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Retrofitting Analysis for Improving Benefits of A/O WWTPs Considering Process Control Aspects

PhD THESIS

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A perfection of means, and confusion of aims, seems to be our main problem.

Albert Einstein

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Abstract

A methodology for retrofitting existent Anoxic/Oxic (A/O) wastewater treatment plants (WWTP) to perform the Enhanced Biological Phosphorus Removal (EPBR) in order to biologically remove organic matter (COD), nitrogen (N) and phosphorus (P) at the same time, considering process control aspects, was developed. The proposed methodology exhaustively searches a process model, using existent plant data to determine the current kinetic parameters. The plant model is calibrated using a methodology based on the *Fisher Information Matrix*. Using the plant model structure, new plant configurations are proposed and a set of criteria are used to identify what is the best alternative. Amongst the criteria are: the robustness of the process control structure, operating costs, investment costs to perform changes in the plant layout and equipments and the effluent quality. The feasibility of phosphorus accumulating organisms (PAO) growth and the effect of these species in the existent process control structure are also studied.

Resumen

En este trabajo se ha desarrollado una metodología para implementar la eliminación biológica de fósforo (EPBR) en las plantas de tratamiento de aguas residuales urbanas (EDAR) con configuración anóxica / óxica (A/O) diseñadas para eliminar únicamente materia orgánica (DQO) y nitrógeno (N). El objetivo es eliminar biológica y simultáneamente DQO, N y fósforo (P) teniendo en cuenta aspectos de control de procesos y con el mejor rendimiento de operación. La metodología propuesta busca exhaustivamente un modelo del proceso, utilizando los datos existentes de la planta para determinar los parámetros cinéticos. El modelo de la planta se ha calibrado utilizando una metodología basada en la matriz de información de Fisher (FIM). Usando la estructura del modelo de la planta y las nuevas configuraciones de plantas que se proponen, se utiliza un conjunto de criterios para identificar cuál es la mejor alternativa. Entre los criterios utilizados se encuentran: calidad del efluente, solidez de la estructura de control del proceso, costos de operación y costos de inversión para compra de equipos y para llevar a cabo cambios en la distribución de la planta. También se estudia la viabilidad de los organismos acumuladores de fósforo (PAO) y el efecto del crecimiento de estas especies con diferentes estructuras de control del proceso.

Resum

En aquest treball s'ha desenvolupat una metodologia per implementar l'eliminació biològica de fòsfor (EPBR) en les plantes de tractament d'aigües residuals urbanes (EDAR) amb configuració anòxica / òxica (A/O) dissenyades per eliminar únicament matèria orgànica (DQO) i nitrogen (N). L'objectiu és eliminar biològicament i simultàniament DQO, N i fòsfor (P) tenint en compte aspectes de control de processos i amb el millor rendiment d'operació. La metodologia proposada cerca exhaustivament un model del procés, utilitzant les dades existents de la planta per determinar els paràmetres cinètics. El model de la planta s'ha calibrat utilitzant una metodologia basada en la matriu d'informació de Fisher (FIM). Usant l'estructura del model de la planta i les noves configuracions de plantes que es proposen, s'utilitza un conjunt de criteris per identificar quina és la millor alternativa. Entre els criteris utilitzats es troben: qualitat de l'efluent, solidesa de l'estructura de control del procés, costos d'operació i costos d'inversió per a compra d'equips i per dur a terme canvis en la distribució de la planta. També s'estudia la viabilitat dels organismes acumuladors de fòsfor (PAO) i l'efecte del creixement d'aquestes espècies amb diferents estructures de control del procés.

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List of Variables

Symbol	Description	Chapter
$\overline{\sigma}$	Maximum singular value in singular value decomposition (SVD).	3
$\underline{\sigma}$	Minimum singular value in singular value decomposition (SVD).	3
$X_{TSS}^{Q_W}$	Total suspended solids in purge stream.	4
θ	Time delay in transfer functions.	3,4, appendix
ω	Frequency.	3,4
γ	Condition number.	3,4
γ^*	Minimized condition number.	3,4
τ	Process constant time.	3,4, appendix
τ_{CL}	Closed loop constant time (setting parameters of tuning rules PI/PID controllers).	appendix
τ_D	Rate (Derivative action - PI/PID parameter).	appendix
τ_I	Reset (Integral action - PI/PID parameter).	appendix
Δ	Difference between two variables.	4
$\Delta\alpha_j$	Slope of the curve effluent fines per cubic meter of effluent versus pollutant concentration before to reach the effluent discharge limit of pollutant "j". The sub-index "j" can be or ammonium, or total nitrogen or phosphate.	4
$\Delta\beta_j$	Slope of the curve effluent fines per cubic meter of effluent versus pollutant concentration after to reach the effluent discharge limit of pollutant "j". The sub-index "j" can be or	4

	ammonium, or total nitrogen or phosphate.	
$\beta_{0,j}$	Increment of the value of effluent fines per cubic meter when the effluent concentration of pollutant “j” is superior to the legal limit. The sub-index “j” can be or ammonium, or total nitrogen or phosphate.	4
γ_E	Cost of kWh in €.	4
λ_{ij}	Element “ij” of the relative gain array.	3
γ_{SP}	Cost of the treatment of one kg of purged sludge.	4
s	Complex variable – transfer function models in the continuous time-domain	appendix
A_E	Aeration energy, in kWh d^{-1}.	4
CCF	Calibration cost function (calculated with calibration plant data)	4
C_j^{EFF}	Effluent concentration of the pollutant “j”. The sub-index “j” can be ammonium, total nitrogen or phosphate.	4
$C_{L,j}$	Limit of concentration of pollutant “j” in the effluent.	4
EF	Effluent fines, € d^{-1}.	4
G(ω)	Process response at frequency ω.	3
G(0)	Process response at frequency 0 (steady-state).	3
J (Janus)	Calibration index used for comparing the performance of the model calibration subset that involves both calibration and validation data.	4
K, K(0)	Process gain matrix.	3,4, appendix
K_P	Controller gain (Proportional action - PI/PID controller).	appendix
K_{ij}	Element “ij” of K.	3
K_{ij}^C	Element “ij” of the process gain matrix under closed loop	3

	operation.	
k_La_i	Oxygen transfer coefficient.	4
modE	The ratio between the highest eigenvalue of the FIM and the lowest eigenvalue of the FIM, used as calibration criterion. Lower values of modE indicate poor correlations amongst the calibration parameters in the calibration subset, which means a good subset is being chosen.	4, appendix
normD	Determinant of the FIM, used as calibration criterion. High values of norm D indicates calibration parameters are suitable for explaining the plant behaviour.	4, appendix
OC	Operation cost, € d^{-1}.	4
PE	Pumping energy, in kWh d^{-1}.	4
P_F	Pumping factor. It converts flow rate units in energy units.	4
Q_{IN}	Influent flow rate, m^3d^{-1}.	3,4, appendix
Q_{RAS}	Activated sludge recycle, m^3d^{-1}.	3,4,5, appendix
Q_{RINT}	Internal recycle flow rate, m^3d^{-1}.	3,4,5, appendix
Q_W	Purge flow rate, m^3d^{-1}.	3,4,5, appendix
RDE	Ratio between normD and modE criteria. High values of RDE indicate that parameter calibration subset is able to explain the plant behaviour without correlated calibration parameters.	4, appendix
RGA(0)	Relative gain array calculated with steady-state gains.	3,4
S_A	Fermentation products, gCOD m^{-3}.	4, appendix
S_F	Readily biodegradable substrate, gCOD m^{-3}.	4, appendix
VCF	Validation cost function (calculated with validation plant data)	4

