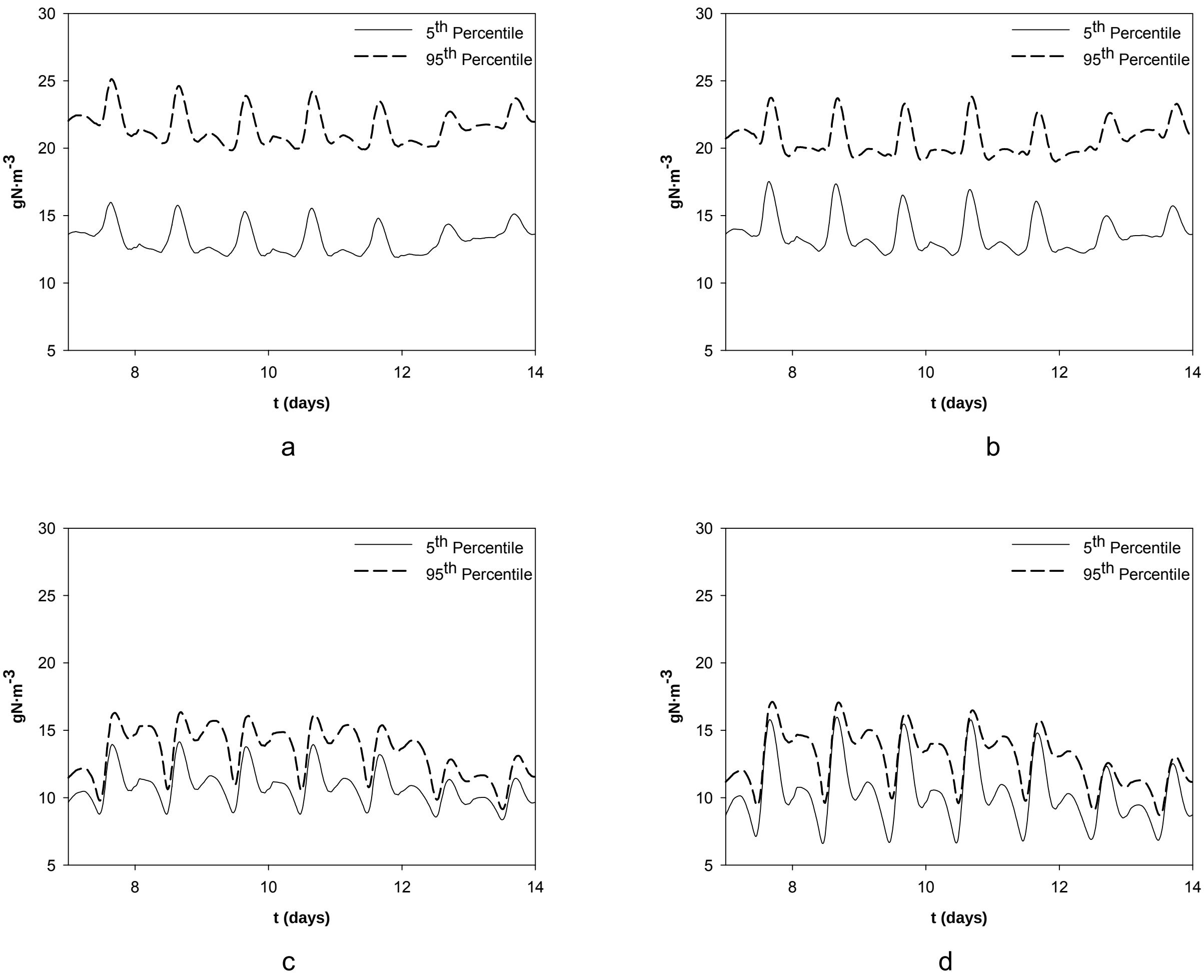


Figure 7.8. Dynamic uncertainty ranges for TN during the evaluation of alternative A_2 (a), A_3 (b), A_4(c) and A_6 (d) under ASM parameters uncertainty. The TN profiles corresponding to the 5th and the 95th percentile resulting from the Monte Carlo simulations are shown.

7.2.4. *Step 9.* Selection of the best alternative

From the results of the previous analyses it is possible to know the contributions of environmental, economic, legal and technical objectives to the variance in the control objectives' overall degree of satisfaction. In this way, Alternatives A_4 and A_6 are the least favoured alternatives because they have the lowest scores in objective OBJ_2 (*minimize economical costs*); i.e. high absolute value and high variability in plant operating cost. This is mainly due to the extra cost of the carbon source and additional sludge production that is induced by applying this strategy. Nevertheless, it must be pointed out that these two alternatives provide the best accomplishment and the lowest variation in objectives OBJ_1 (minimize environmental impact) and OBJ_4 (comply with legal effluent discharge limits). Alternative A_1 is also rejected because of the bad scores in operating costs (OBJ_2), environmental (OBJ_1) and legal objectives (OBJ_4). The lack of instrumentation in this strategy makes the operation really unfeasible, because the plant is always running under the same operating conditions and is not capable to adapt to the different perturbations

It is important to point out that the results demonstrate that when *uncertainty* in the ASM model inputs is considered, then the decision to implement alternative A_5 that was derived from the (deterministic) base case evaluation might be questioned. Despite the fact that alternative A_5 obtained good scores in some of the criteria used to quantify the degree of satisfaction of the considered objectives, it can also be concluded that its performance strongly depends on the selection of the model inputs, i.e. kinetic and stoichometric parameters, and influent fractions. If those inputs are changed from the default values, as is done when performing the Monte Carlo simulations, the same level of accomplishment of the plant objectives can no longer be ensured. For this reason, when considering *uncertainty* on model inputs alternative A_3 comes out as the most desirable alternative that has a higher chance of success, since A_3 has good scores in all the objectives and can thus be considered as the most balanced of the alternatives. Also, the good value in terms of multi-objective mean and standard deviation ensure the robustness of the decision. Hence it cannot be said that alternative A_5 is better than A_3, as was concluded in the deterministic case. Instead, it is now probable that alternative A_3 is better than A_5. This analysis – including *uncertainty* – thus brings about a better documented decision about which alternative to choose, since balancing the accomplishment of the objectives is combined with taking into account the deviations created by the input uncertainties that are considered.