List of Acronyms

Symbol	Description
A/O	Anoxic and Aerobic (WWTP configuration)
A^2/O	Anaerobic, Anoxic and Aerobic (WWTP configuration)
ASM2d	Activated Sludge Model 2d
ASP	Activated Sludge Process
BABE	Bio-augmentation Batch Enhanced
BOD	Biodegradable Oxygen Demand
COD	Chemical Oxygen Demand
CSD	Control Structure Design
CSTR	Continuous Stirred Tank Reactor
EBPR	Enhanced Biological Phosphorus Removal
FF	Feed-forward action
FIM	Fisher Information Matrix
FODT	Transfer Function of First Order with Dead Time
ITAE	Integral Time-Average Error (method for tuning PI/PID controllers)
IWA	International Water Association
MBR	Membrane Bioreactor
OE	Output Error (black-box model structure)
PAO	Phosphorus Accumulating Organisms

PHA	Poly-HydroxyAlkanoate
PP	Poly-Phosphate
RGA	Relative Gain Array
SBR	Sequential Batch Reactor
SRT	Sludge Retention Time
UCT	University of Cape Town (WWTP configuration)
VFA	Volatile Fat Acids (acetic, propionic, butyric, etc.)
WWTP	Wastewater Treatment Plant (s)

Chapter 1: Introduction

Wastewater treatment plants (WWTPs) are industrial facilities of great importance these days since they remove organic matter and nutrients from wastewater, allowing the return of great amount of water to the river basins for human (re)use and to keep the equilibrium in several ecosystems. It is possible to affirm, in a global point of view, that WWTPs improve the environmental conditions as well as provide health and well-being to the citizens, even though their benefits are extremely difficult to be acknowledged by the people due to the slow dynamics of the ecosystems processes.

The most popular technology for treating the wastewater is the Activated Sludge Process (ASP). The activated sludge process was developed in 1914 by Andern and Lockett and was named this way because sludge naturally produced in the organic matter decomposition, containing different kind of microorganisms, stabilized the wastewater. The stabilization processes involved release of energy since organic matter is oxidized to carbon dioxide and water. Energy associated to the carbon sources present in the wastewater allows the biomass growth. The generated sludge, which should be separated from the treated liquid mass, is mixed with new portions of incoming wastewater and again the same behaviour happens. Thereby, even more wastewater flow rates could be treated (Crites and Tchobanoglous, 1998). With the constant increase of world population, the use of soil stimulants (like the products based on the NPK, Nitrogen, Phosphate and Potassium elements), the massive use of detergents and new cleaning products, the WWTPs had to be converted into new WWTPs for removing not only organic matter but also N and P nutrients and even more amounts of wastewater. The need for changes in the first WWTP design was motivated by the minimization of the undesired consequences of the eutrophication effects.

The organic matter and the nutrient removal processes take place in the secondary or biological step of the wastewater treatment (water line). Before, the influent has been pre-treated and oils, greases and macrosolids (gross material) have been removed. Following, a primary sedimentation is done. After the biological treatment, two streams are generated: a final effluent, which in theory could be dispensed into water bodies (lakes, rivers…) and a waste sludge stream that should be treated. Usually, the sludge treatment is performed anaerobically in digesters, where biogas composed mainly of methane and CO_2 is generated providing a renewable energy source. The treated sludge is dewatered and the liquid phase resulted is returned to the primary treatment. The dewatered sludge is sent to composting units, in general. Figure 1.1 shows a schematic AS plant diagram, including the different steps. The processes around the activated sludge reactors promote strong disturbances to the biological processes, specially the dewatering processes used to treat the waste sludge. One of these disturbances is the production of ammonium, which returns to the process mixed with the influent wastewater.

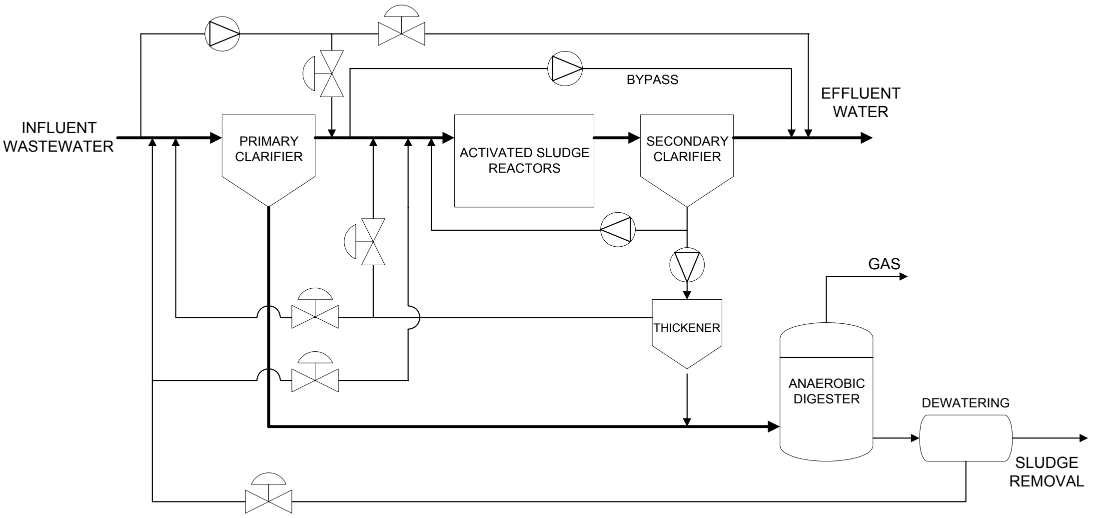


Figure 1.1: Schematic representation of a typical activated sludge plant.

Nutrient removal is dependent on one or more carbon source(s). The activated sludge technology has been employed successfully because it couples organic matter and nutrient removal processes providing naturally carbon sources for N and P removal. Nevertheless, a trade-off is established between cost reduction and level of process interactions. With these interactions the plant becomes harder to control, since multiple manipulated variables affect simultaneously all the important process variables. One of these manipulated variables is the dissolved oxygen (DO) in the aerobic reactors. High concentration of DO promotes faster organic matter oxidation and nitrification processes than in the nature cycles. The DO concentration is a function of the contact of the wastewater and the air. So, a first way to increase the oxygen concentration is by means of mixing. However, an easier and economic manner to achieve high DO concentrations is putting atmospheric air in contact to the reactors bulk solution through air diffusers and blowers. The oxygen dissolved concentration is dependent on temperature, pressure, salt concentration and ratio between the air mass and the wastewater mass (mixed liquor). All these factors are lumped in the oxygen transfer coefficient, k_La given in [d^{-1}].