The key to solving this *multicriteria* decision making problem is not easily found, and the solution is based on realizing that different process alternatives have many uncertainties in common. For example, all the generated WWTP control strategies are subjected to identical uncertain influent fractions and kinetic and stoichiometric parameters, but depending on the evaluated alternative, the *uncertainty* will be propagated in a different way. Assuming that the decision maker is particularly interested in a control strategy that promises the lowest environmental impact, then the selected alternative would be A_4. On the other hand, if a compromise between operating costs and risk wants to be ensured that the selected alternative should be A_3.

7.2.5. Sensitivity analysis

The sensitivity analysis of the weights applied to the multi-objective function (**equation 1**) presented in this last part of the chapter is intended to contribute to clarifying how the selected alternative resulting from the *multicriteria* decision making procedure under activated sludge model input uncertainties will vary when the relative importance of the different objectives is changed. The weight represents the desires or preferences of the decision makers to obtain an alternative that maximises the degree of satisfaction and reduces variability for a determined objective.

The results are presented in a bi-plot fashion, where the changes in the selected alternative (z – axis) are represented when the relative importance of the control objectives (x and y axis) is changed. The first example consists of a simplified analysis amongst objectives OBJ_1 (*minimize environmental impact*), OBJ_2 (*minimize economical costs*) and OBJ_3 (*maximize technical reliability*). The importance of the fourth objective (comply with the limits set by the law; OBJ_4) remains constant i.e. $w_4 = 0.25$. The coefficient of variation of the multi-objective function s(A_j) for the six competing alternatives is recalculated to obtain a rank (see also **Chapter 4**)

From the results of **Figure 7.9a** it can be noticed that high values of OBJ_1 clearly favour alternative A_4 above the other alternatives. This is mainly due to the fact that the addition of external carbon source in this strategy will reduce the impact on water by improving the overall nitrogen removal efficiency while simultaneously reducing the variability in the effluent quality as shown in **Figure 7.4**. Nevertheless, as w_2 increase in value the most desirable alternative changes from A_4 to A_3 because alternative A_2 presents lower operating costs and variability as shown in **Table 7.**. It is important to mention that all the alternatives with an ammonium controller (A_4, A_6), although having the lowest values in operating costs, are anyhow not selected when the economic objectives are prioritized. This is mainly due to the high sensitivity of the ammonium controller to the input *uncertainty*, increasing the variance of the *multicriteria* index and thus reducing the coefficient of variation. Finally when objective OBJ_3 is prioritized, the selected alternative depends on the relative contribution of OBJ_1 and OBJ_2 because both alternatives satisfy OBJ_3 in a similar way. Again, it can be said that alternative A_4 improves the coefficient of variation of OBJ_1 (minimize environmental impact) at the expense of sacrificing (to an extent) its economical variability (OBJ_2).

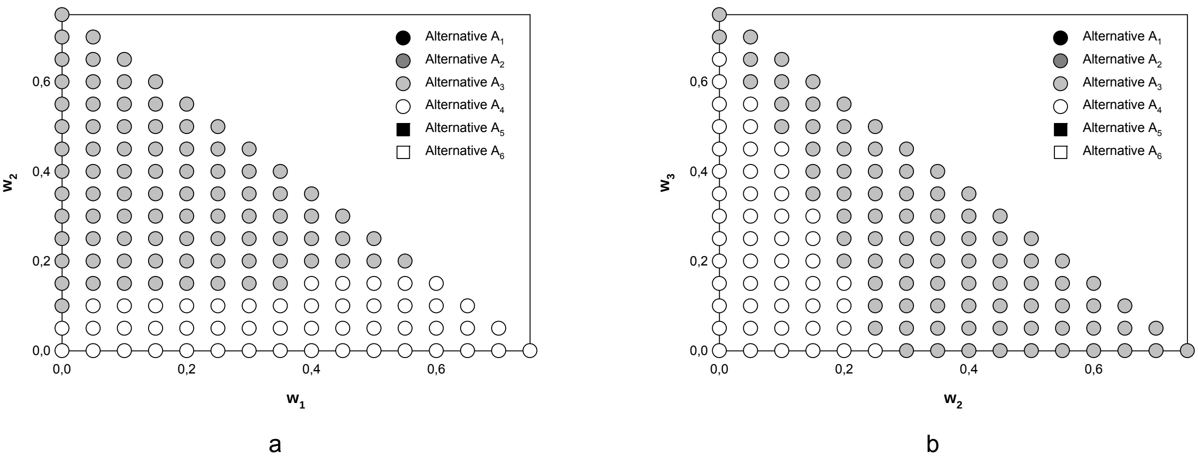


Figure 7.9. Sensitivity analysis of the weights of OBJ_1, OBJ_2 and OBJ_3 (a) and OBJ_2, OBJ_3 and OBJ_4 (b)

If the sensitivity analysis is made amongst OBJ_2 (*minimize economical costs*), OBJ_3 (*maximize technical reliability*) and OBJ_4 (*comply with the legal effluent discharge limits*) the solution also switches between A_3 and A_4. If economic objectives are prioritized (OBJ_2) at the expense of the technical reliability (OBJ_3) and the degree of accomplishment of the effluent discharge limits (OBJ_4), the most favoured alternative would be A_3. Nevertheless as soon as OBJ_4 gains in value alternative A_4 results as the better candidate because never violates legal limits, as shown in **Figure 7.9b.** Again, a similar degree of accomplishment of OBJ_3 by A_3 and A_4 can be observed which depends on the relative importance of OBJ_1 or OBJ_4. This analysis opens up for a number of discussions. One can note that the preliminary selected alternative A_5 (deterministic case) is no longer selected as the best for any of the possible combinations of weights. The considered input uncertainties had a large impact on the behaviour of this controller (cascade ammonium), where in some cases this controller was not capable to compensate for the different disturbances. After this analysis, it was possible to conclude that this alternative was only the best for a limited range of conditions. Thus, when considering *uncertainty* in the *multicriteria* decision making it is possible to answer questions such as: What would happen if there is a change in the influent composition? What are the expected effects of either temperature changes or toxic spills and how can the controller handle them? Secondly, this type of representations clearly distinguishes the different processes and their more important features, while at the same time it highlights their main weaknesses. Finally, it is highly encouraged to perform this type of analysis because it can better guide decision makers on such important questions as whether to go ahead with the implementation of a controller and what is the potential risk of failures in the event of the selection of an alternative.

7.3. CONCLUSIONS

This chapter has presented a systematic procedure to consider the influence of model parameter input *uncertainty* in the decision making process during the *multicriteria* evaluation of WWTP alternatives. In the first section several WWTP alternatives are tested and evaluated using standard deterministic *multicriteria* decision analysis setting those parameters at their default value. In the second part, the *uncertainty* in those parameters was quantified by means of model input probability distributions that were based on the available knowledge about the different parameters. Next the plant mechanistic model was coupled to a Monte Carlo engine that randomly selected parameters from the previously defined distributions using Latin Hypercube Sampling, i.e input *uncertainty*, solving the model for each set of model inputs. Such approach gave a range of possible solutions for the desired WWTP performance criteria representing their possible variation. The results were analyzed using several descriptive statistical tools and it was possible to see how these input uncertainties were propagated through the model and affected the different outcomes

From the evaluated controllers in the case study, alternatives with an external carbon source (Alternatives A_4 and A_6) reduced the *uncertainty* in the degree of satisfaction of environmental, legal and technical objectives but increased the economical costs and its variability as a trade-off. The alternatives with DO and NO controller (A_2 and A_3) reduced operating costs while at the same time improving the effluent quality. Finally, it was shown how the preliminary selected alternative A_5 – resulting from a deterministic *multicriteria* decision analysis became less desirable when the input *uncertainty* was considered. When considering *uncertainty*, a simpler controller structure (A_3) was evaluated to have a higher chance of success.

The relative importance of the control objectives (weights) on the selection of alternatives was investigated. On the one hand it was discovered the affinity of alternative A_4 for the objectives OBJ_1 and OBJ_4. On the other hand the sensitivity analysis revealed that when OBJ_2 was favoured alternative A_3 would be selected. Finally the need to carry out this type of analysis in order to obtain more information about how the process may vary was emphasized: identification of potential WWTP problems early on, reducing risk of controller failures and finally improving the whole decision making process are the benefit

7.4. REFERENCES

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CONCEPTUAL DESIGN OF WWTPs USING MULTIPLE OBJECTIVES

CHAPTER 1	*INTRODUCTION*
CHAPTER 2	*LITERATURE REVIEW, LIMITATIONS OF CURRENT APPROACHES AND DESCRIPTION OF NEW CONCEPTUAL DESIGN METHODOLOGY*
CHAPTER 3	*DESCRIPTION OF PROCESS MODELS*
CHAPTER 4	*HIERARCHICAL GENERATION AND MULTICRITERIA EVALUATION OF WWTP ALTERNATIVES*
CHAPTER 5	*SYSTEMATIC PROCEDURE FOR HANDLING CRITICAL DECISIONS DURING MULTICRITERIA EVALUATION OF WWTP ALTERNATIVES*
CHAPTER 6	*MULTIVARIATE ANALYSIS DURING MULTICRITERIA EVALUATION OF WWTP ALTERNATIVES*
CHAPTER 7	*UNCERTAINTY ANALYSIS DURING MULTICRITERIA EVALUATION OF WWTP ALTERNATIVES*
CHAPTER 8	***CONTRIBUTIONS, DISCUSSION AND FUTURE RESEARCH***

PhD THESIS

CHAPTER 8. CONTRIBUTIONS, DISCUSSION AND FUTURE RESEARCH

This chapter is a summary of the thesis results. Conclusions are drawn and future research is outlined.

8.1. SUMMARY OF THE KEY FINDINGS

This thesis proposes a new systematic procedure for supporting the conceptual design of Wastewater Treatment Plants (WWTP) using multiple objectives.

The proposed conceptual design method addresses design/redesign problems in a WWTP with respect to multiple objectives and multiple performance measures. The proposed approach selects the alternative that maximizes effluent quality while at the same time keeping both the construction and operating costs at minimum. Additional criteria, such as adaptability to short and long term perturbations, control performance and risk of microbiology-related solids separation problems, are included in the decision procedure in order to improve the overall effectiveness of the resulting WWTP. Since all the decisions (i.e. sequence of aerobic, anoxic, aerobic sections, selection of the biological removal process and implementation of a control strategy) are evaluated systematically using multiple criteria in the early stages, the future plant design and operation is influenced by all of these.

This thesis has contributed to solving certain key challenges in the conceptual design of WWTPs such as reducing the number of alternatives that must be evaluated, allowing different objectives to be included during the decision process, dealing with the problem of *critical decisions*, improving the analysis and interpretation of *multicriteria* matrixes and finally handling the *uncertainty* in the model parameters used while analyzing alternatives.