A part of the nutrient removal is the biological nitrogen removal (BNR). Such process converts ammonium in nitrogen gas in ASP plants through nitrification/denitrification processes. Denitrifying bacteria need organic matter to perform the conversion of nitrate/nitrite to nitrogen gas. Denitrifying bacteria are heterotrophic and facultative, hence, if DO is present concomitantly with nitrate, oxygen would be consumed instead of nitrate and the performance of N removal process would decrease. That is the reason why denitrification process should occur under anoxic conditions (without oxygen but with nitrate/nitrite, saving money spent in the aeration process). If methanol is used as carbon source, the following chemical reaction is obtained:

$$NO_3^- + 1.183\, CH_3OH + 0.273\, H_2CO_3 \rightarrow 0.091\, C_5H_7O_2N + 0.454\, N_2 + 1.820\, H_2O + HCO_3^- \qquad \text{Eq.1.1}$$

The molecule $C_5H_7O_2N$ is an accepted representation of the biomass constitution. It is simple to note that denitrification increases the alkalinity of the system. As methanol seldom is present in the urban wastewater, the common way to provide readily biodegradable organic matter is by means of hydrolysis of the large carbonaceous chains, carried out by heterothophs.

The nitrate amount to be denitrified is a consequence of the nitrification performance. Nitrification is aerobically performed by autotrophic microorganisms. Besides oxygen, a carbon source in the form of inorganic carbon is needed to constitute the cells. Nitrification occurs in two steps: the first step is called nitritation, where ammonium oxidizing bacteria (AOB) convert ammonium into nitrate and in a second stage, named as nitratation, nitrite is converted to nitrate through nitrite oxidizing bacteria (NOB). The stoichiometry of both steps is presented as follows.

Nitritation – first step (AOB)

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + 2H^+ + H_2O \qquad \text{Eq. 1.2}$$

Nitratation – second step (NOB)

$$NO_2^- + 0.5O_2 \rightarrow NO_3^- \qquad \text{Eq. 1.3}$$

As can be observed, organic matter removal and biological nitrogen removal are coupled. Heterotrophic and autotrophic biomasses can work together in an Anoxic/Aerobic (A/O) plant configuration (as the modified Lutzack Ettinger configuration, Metcalf and Eddy, 2004). In the anoxic part, denitrification takes place, consuming BOD and in the aerobic one, nitrification occurs. Nitrate and nitrite are returned by a recycle stream from the aerobic basin to the anoxic reactors. As the plant has to treat continuously the influent and this stream could provoke biomass wash out, settling devices have proved to be an appropriate way to retain the microorganisms inside the system. Hence, a biomass recycle stream is necessary in the plant configuration, carrying out the settled biomass to plant inlet to maintain the process operative.

The necessity of removing phosphorus, as a consequence of the negative effect of its presence in the water basins which promotes eutrophication effects, new plant configurations had to be created. Basically, these modifications consist of the insertion of an anaerobic volume in the A/O configuration to yield enough amounts of fermentation products which will be consumed by the PAO (Phosphorus Accumulating Organisms) (or also building an oversized primary settler to guarantee that outlet wastewater is free from DO) or adding chemicals (inorganic compounds like $FeCl_3$, lime and alum, or also polyelectrolyte), stimulating chemical precipitation of the phosphate ions. The latter physicochemical route for removing phosphorus is the easier and well established route from the operating point of view and does not demand a systematic study of the involved biomasses to modify the existent A/O plant (US-EPA, 1976). By its turn, enhanced biological phosphorus removal (EBPR) requires investment costs as opposite to the operating costs required for the chemical precipitation. EBPR also improves settleability of the sludge in the secondary settlers since anaerobic reactors produce VFA (volatile fatty acids) that are easily biodegradable by floc-forming biomass, avoiding bulking problems caused by the filamentous bacteria in the settlers (Loosdretch *et al*, 1998). The plant configuration with an anaerobic zone before the A/O configuration is called anaerobic-anoxic-oxic (A^2/O) configuration. It is worth noticing that the presence of an anaerobic zone, which promotes the fermentation processes, will decrease the necessity for aeration in the aerobic zone to remove COD. Also, the fermentation products will provide better denitrifying rates since more VFA molecules will be available for converting the nitrate into nitrogen gas (Henze *et al*., 1999).

EBPR depends on the organic matter availability and the presence of nitrate/nitrite or DO (Metcalf and Eddy, 2004). Although all details of phosphorus removal processes are not completely understood, such processes occur in two stages, as investigated by Smolders *et al*, 1994. In a first stage under anaerobic conditions, fermentation products are yield and the microorganisms are able to store them into internal polymers releasing orthophosphate. Then, an anoxic or aerobic stage is necessary to make the microorganisms grow using the internal polymers and store phosphate as poly-phosphate (PP). As the phosphate uptake is greater than the phosphate released, phosphate is removed being part of the cells structure. However, a possible presence of nitrite/nitrate or oxygen in the first stage, due to malfunctioning plant operation, would decrease the amount of orthophosphate released producing a lack of phosphate storage in the aerobic stage.

Fermentation processes, which convert molecules with long chains into small molecules, especially into volatile fat acids (VFA), play an important role in phosphorus removal. PAO accumulate the VFA molecules as polyhydroxyalkanoate macromolecules (PHA) under anaerobic conditions. Under anoxic or aerobic conditions, PAO use internal reserves of PHA to grow. Differently of N removal, P removal is not irreversible as there is not an insoluble gaseous product made of P in the PAO metabolisms, which keeps P inside the biomass. Moreover, the lack of VFA in the anaerobic zone or the presence of oxygen/nitrate in the same zone limits the accumulation of PHA and as a consequence, PAO will not have enough energy accumulated as PHA to grow in aerobic conditions. Figure 1.2 shows profiles of soluble BOD and phosphates in a batch reactor under different operating conditions. Basically, these conditions are determined by the presence/absence of electron acceptors, as DO and nitrate.

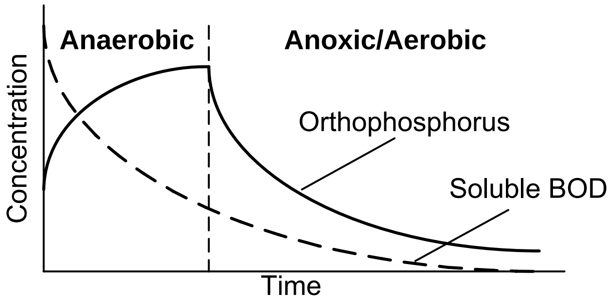


Figure 1.2: Phosphorus and soluble BOD profile under different conditions in presence of PAO.