The conceptual design method includes a more reliable decision procedure that shows in a systematic, objective, communicable and transparent way the rationale for prioritizing a certain alternative amongst the others. The decision procedure developed for this thesis provides the alternative that best fulfils the defined objectives, showing its main advantages and weaknesses, the different correlations between alternatives and evaluation criteria and highlighting the conditions in which an alternative/decision is feasible.

The proposed procedure follows a modular and evolutionary approach that combines techniques from different disciplines such as: the *hierarchical* decision approach (Douglas 1988, Smith 2005), *multicriteria* decision analysis (see for example Vincke 1992, or Belton and Stewart 2002), preliminary multiobjective optimization using sensitivity functions (Douglas *et al.*, 1985), knowledge extraction and data mining techniques (Quilan 1993), *multivariate* statistical techniques (Johnson and Wichern, 1992; Hair *et al.*, 1998) and *uncertainty* analysis using Monte Carlo simulations (McKay *et al.*, 1979; Iman *et al.*, 1981). The conceptual design method is comprised of different blocks as described in Section 2.4.

[1] *Hierarchica*l generation and *multicriteria* evaluation of the WWTP alternatives

[2] Analysis of *critical decisions*

[3] Application of *multivariate* statistical techniques

[4] *Uncertainty* analysis

It is important to point out that although in the presented thesis all the blocks are linked together (as shown in **Figure 2.1** in **Chapter 2)**, each block can be used separately and even combined with other design/evaluation methodologies that can be found in the literature, e.g. Uerdingen (2003), Chen and Shonnard (2004).

The following paragraphs summarize the methodological aspects of each developed block and the main results of each case study. Finally, we conclude by detailing the main contributions to the conceptual design of WWTPs.

8.1.1. Block 1: *Hierarchical* generation and *multicriteria* evaluation of WWTP alternatives

The first block of the presented thesis supported the conceptual design of a WWTP by combining a *hierarchical* decision approach with *multicriteria* analysis. The block, which was expressed as a systematic procedure, was comprised of several steps: i) initial state in the exploration for collecting all the available information for carrying out the evaluation; ii) defining the objectives and the criteria used to quantify their degree of satisfaction; and finally iii) the decision procedure, which involved identifying the issue to be solved, generating the alternatives, and evaluating these alternatives in order to finally select one according to its performance and the relative importance of the defined objectives.

In the case study, three different alternatives were generated by applying the *hierarchical* decision process to an organic carbon removal and nitrification activated sludge WWTP. These configurations were grouped according to whether the anoxic phase was located before, after or within the aerobic zone, i.e. predenitrification, postdenitrification and simultaneous nitrification and denitrification. For each generated alternative the degree of satisfaction of the four objectives, i.e. economic, technical, legal and environmental, was calculated by means of a set of ten criteria using both dynamic simulation and model based cost estimation. After following all the steps described in **Chapter 4,** postdenitrification was found to be the most desirable alternative, taking into account the design objectives and process performance. Basically, this was because this alternative fulfilled OBJ_1 (*minimize environmental impact*), OBJ_3 (*maximize technical reliability*) and OBJ_4 (*comply with the limits fixed by law*) most satisfactorily despite the high operating costs linked to purchasing an external carbon source and sludge disposal. Thus, predenitrification and simultaneous nitrification/denitrification were not selected because their potential advantages were not sufficient to warrant further consideration and more study was devoted to the family of alternatives with postdenitrification. Nevertheless, the sensitivity analysis showed that although postdenitrification was the most preferred alternative for the widest range of situations, when the economic objectives were prioritized (OBJ_2) the situation changed so that predenitrification was the candidate implemented. This was due to the lower operating costs of this alternative at the expense of effluent quality (OBJ_1) and complying with the law (OBJ_4).

In the second case study the proposed methodology was used to select the optimum combination of set points for a couple of PI controllers implemented in a nitrogen removal activated sludge WWTP. The objective was to control both the dissolved oxygen and nitrate by manipulating the aeration flow and the internal recycle. The proposed methodology was used to evaluate the different states of the controllers within a range between 0.25 to 4 $gN \cdot m^{-3}$ and 0 to 4 $g(-COD) \cdot m^{-3}$ for the nitrate and dissolved oxygen controllers respectively. These set point combinations were evaluated using the same four objectives described in the previous case. Their degree of satisfaction was quantified with different criteria by means of dynamic simulation. Analyzing the results showed that the combination of set points that ensured the best plant performance was low dissolved oxygen (DO = 0.5 $g(-COD) \cdot m^{-3}$) and a high nitrate set point (NO = 3.5 $gN \cdot m^{-3}$). This was mainly because this combination achieved better denitrification efficiency and lower operating costs (i.e. low aeration energy) in spite of the low performance in terms of plant adaptation to short term and long term perturbations and control performance. In addition, several sensitivity analyses were run in order to study the variations in the set point combinations when the relative importance of the objectives was changed. The results showed that although the relative importance of the control objectives was modified, the combination of set points did not change substantially.

This block has contributed in the field of conceptual design of WWTPs in several ways: Firstly, it reduced the large number of WWTP alternatives that have to be evaluated using a *hierarchical* decision approach. The *hierarchical* decision approach broke the conceptual design down into a number of issues that were easier to analyze and evaluate. Thus, it is avoided to evaluate at further levels of detail alternatives that at lower levels of abstraction result not viable. Secondly, multiple objectives were included when evaluating the WWTP alternatives. *Multicriteria* decision analysis provided with a solution that maximized the degree of satisfaction of the different objectives considered, taking into account their relative importance and the process performance. Thus, the final WWTP design and operation was influenced greatly by environmental, technical, economical and legal aspects. Finally, a sensitivity analysis of the weights was also included to determine the variations in the selected alternative when the relative importance of the objectives was changed.