Figures 1.3 and 1.4 present a schematic model with the internal chemical species that made up the whole biological P-removal processes (Smolders *et al.*, 1994).

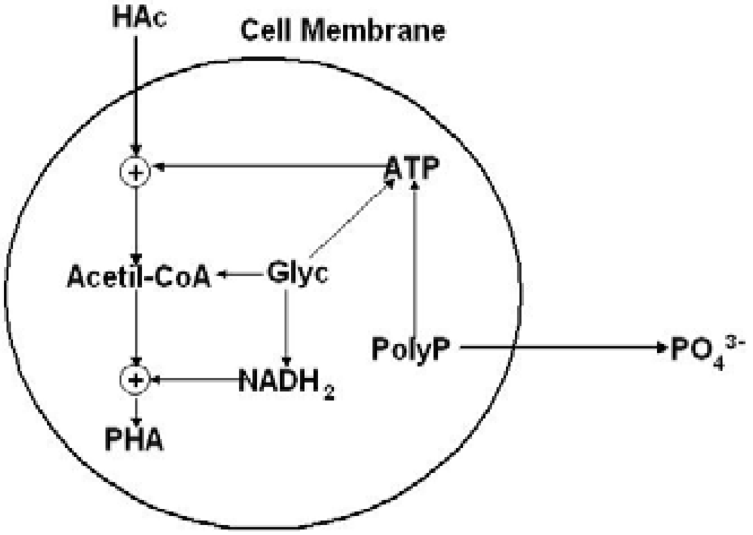


Figure 1.3: Schematic representation of anaerobic phase of phosphorus removal process.

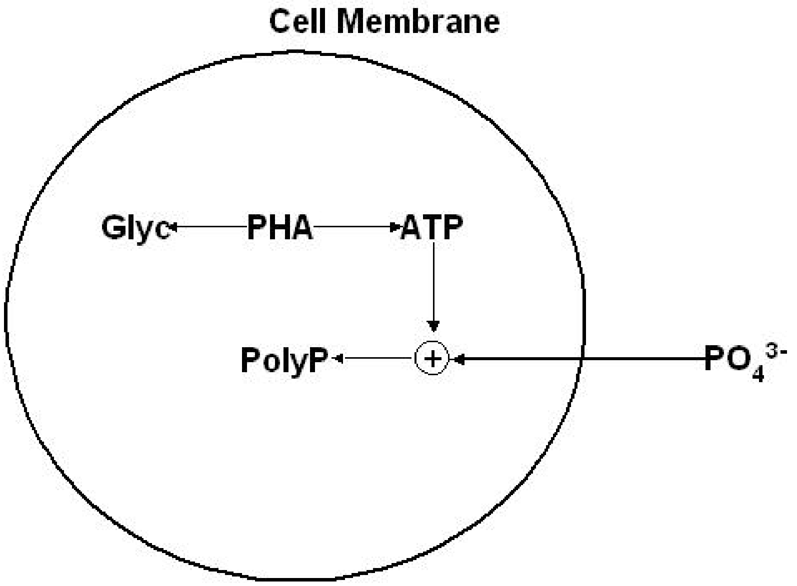


Figure 1.4: Schematic representation of aerobic phase of phosphorus removal process.

Several configurations of AS plants that allow biological phosphorus removal besides the A^2/O one are presented in the literature (MetCalf and Eddy, 2004). Figure 1.5 shows some of them, including the own A^2/O layout. The Bardenpho process has five stages in series: anaerobic, anoxic, aerobic, anoxic and aerobic. A recycle stream connects the first and more important aerobic stage to the first anoxic stage. The apparently large number of stages of the Bardenpho process is a function of the difficulties to remove all nitrate after the third stage. So, an anoxic stage was inserted to promote denitrification. However, nitrogen bubbles were carried forward to the settler, bringing difficulties to the settling process. So, an aerobic step had to be coupled as a fifth stage to help to remove the nitrogen gas bubbles and become sludge better settleable. As nitrifiers grow slowly, there is the possibility to include an especial tank to promote the nitrification using part of the sludge returned from the secondary settlers and a nitrogen source with high N concentration from other parts of the WWTP. Such modification of the A^2/O system is called BABE (Bio-Augmentation Batch Enhanced) process (Salem *et al.*, 2003). The University Cape Town (UCT) configuration has four stages: anaerobic, anoxic I, anoxic II and aerobic. Two recycles of mixed liquor (internal recycles) are present in this configuration: recycle 1 from the anoxic I to the anaerobic and recycle 2, from the aerobic to the anoxic II. The activated sludge recycle stream goes from the bottom of the settler to the anoxic I stage. Such configuration minimizes the risk of presence of DO and nitrate in the anaerobic zone (Loosdrecht *et al.*, 1998). The BFCS® process (*Biologische-*

Chemische-Fosfaat-Stikstof verwijdering) is a modification of the UCT process to allow chemical precipitation of phosphorus (Loosdrecht *et al*., 1998).

In order to save space and win configuration flexibility, Sequential Batch Reactors (SBR) have been developed. In such technology, instead of different reactors to perform each step of the treatment (anaerobic, anoxic and aerobic), there is just one that operates by cycles. Many research works are published about this process technology, even though few of them are applied as a retrofit of an existent WWTP (Andreottola *et al*., 2001). Besides SBR technology, attached-growth processes, like membranes (MBR), have arisen to save space and guarantee more biomass stability, since pollutant removal occurs inside biofilms in which the cells are less exposed to external changes in the reaction conditions. Other use of MBR technology is to substitute the conventional secondary settlers to MBR reactors to save space. (Lee *et al*., 2002). Also, few references about the usage of MBR as a solution of a retrofit problem are found (Brepols, *et al*., 2008).

As can be seen in Figure 1.5, there are robust alternatives for biologically removing phosphorus. Nevertheless, there are many WWTP that were not designed for its removal. In Catalonia, the number of plants that biologically or chemically remove phosphorus is equal to 73 (ACA – Agència Catalana d'Aigües, 2011). Although this number is increasing, there is more than 50% of WWTPs in Catalonia that only removes organic matter. Figure 1.6 shows a distribution of types of WWTP configuration in Catalonia (390 WWTP are working in Catalonia nowadays).