8.1.2. Block 2: Systematic procedure for handling *critical decisions* during the *multicriteria* evaluation of WWTP alternatives

The *critical decisions* were analyzed in the second chapter of the presented thesis with a three-step procedure. This procedure combined sensitivity analysis, preliminary multiobjective optimization and knowledge extraction to assist the designer when selecting the best alternative amongst the most *promising alternatives,* i.e. options that satisfy the design objectives to a similar degree but which have completely different implications for the future plant design and operation.

The analysis was carried out while redesigning an activated sludge plant to achieve simultaneous carbon, nitrogen and phosphorus removal. After following the steps described in Block I, i.e. *hierarchical* generation and *multicriteria* evaluation, three different alternatives were generated and evaluation was performed in relation to more than a dozen criteria. Next, two alternatives, i.e. biological phosphorus removal and chemical phosphorus precipitation, were found to be similar in terms of accomplishing the objectives but to have different implications for the future plant design and operation. For this reason it was recommended to carry out a further analysis in order to get a wider picture of the design space. Thus, once the most *promising alternatives* were optimized and characterized, and the trade-offs had been evaluated, it was concluded that the best treatment alternative was biological phosphorus removal. Even though biological phosphorus removal implied constructing additional anaerobic volume, it resulted in lower operating costs and a more balanced removal of nitrogen and phosphorus. Furthermore, this option undergoes a smaller variation in the overall process performance at the time to improve the criteria identified as a weak. In addition, it was discovered – by means of the extracted rules – that chemical precipitation was not able to achieve good phosphorus removal levels without decreasing the operating costs, as well as the fact that the bad performance in terms of nitrogen removal would make this alternative a very expensive activated sludge plant in terms of operating costs if these limitations had to be overcome.

This chapter has contributed to improve the conceptual design of WWTPs and dealt with the problem of *critical decisions* with several *multicriteria* evaluation tools: first, with a preliminary multiobjective optimization method in which the most *promising alternatives* were compared close to the optimum conditions based on the results of dynamic simulations; second, a data mining based technique that identified both the strong and weak points of each option by means of classification trees and the rules that were subsequently extracted; and third, with a trade-off evaluation that balanced the improvement of the criteria identified as weak points of the option and the loss of the overall process performance by applying, in an integrated way, dynamic simulation and qualitative knowledge extracted during the design process.

8.1.3. Block 3: *Multivariate* analysis during the *multicriteria* evaluation of WWTP alternatives

The third block of the thesis presented a *multivariate* based methodology that mined the *multicriteria* matrixes obtained while evaluating conceptual design WWTP alternatives. The proposed approach combined cluster analysis, principal component/factor analysis and discriminant analysis.

In the third case study, these techniques were applied in order to mine the simulation output results of implementing 11 control strategies in the BSM2 WWTP. The overall plant performance was tested with different combinations of six controllers: i) DO controller manipulating the airflow rate, ii & iii) NO controller manipulating either an external carbon source or an internal recycle, iv & v) OUR and ammonium controller manipulating the DO set point and finally vi) a TSS controller manipulating the waste flow rate. Cluster analysis identified similar performance patterns with alternatives with and without an external carbon source and TSS controller. Principal component/Factor analysis showed the main correlations between different groups of criteria and the control strategies influencing these criteria. Thus, it was possible to find synergies in some of them, e.g. better denitrification capacity with a lower risk of rising, and trade-offs, e.g. better nitrification efficiency and higher aeration costs. In addition, it was possible to characterize groups of control strategies with the extracted and labeled factors, e.g. the group of control strategies with an external carbon source was characterized for high operating costs and good effluent quality. Discriminant analysis identified six useful criteria for discriminating the classes obtained by cluster analysis. Thus, it was possible to determine that the differences in the plant performance for these groups of control strategies were due to external carbon source addition, methane production and the risk of microbiology-related solids separation problems.

The third results chapter of the thesis contributed with a *multivariate* based methodology that extracted meaningful information from the matrixes resulting from *multicriteria* evaluation of WWTP alternatives. Thus, there was an improvement in accessibility of the information needed for effective evaluation, giving groups of alternatives with similar performances, finding correlations between multiple criteria and justifying the reason why the identified alternatives were different from the others.

8.1.4. Block 4: *Uncertainty* analysis during the *multicriteria* evaluation of WWTP control alternatives

The last block of the thesis presented an optional systematic procedure that supports the *multicriteria* evaluation of WWTPs under *uncertainty* model parameters. The WWTP model was coupled to a Monte Carlo engine that randomly sampled parameters from predefined probability distributions, thus solving the model for each parameter, propagating the input *uncertainty* through the WWTP model and quantifying the output *uncertainty* i.e. evaluation criteria for each evaluated WWTP alternative.

Using a modified version of the BSM2 as a case study, the chapter showed the variations in the decision making when the *uncertainty* in the activated sludge model parameters was either included or not. From the evaluated control strategies, alternatives with an external carbon source reduced the *uncertainty* to a satisfying degree for the environmental, legal and technical objectives but increased the economical costs and variability as a trade-off. The alternatives with a DO and NO controller reduced operating costs while at the same time improving the effluent quality. Finally, it was shown how the alternative selected initially, which included a cascaded ammonium controller resulting from a deterministic multicriteria decision analysis, became less desirable when the input *uncertainty* was considered. Simpler control structures (DO and NO) had a greater chance of being successful. In addition, a sensitivity analysis of the weights showed that high values in OBJ_1 (*minimize environmental impact*) clearly favored alternatives with an external carbon source over the other controllers. This was mainly due to the fact that adding an external carbon source in this strategy reduced the impact on water by improving the overall nitrogen removal efficiency while simultaneously reducing the variability in the effluent quality for this WWTP. Nevertheless, as w_2 (*minimize economical costs*) increased in value the most desirable alternative changed from the external carbon source nitrate controller to the internal recycle nitrate controller since this alternative had lower operating costs and variability.

This chapter has contributed to the conceptual design of WWTPs with a tool that provided more information about how the process may vary: first, by quantifying the variation in the overall degree of satisfaction of the control objectives for the generated WWTP alternatives; second, by identifying the contributions of environmental, legal, technical and economic objectives to the existing variance; and finally, by analyzing the influence of the relative importance of the defined objectives when selecting the alternatives. Thus, it was possible to identify potential WWTP problems early on, which reduces the risk of failure and improves the decision making process as a benefit.

8.2. OPPORTUNITIES AND LIMITATIONS OF THE CONCEPTUAL DESIGN METHOD

In this section we draw conclusions about the opportunities and limitations of the proposed conceptual design procedure in relation to the results obtained from the different case studies. Strong emphasis is also placed on general conclusions about the structure of the conceptual design method.

8.2.1. Opportunities

The conceptual design method proposed in this thesis is a typical example of a divide-and-conquer-type of strategy. The general principle consists in subdividing a complex problem into a number of subproblems and usually requires abstraction, idealization, and consideration of a relationship between the subproblems. Although there is a fair chance that some aspects of the master problem will be lost when employing this procedure, the reduced complexity in each subproblem facilitates the search for good and partial solutions. In the proposed conceptual design method, the subproblems are dealt with by the different tools developed throughout this thesis, i.e. analysis of *critical decisions*, inclusion of different design objectives and both *multivariate* and *uncertainty* analysis. These tools have contributed to solve parts of the master problem concerning the whole design problem.

One of the main benefits of the conceptual design method consists in guiding the decision maker systematically through the steps of evaluating the different process alternatives. The decision maker is thus forced to evaluate a broad range of possible conceptual design alternatives. Many times selecting the best alternative is almost obvious. However, the advantage of a systematic evaluation provides the possibility of finding a not so straightforwardly apparent alternative. A good example of this kind of situation was found while selecting the biological nitrogen removal process (case study #1). It is commonly believed that predenitrification has the most potential for improving the overall nitrogen removal. However, the alternative based on an external carbon source deserved much more attention as a consequence of both low readily biodegradable influent substrate and short hydraulic retention time in the biological reactor for the studied WWTP. Also, this systematic evaluation has clear advantages related to the extraction and maintenance of the design process record. Thus the geographical and temporal reuse of the generated knowledge that would otherwise be tacit and usable by a single designer is now possible.

Moreover, data gathered during the different sensitivity analyses can be introduced during different steps of the proposed conceptual design method. For example in *Step 5* it was possible to identify both strong and weak points for each evaluated alternative, while in *Step 6* the provides with the information about the links between criteria and improvement/damaging of process performance.Thus, during the redesign of the nitrogen removal WWTP to achieve simultaneous organic carbon, nitrogen and phosphorus removal, it was possible to unravel by means of the combined evaluation by both dynamic simulation and qualitative knowledge the expensive costs in terms of plant performance at the time to improve the identified limitations of the alternative chemical phosphorus removal. In addition, the plant could not carry out complete denitrification and additional measures, such as adding an external carbon source or increasing the anoxic section, were therefore necessary worsening even more a poorly satisfied economic objective.

Analyzing the evaluation matrixes obtained with *multivariate* analysis has a number of advantages. Firstly, it was possible to discover groups of alternatives with similar behavior in terms of plant performance. Secondly, *multivariate* statistical techniques were capable of determining the complex correlations existing between multiple criteria by means of extracting several factors, i.e. a linear combination of criteria. Moreover, it showed the relationships with the different alternatives and the extracted factors. Finally, it facilitated identifying the most discriminant criteria for a single/group of control strategies. All this information can be used to assist the decision maker and improve how the information is used in order to make a more effective evaluation.

Uncertainty is a crucial factor in engineering practice. A number of advantages have been listed in favour of the proposed approach with respect to include model parameter *uncertainty* while evaluating WWTP alternatives. The representation of the input *uncertainty* as a probability distribution function could be used as a quantitative representation of the parameter variation. Since there is good communication between the random generator engine and the WWTP model, Monte Carlo simulations are a straightforward option for propagating the input *uncertainty* through the whole model and study its propagation. Further, it was possible to show, as in case study # 5, how the decision making could change (e.g. an alternative with an ammonium controller to a simpler alternative) when input *uncertainty* was included. The results of this analysis open up for a continued discussion on several points: for example, certain options were only performing well for a limited range of conditions. Thus, when *uncertainty* was considered it was possible to answer questions such as: What would happen if there was a change in the influent composition? What are the expected results of temperature changes or toxic spills and how can the selected alternative handle these? Finally, more information was obtained during this analysis and therefore potential problems could be identified early on, which reduced the risk of failures and improved the whole decision making process.

8.2.2. Limitations

As with any method, the proposed conceptual design procedure also has a number of limitations. One of the main disadvantages is the lack of systematization when using the different optional tools developed for this thesis such as: analysis of *critical decisions*, *multivariate* analysis or *uncertainty* evaluation. So far, this step is quite empirical and solely relies on the experience/ the time/ knowledge of the decision maker.

A minor disadvantage consists in the fact that there is no automatic generation of alternatives in the first block of the proposed conceptual design method. For example in the different case studies presented in this thesis the different alternatives were generated based on the designer's experience or a literature review once the initial state in the exploration (*Step 1*) was completed.

A major disadvantage consists in the fact that the method does not automatically reject alternatives when they do not comply with minimum requirements. Even though value functions penalize an alternative when it satisfies a certain objective poorly, as an effect of the multiobjective function it could be selected as the best alternative if it fully satisfies another objective. A lot of effort has been put into this point throughout the thesis by developing tools to inform the designer about these drawbacks, e.g. identification of strong and weak points by means of classification trees or clusters of alternatives with an undesirable performance, evaluation of trade-offs by means of dynamic simulation and knowledge based rules or even *uncertainty* analysis. Therefore, the final decision rests with the process designer

Also, as in the other type of preference ranking methodologies to solve a specific issue, the presented conceptual design method calculates the degree of satisfaction of the different objectives by the generated alternatives even though it is possible that none of these technologies are suitable solutions.