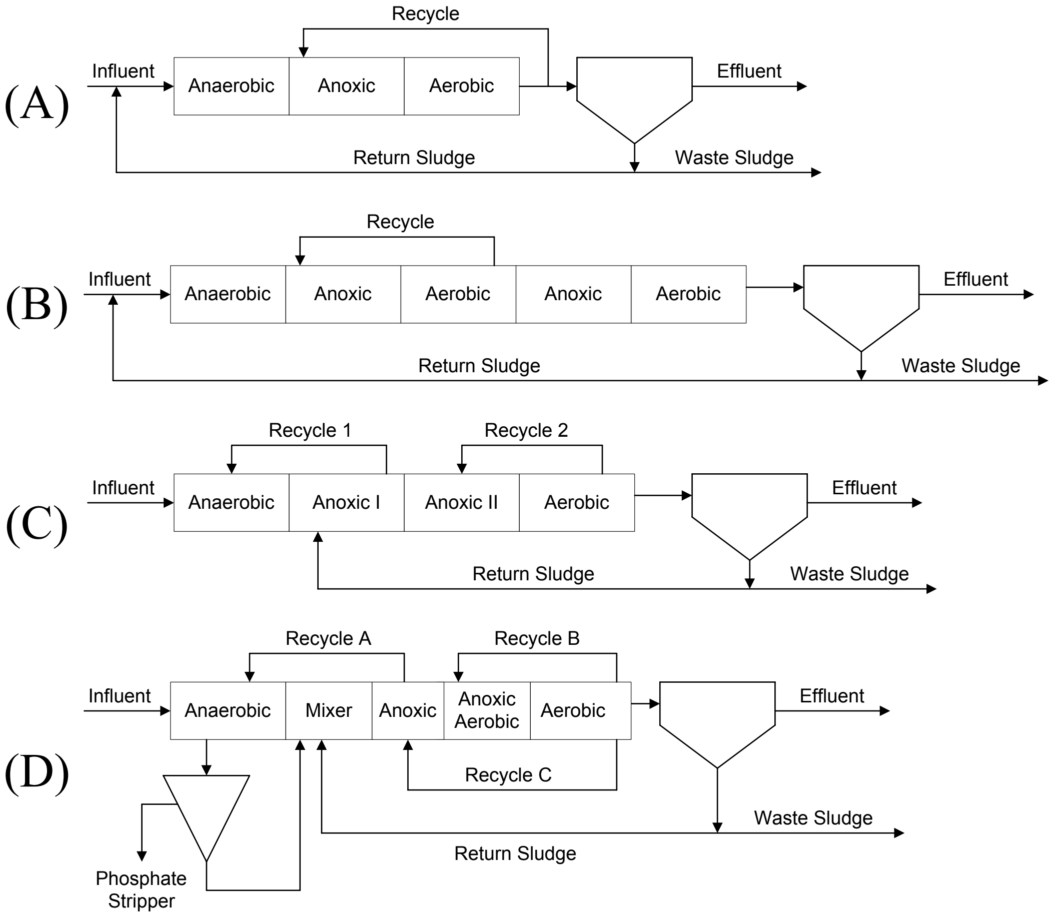


Figure 1.5: Some AS plant configurations including EBPR. (A) A^2/O system; (B) Bardenpho; (C) UCT; (D) BCFS®.

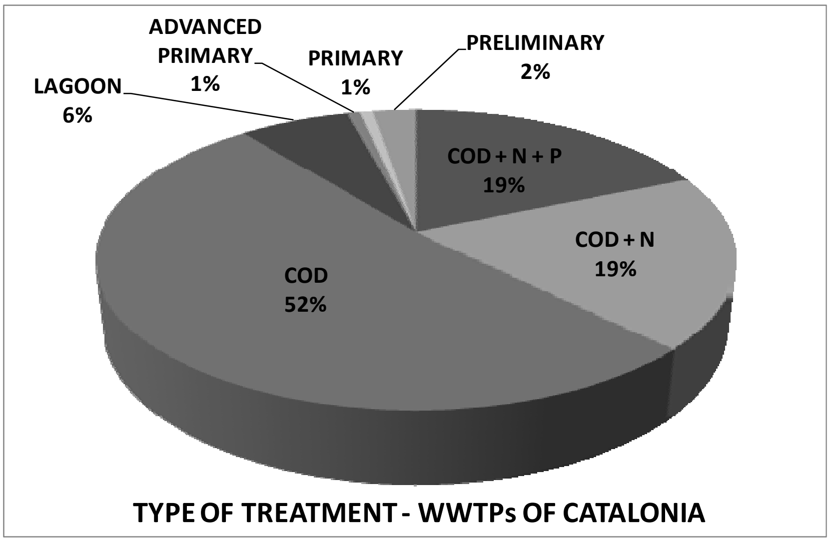


Figure 1.6: Distribution of type of current process treatment of the sludge on WWTPs of Catalonia (source, ACA – Catalonian Water Agency, 2011).

Thereby, there is a strong necessity for retrofitting these plants in order to convert them into plants able to biologically remove COD, N and P simultaneously. The appeal for using EBPR arises from the need to reduce operating costs of chemical P precipitants, with cleaning basins with considerable amounts of chemical sludge and with the transportation / disposal of this sludge.

Such retrofitting process of existent WWTP into WWTP able to perform EBPR should take advantage of all the process history of the current WWTP and need to respect the legal limits of discharge, the physical and economical constraints, keep the maximum plant stability to face external disturbances and to achieve the same performance of pollutant removal of the existent plant (Flores-Alsina, 2008). Figure 1.7 schematically represents the desired retrofitting process for implementing the EBPR in existent WWTPs.

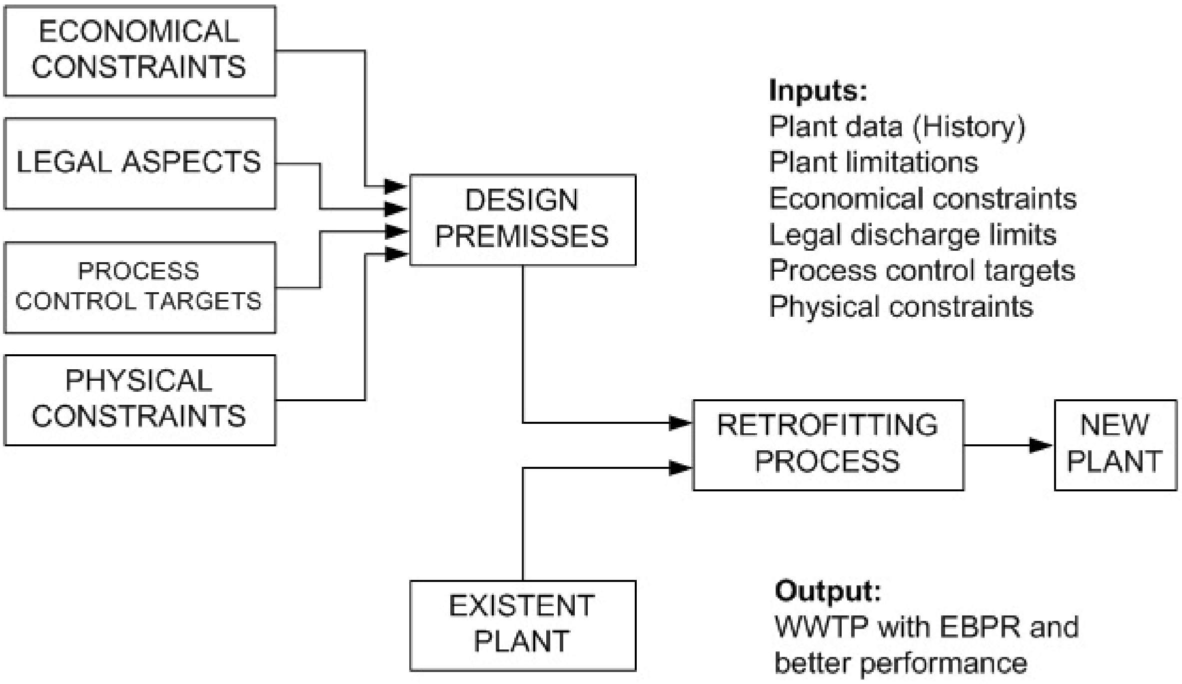


Figure 1.7: Philosophy of a retrofitting methodology.