The conceptual design method is objective through the analysis phase and criteria quantification (*Step 3.4.1*). Nonetheless, defining the extreme profiles for criteria quantification (*Step 3.4.2*), assigning weights according to the relative importance of the different objectives (*Step 3.4.3*), identifying the *uncertainty* factors and their probability distribution functions (*Step 8.1*), are very subjective and rely on the judgment of the decision maker.

Another inconvenience consists in the fact that some of these blocks cannot be safely established in the conceptual design method developed in this thesis without intense use of dynamic simulation. The inherent problem lies in the non-linearities of the wastewater treatment process, which make linear interpolation unreliable, for example during sensitivity and *uncertainty* analysis. Closely related, it is important to highlight that the presented format of the conceptual design method is extremely dependent on a good model describing the process in order to obtain reliable results. Even though in this thesis the list of criteria is quantified by either dynamic simulation of model based estimations, in some of the developed blocks more qualitative values could be included

Another point to emphasize is the required knowledge to make the analyses reliable. Some points where knowledge is required is the *multivariate* analysis and knowledge extraction. Dynamic simulation of wastewater treatment plant models also demands for an expert. Then there is the *uncertainty* analysis, where especially the selection of the probability distribution functions asks for expert knowledge. Expert knowledge is one limitation, combined with the previously stated computational burden is another important limitation. Monte-Carlo analysis and dynamic simulation take a lot of computer time.

In addition to the previously mentioned problems, the author recognizes the difficulties that will suppose for those employees in consulting and engineering companies that design plants to benefit of the work presented in this thesis. Perhaps the designers that are used to work with empirical rules and safety factors will think this new group of conceptual design methods, although the described numerous benefits, are far too time consuming to apply in practice.

A further disadvantage of this method is that it does not recognize important differences between grassroot and retrofit design. The importance of rating the equipment used under different operating conditions, either by plant experience or by calculation, is often not given enough attention in the analysis and evaluation of the process alternatives.

In the present form the conceptual design method is only applicable to wastewater treatment plants based on activated sludge systems. In this present structure, another type of biochemical process cannot be included in the proposed conceptual design method. For example, some biochemical processes are discontinuous and are subjected to different cost structures (e.g. costs for non-occupation time in a multi-purpose plant) which would thus require a modification of the economic indicators of the conceptual design method. However, the method leaves open the possibility of defining new performance indicators for other conceptual design applications in the analysis phase.

8.3. SCOPE AND APPLICABILITY OF THE CONCEPTUAL DESIGN METHOD

Most methods applied in industrial practice are team-oriented so that specific knowledge and experience can be included during the problem analysis when generating the alternatives and decision making. As generating the possible alternatives (*Step 3.2*) is a crucial step in the conceptual design method, the authors propose generating these options using team work. In addition, team work can be used to define the extreme profiles in the value functions (*Step* 3.4.2), and to assign the relative importance of weights or define the *uncertainty* factors and probability distributions (*Step 8.1*) before Monte Carlo analysis. To do this, the procedure described in this thesis should be used with well-known creativity techniques such as brainstorming and morphology.

The conceptual design presented can be used to design new plants along the entire process life cycle, improve their feasibility putting operating strategies in practice or redesigning plants. It could be possible to collect and integrate the gathered process-specific knowledge generated during the design process and use it as a communication tool for future process engineers dealing with a specific problem. For example, in the event that the effluent nitrogen needs to be improved in the redesigned plant of case study #2, a list of actions could be provided to the process engineers that will outline the advantages/disadvantages of applying certain alternatives and their degree of affectation.

In addition, it could be used to extract relevant information from WWTP benchmark studies. In this field the problem of extracting meaningful information when several control strategies are evaluated with the multiplicity of required criteria is well recognized. Some of the tools presented in this thesis have proved to be useful for improving accessibility to information for both analyzing and evaluating the results. Therefore, the complexity of this evaluation is reduced to aggregate indexes, e.g. clusters of controllers, principal components and discriminant functions.

Finally, the *uncertainty* analysis block could be used to evaluate the robustness of some decisions, such as whether to implement a certain technology or not. A clear example can be found in last chapter of the thesis in which the ammonium controller alternative selected initially became less desirable when input *uncertainty* was included. Moreover, this methodology could be included during the benchmark studies in order to determine if the proposed control strategies are only reliable for a certain range of conditions.

8.4. FUTURE RESEARCH

8.4.1. Extending the conceptual design method to support the evaluation of other types of biochemical processes

Most industrial biochemical processes, e.g. pharmaceutical and food production, are operated in a batch or semi-batch regime in mono or multi-purpose plants depending if it is uniquely designated for an specific product.

Some additional work should be done if the proposed method has to be applied to multi-purpose processes. Before each campaign starts, the production recipe has to be defined for the desired product. Since multi-purpose plants generally comprise a large number of equipment items (e.g. reaction vessels, storage tanks, filters, centrifuges and dryers), a good arrangement of equipment regarding space-time yield has to be found prior to each campaign in case the optimal arrangement is not readily found in the first run. In this sense the conceptual design method should be modified in order to take all these aspects into account i.e. create a new facility or optimize the batch schedule.

8.4.2. Generating redesign alternatives

In the proposed conceptual design method the decision maker generates structural alternatives based on the proposed hierarchy and the available process knowledge. For example a number of heuristic rules could be generated after each alternative is evaluated to specifically target a design/redesign problem. A systematic study of these rules could reveal important information for pre-selecting alternatives and therefore reduce the evaluation time. In addition, the designer would be informed of the specific reasons why he/she does not have to spend more time evaluating a determined alternative by analyzing the initial state in the exploration.