The usual alternatives of plant configurations for implementing EBPR presented in Figure 1.5 also show a considerable degree of mass integration. All the schemes of AS plants in Figure 1.5 have biomass recycles or nitrate recycles. This fact brings extra difficulties for the control of the process, since the performance of a determined process could affect the performance of processes that occur in the upstream zone. For instance, if the denitrification process works poorly because of lack of COD and then nitrate recycle is increased, maybe DO is carried out to the anoxic zone and denitrification would be even more inhibited.

In addition to this mass integration, WWTP effluent discharge limits have become even more stringent along the years, with regard to the pollutant concentration, in special COD, BOD$_5$, total N and total P. Naturally, this progressive change in legal restrictions was not motivated to make harder to control WWTPs but for avoiding to exceed the capacity of the environment to keep its cycles free of disturbances provoked by the human activities. Hence, controlling the plant is even more complex since the process is pushed up to its physical limitations (for example, the lack of volume of nitrification to achieve the legal limits). In the case of Europe, the European Community directive for regulating effluent concentrations, published in 1991, has defined discharge limits for WWTP effluent. These limits are presented in the Table 1.1 (Sintic *et al.*, 1998).

Table 1.1: Effluent limits for WWTP discharges according to the EC-directive.

Variables	**Requirements**			
	10.000 – 100.000 p.e.		**More than 100.000 p.e.**	
	Minimum reduction (annual mean)	**Maximum concentration (annual mean)**	**Minimum reduction (annual mean)**	**Maximum concentration (annual mean)**
COD	75%	125 mgL^{-1}	75%	125 mgL^{-1}
BOD$_5$	70-90%	25 mgL^{-1}	70-90%	25 mgL^{-1}
total N	70-80%	15 mgL^{-1}	70-80%	10 mgL^{-1}
total P	80%	2 mgL^{-1}	80%	1 mgL^{-1}

Observation: “p.e” means “population equivalent”.

1.1 Process modelling and simulation

To understand the process behaviour of the WWTP is the fundamental stone to improve performance through identifying bottlenecks and proposing modifications of existent plants or even design a completely new WWTP. Besides the experimental knowledge, mathematical models are a set of tools for predicting plant behaviour under different conditions from the ordinary outlook of the WWTP or even under unexpected operational scenarios (Jeppsson, 1996).

In practical terms, there are two kind of models that are useful for WWTP: (1) the black-box models, based exclusively on plant data which brings correlations amongst input (biological requirements or manipulated variables of the control system) and output variables (variables of interest or controlled variables of the control system) (Machado, 2007); (2) the phenomenological models, based on the mass, energy and momentum balances supported by the biological relationships between biomasses and substrates previously described and documented in the literature. The former kind of models does not explicitly show how the dissolved oxygen concentration affects the heterotrophic biomass amount which by its turn affects the ammonium concentration in the effluent. However, based on the plant history, a simple transfer-function between the dissolved oxygen and the ammonium concentration in the effluent can be correlated. On the other hand, the phenomenological models stand for declaring all the relationships of all the important variables. A complete review of the WWTP models can be found in Jeppsson (1996).

Usually, COD and nutrient removal processes in WWTPs are modelled using the International Water Association (IWA) activated sludge models (ASM). These models are mainly used for the design or redesign of WWTP (i.e., Benedetti *et al.*, 2008, Ferrer *et al.*, 2008, Rivas *et al.*, 2008), development of control strategies for WWTP (i.e. Flores-Alsina *et al.*, 2008b) and control design for integrated urban wastewater systems (i.e., Vanrolleghem *et al.*, 2005, Fu *et al.* 2008). Since the release of ASM1 by Henze *et al.* (1987), four versions of ASM for organic matter and nutrients removal processes have been proposed by the IWA Task Group on mathematical modelling: ASM1, ASM2, ASM2d and ASM3 (Henze *et al.*, 2000). ASM2d was proposed to provide a useful framework for the description of WWTP with biological N and P removal. Three types of microorganisms are defined in ASM2d. Heterotrophic microorganisms (X_H) grow on readily biodegradable organic substrates (S_F) and fermentation products (S_A). Autotrophic microorganisms (X_A) are involved in the aerobic process of nitrification, where ammonium (S_{NH4}) is converted to nitrate (S_{NO3}). Finally, PAO microorganisms are responsible of enhanced biological phosphorus removal (EBPR) and are modelled considering three state variables: cell internal storage products (X_{PHA}), stored poly-phosphate (X_{PP}) and PAO (X_{PAO}), as commented before.

Commonly, an approximate description of a WWTP with N and P removal can be achieved by using the default values of ASM2d parameters, but calibration of the model is required for an accurate description of experimental data. Moreover, determining the best parameter values, according to a cost function is only part of the problem and should be followed by a confidence assessment of the estimates (Checchi *et al.*, 2007). The high number of parameters of complex models as ASM makes difficult to choose which parameters must be selected for calibration. This is usually based on process knowledge and previous experience, but some authors have proposed a systematic approach based on mathematical tools for parameter selection. The knowledge-based approach makes use of the large amount of experience reported from activated sludge systems (Ruano *et al*, 2007) as the protocols developed by WERF (Melcer *et al.*, 2003), BIOMATH (Vanrolleghem *et al.*, 2003), STOWA (Hulsbeek *et al.*, 2002) or CALAGUA (García-Usach *et al.*, 2006).

The systematic approach studies the identifiability of ASM models relying on the sensitivity and correlation analysis of model parameters (Weijers and Vanrolleghem, 1997, Brun *et al.*, 2002, de Pauw, 2005). These systematic methodologies firstly calculate a ranking of parameters (local sensitivity analysis) based on its influence on model outputs and then study the correlation analysis of parameter subsets. Weijers and Vanrolleghem (1997) developed a procedure based on the Fisher Information Matrix (FIM) to study the identifiability of ASM1 models. The D and modE criteria of the FIM were used to find an identifiable parameter subset among numerous combinations. This methodology was also successfully applied to other kinetic models (Reichert and Vanrolleghem, 2001, de Pauw, 2005, Checchi and Marsili-Libelli, 2005 or Marsili-Libelli and Giusti, 2008). On the other hand, Brun *et al.* (2002) developed a systematic approach for ASM2d calibration based on full-scale plant data by applying identifiability analysis and a subsequent iterative parameter subset selection and tuning using comparable criteria to the D and modE criteria. They defined the collinearity index (γ) and the determinant measure (ρ).The γ index represents the interdependence of all the analyzed parameters and ρ is a relative measure suited for comparison of parameter identifiability of different parameter subsets. In addition, Brun *et al.* (2002) studied the problem of parameter interdependencies and the effect of fixed parameter values on parameter estimates (bias problem). Recently, a similar methodology was applied for water body quality modelling where the water drainage system was the focus instead of the biological wastewater treatment (Freni *et al.*, 2009). Finally, a novel methodology for selecting the most important parameters that are able to better explain the behaviour of the WWTP processes avoiding overfitting effects was also elaborated (Machado *et al.*, 2009) based also on the ratio of both main FIM criteria (D and modE criteria).

Process models of WWTPs, once built, should be simulated under specific conditions to predict the plant behaviour during a certain period of interest. The simulation itself is an initial value problem that can be solved with a wide set of standard methods found in the literature (Rice and Do, 1995). Such methods are also implemented in simulation and mathematical softwares like BioWin^{TM}, EFOR^{TM}, GPS-X^{TM}, Matlab/Simulink^{TM}, Simba$^{®}$, STOAT^{TM}, WEST$^{®}$ and so on (Krause *et al.*, 2002; Meijer *et al.*, 2002; Gernaey *et al.*, 2004b).

1.2 Process control aspects of WWTP

More stable operation of wastewater treatment has been achieved since the automatic control was adopted in some wastewater treatment facilities. Digital Proportional, Integral and Derivative controllers (PID) allowed moving process operators to a higher level in the process control hierarchy since fast control loops passed to be managed by an auto-operated regulatory system. Thereby, the plant operators could save time and passed to analyse the processes bringing new ideas for maximize plant benefits. In addition, a supervisory layer is making use of “if-then” rules to deal with process disturbances and frequent operation problems (Baeza *et al.*, 2000, 2002b). In this way, for instance, feedforward and model predictive controllers also provide automatic solutions for refusing external disturbances, but few wastewater treatment units get the benefits of them or such controllers are applied only in pilot plants instead of full-scale plants (Brouwer *et al.*, 1998; Samuelsson and Carlsson, 2001; Ingildsen *et al.*, 2002; Krause *et al.*, 2002; Stare *et al.*, 2006; Vrecko *et al.*, 2006).

In particular, as biological wastewater treatment processes depend on complex biological reactions of live organisms and not on ordinary chemical reactions, converting experimental observations and data in process information demands a higher effort. The set of the IWA AS models is an expressive example of this effort. The ASM1 (Henze *et al.*, 1987), the ASM2 (Henze *et al.*, 1995) and the ASM2d (Henze *et al.*, 1999) synthesize in a comprehensive way the most important reactions involved in the biological COD, N and P removal processes, observed by many researches (Smolders *et al.*, 1994; Mino *et al.*, 1995; Kuba *et al.*, 1996). For taking advantage of this biological modelling effort, a reasonable number of scientific works perform the modelling task of the whole WWTP for process control with such models, combined with calibration protocols and methodologies where experimental data (routine analysis) as COD, BOD, total P, total N, dissolved oxygen in aerobic basins, TSS, MLSS, VLSS, Kjeldhal nitrogen of the influent and the effluent are extensively used as the primary source of information of the plant behaviour (Brdjanovic *et al.*, 2000; Ayesa *et al.*, 2005; Ingildsen *et al.*, 2005). Biological models calibrated with full-scale plant data have been applied to design control structures for guaranteeing plant stability, minimizing operating costs and maximizing the effluent quality even during undesired weather scenarios (rain events for instance) (Suescun *et al.*, 2001; Meyer and Pöpel, 2003; Cadet *et al.*, 2004).

Along the years, practical experience with activated sludge plants has emphasized the control of inventory variables (Olsson, 2006). In the case of AS plants, the sludge retention time (SRT) and DO in the aerobic reactors are the most important inventory variables.

The sludge retention time is a determinant variable in organic matter, N and P removal. By definition, SRT is given as follows:

$$SRT\left[d^{-1}\right]=\frac{\sum_{1}^{j}V_jX_j}{Q_{EFF}X_{EFF}+Q_WX_W} \qquad \text{Eq. 1.4}$$

where V_j and X_j are the reactor volume and biomass concentration (solids) of the reactor j, respectively, given in m^3 and g $TSSm^{-3}$. Q_{EFF} and Q_W are the effluent and purge flow rates, respectively, while X_{EFF} and X_W are the biomass concentration in the effluent line and in the purge flow line. Flow rates are given in m^3d^{-1}. High retention times increase the performance of the N removal, while low ones provide better P removal. This difference arises from the specific growth velocity of the different biomasses (autotrophs grow slower than PAO biomass). The manipulated variable to control SRT is the purge flow rate, Q_W. Nevertheless, changing Q_W not only the SRT will change because the mathematical relationship of Eq. 1.4 but also because Q_W affects the solid concentration in all reactors and consequently the dynamic of all the biological processes involved.

According to Eq. 1.4, SRT control requires the measurement of the solids concentration in different parts of the plant,. However, if the solids are controlled in only one point of the plant, for instance in the last aerobic reactor, an equivalent result can be obtained. In some cases, instead of controlling SRT, the sludge blanket height in the settler is controlled, for example in the work developed by Suescun *et al.* (2001).

At the same time, DO is a key variable in the nitrification processes and its absence is required in part of P removal and in the denitrification process to obtain better performances of these processes. It is known that the dissolved oxygen increases the nitrification rate while decreases asymptotically the denitrification rate as shows Figure 1.8 (Crites and Tchobanoglous, 1998).

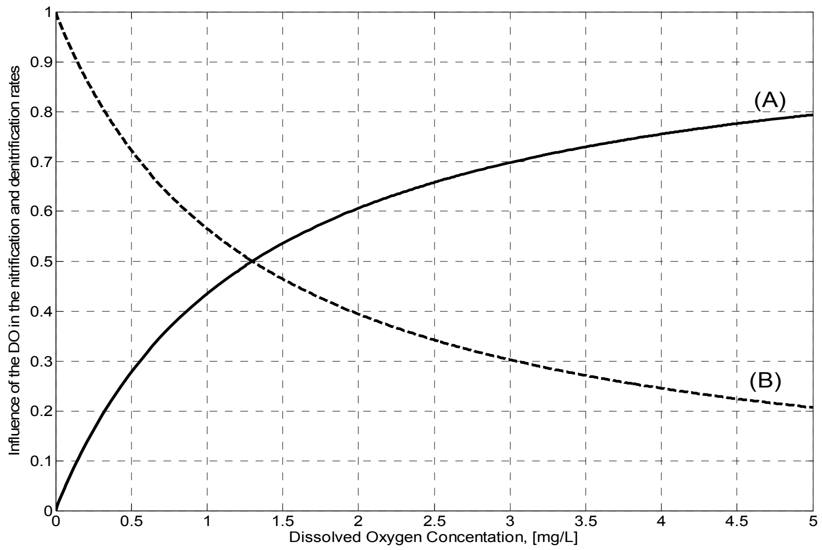


Figure 1.8: Influence of DO in the nitrification rate (A) and in the denitrification rate (B).