8.4.3. Experience re-use to systematize the communication amongst the developed blocks

Case base reasoning (CBR) systems can be defined as knowledge based techniques that permit the use of past experiences to solve new problems that arise in a process. The basis idea behind its functionality would be that second time we solve a problem it is usually easier than the first because we remember and repeat the previous solution or recall our mistakes and try to avoid them (Kolodner, 1993).

In the proposed conceptual design method, CBR could be used taking advantage of past experiences that the designer keeps in mind at the time to decide whether or not going through a complicated and time consuming analysis e.g. *uncertainty* analysis or critical decision analysis . Let us suppose that in posteriors projects a designer finds out that an ammonium controller is the selected alternative after carefully evaluation. It would be worthwhile running an *uncertainty* analysis because according to his/her past experience, i.e. in this thesis for example; this controller only behaved fulfilling the control objectives under certain conditions.

8.4.4. Differentiating the grassroot and retrofit designs

Retrofit problems should be analyzed and evaluated with tools that have been specifically developed for grassroot design. However, there are fundamental differences between the two approaches. First, retrofit is highly specific and some of the retrofit problems can often be predetermined, to a certain degree, from the historical evolution. Second, implementing a solution to a retrofit problem has to be coordinated in a way that minimizes the impact on plant operation. Third, grassroot design requires different mathematical tools; the so-called rating models are much more complex than design models generally used in grassroot design.

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ACRONYMS AND NOMENCLATURE

AD = anaerobic digestion

ADM1 = anaerobic digestion model N^{o}1

AE = aeration energy (kw·h·day^{-1})

AER = aerobic reactor

A_j = design option, total number of design options m for a given issue I_i

$Ac_{j,l,f}$ = action to improve a criterion X_i, of the alternative A_j using the design/operating variable V_f

ANAER = anaerobic reactor

ANOX = anoxic reactor

AOB = ammonium oxidizing bacteria

AS = activated sludge

ASM1 = activated sludge Model N^o 1

ASM2d = activated sludge model N^o 2d

ASM3 = activated sludge model N^{o}3

BOD_5 = biochemical oxygen demand concentration

C = carbon

CA = cluster analysis

CAPDET = Computer Assisted Procedure for Design and Evaluation of wastewater Treatment systems

COD = chemical oxygen demand

CS = external carbon source (kg COD·day^{-1})

CV = coefficient of variation

D = discriminant function

DA = discriminant analysis

DO = dissolved oxygen

D_u = probability distribution that describes the variability of U_u, total number of distributions U

EQ = effluent quality index (kg pollution·day^{-1})

F/M = ratio food to microorganism (kg DBO_5·kgTSS^{-1})

FE = metal salt (kg X_{MET}·day^{-1})

HE = heating energy (kw·h·day^{-1})

H_h = type of studied uncertainty, total number of studied uncertainties H

I_l = issue to be solved, total number of issues Z

IQ = influent quality index (kg pollution·day^{-1})

ISE = integral squared error (g·m^3)^2·day^{-1}

K_La = oxygen transfer coefficient (day^{-1})

K_p = proportional gain

ME = mixing energy (kw·h·day^{-1})

MINLP = mixed integer non linear programming

MP = methane production (kg CH_4·m^{-3})

N = nitrogen

NO = nitrate and nitrite

NOB = nitrite oxidizing bacteria

NPV = net present value

OBJ_k = design objective, total number of design objectives P

OCI = operating cost index

OUR = oxygen uptake rate ($gCOD \cdot m^{-3} \cdot day^{-1}$)

P = phosphorus

PAO = phosphate accumulating organism

PC = principal component

PCA/FA = principal component/factor analysis

PE = pumping energy ($kw \cdot h \cdot day^{-1}$)

PI = proportional integral controller

Q_{carb} = external carbon source flow ($m^3 \cdot day^{-1}$)

Q_e = effluent flow rate ($m^3 \cdot day^{-1}$)

Q_{in} = influent flow rate ($m^3 \cdot day^{-1}$)

Q_{met} = metal salt flow ($m^3 \cdot day^{-1}$)

Q_r = external recirculation ($m^3 \cdot day^{-1}$)

Q_w = waste flow ($m^3 \cdot day^{-1}$)

R_i = evaluation range between x_{i^*} and x_i^*

$R_{i,j,f}$ = rule containing the relationship amongst the process variable f, the criterion i and a given option j

$r_{j,i,f}$ = loss of objective function for a given option j, moving the variable f, trying to improve the criterion i

S = sensitivity to a given perturbation

$s(A_j)$ = multiobjective function for a given option j

SP = sludge production ($kg\ TSS \cdot day^{-1}$)

SRT = sludge retention time

T_i = integral time constant

TIV = time in violation

TKN = total Kjeldhal nitrogen

TN = total nitrogen

TP = total phosphorus

TSS = total suspended solids

U_u = uncertain input parameter, total number of parameter U

$U_{u,y}$ = Monte Carlo shot for a uncertain parameter u, total number of shots Y

$V(X_i)$ = value function, total number of value functions W

$v(x_{j,i})$ = normalized criterion i for a given option j

V_{ANAER} = Mixing volume of anaerobic tank (m^3)

V_{ANOX} = Mixing volume of anoxic tank (m^3)

VF = varifactor

$V_{j,f}$ = design variable for a given option j, total number of variables for this option is Y

w_k = weight, total number of weights X,

WWTP = wastewater treatment plant

X_i = criterion, total number of criteria W, set of criteria for a given issue n

x_i^* = best situation for a certain criterion X_i

x_{i*} = worst situation for a certain criterion X_i

$x_{j,i}$ = quantified criterion i for a given option j

$x_{j,i}^*$ = identified strong point i for a given option j

$x_{j,i*}$ = identified weak point i for a given option j