Nevertheless, Figure 1.8 shows that simultaneous nitrification/denitrification processes can occur, since in a wide range of DO concentration these biological rates are not null. Air pressure or flow rate are the manipulated variables to control DO, apart from the mixing that helps to put in contact atmospheric air with mixed liquor of the reactors.

SRT and DO, the two most important inventory variables in AS plants, historically were controlled manually. Automatic process control has gave its first contribution to the AS plants in the moment when PID feedback (FB) controllers were used to control them. So, purge flow rate and the amount of air could be adjusted to keep automatically SRT and the DO in certain levels to run properly the plant. The PID controller works over the error value between the desired value (set-point, y_{SP}) and the measured value (y). Basically, its function is to make null this error. It is worth noticing its action is applied each sample time of the control hardware (single PID controllers, PLCs – Programmable Logic Controllers, DCS-Distributed Control Systems, and so on). However, the classical control theory presents the PID equation in a continuous form (position form), as follows:

$$u(t) = u_{BIAS}(t) + \underbrace{K_P\left(y_{sp} - y\right)}_{PROPORTIONAL} + \underbrace{\frac{K_P}{\tau_I}\int_0^t \left(y_{sp} - y\right)dt}_{INTEGRAL} + \underbrace{K_P \cdot \tau_D \frac{d\left(y_{sp} - y\right)}{dt}}_{DERIVATIVE} \qquad \text{Eq. 1.5}$$

where $u(t)$ is the control action (manipulated variable) at the time t, u_{BIAS} is the reference value for the manipulated variable to keep the controlled variable at its open loop value, K_P is the controller gain, τ_I is the reset time and τ_D is the derivative constant. The PID controller is inserted into a feedback control loop, as shows Figure 1.9 for DO control.

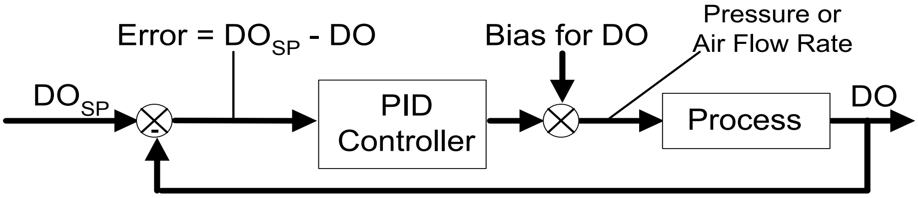


Figure 1.9: Simplified feedback loop for DO control.

Industrial PID controllers take into account the *wind-up* effect, which consists of an uncontrolled increase of the integral action after the manipulated variable has reached its operational limit (saturation problem) (Ogunnaike and Ray, 1994; Aström and Wittenmark, 1997). This effect can be avoided writing the equation 1.5 in the digital velocity form:

$$\Delta u(k) = \quad K_P\left[\left(1+\frac{\Delta t}{\tau_I}+\frac{\tau_D}{\Delta t}\right)\varepsilon(k)-\left(\frac{2\tau_D}{\Delta t}+1\right)\varepsilon(k-1)+\frac{\tau_D}{\Delta t}\varepsilon(k-2)\right] \qquad \text{Eq. 1.6}$$

where $\Delta u(k)$ is the variation of the manipulated variable from the instant k-1 to the instant k (actual instant). Δt is the sample time of the controller in which each control action is applied. And finally, $\varepsilon(k)$, $\varepsilon(k\text{-}1)$ and $\varepsilon(k\text{-}2)$ are the difference between the set-point of the controlled variable and its measurement at the actual instant k, one instant before (k-1) and two before the actual (k-2). As can be observed, equation 1.6 is written in discrete form.

Once the inventory control loops are active, the next control objective is to improve the effluent quality in order to respect legislation. To improve the effluent quality means to reduce COD, N and P concentrations. To achieve this aim, not only the manipulated variables that are adjusted to control inventory variables can be used but also additional control handles such as recycle flow rates (mixed liquor and sludge recycles) and, in some plants, the amount of external carbon source used for improving denitrification (Carlsson and Rehnström, 2002). The possibility of using the same control handles for inventory variables and effluent quality control lies in the fact that there is a relationship among inventory control variables and effluent quality control. In fact, the amount of nitrogen released in the effluent in form of ammonia or nitrate is dependent on the DO concentration. Thereby, *Cascade Control* became common in WWTP linking the DO control to the ammonia control in the last aerobic reactor, for instance. The main advantage of joining hierarchically both controllers and not to use directly the air flow rate or air pressure to perform ammonia control is to avoid interferences of low level measurements (Olsson, 2006). Once the inventory control smoothes its control variables, DO measurement is preferred to be adjusted than air flow rate, to control effluent ammonium. Schematically, cascade control applied to ammonium control is depicted in Figure 1.10.

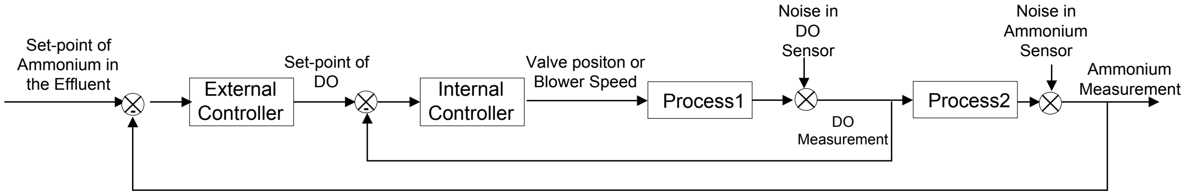


Figure 1.10: Ammonium control by cascade control.

Obviously, such kind of controller could be thought because process instrumentation upgraded. Ammonium on-line sensors to perform its automatic control are available just recently (Olsson, 2006).

As occurs in many continuous processes, influent stream flow rate represents a strong external disturbance. In WWTP, an extra difficulty is added: the influent composition is not constant as well. So, as FB controller actuates according to the error measurement, when changes in the ammonia measurement occur due to changes in the ammonium influent load, the corrective action of ammonia controller is applied with an undesirable time delay. Such problem is one of the limitations of the FB control. In order to overcome this inconvenient behaviour, an anticipative action needs to be calculated. Such control configuration is named Feed-Forward Control (FF), and it is designed based on the knowledge of the relationship between the disturbance variable and the controlled variable. Once being aware of this relationship, a FF-FB controller, which combines the FB action on the error (process variable setpoint and the process variable value) and the FF action based on the knowledge of the disturbance effect on the process variable, should be designed and the control action would be taken as the bias action. So, the ordinary FB loop would have a time-variant reference action, besides the normal action calculated by the ordinary PID controller. In the case of ammonia control, the control loop with combined feedback/feed-forward action could be represented by the picture in Figure 1.11.

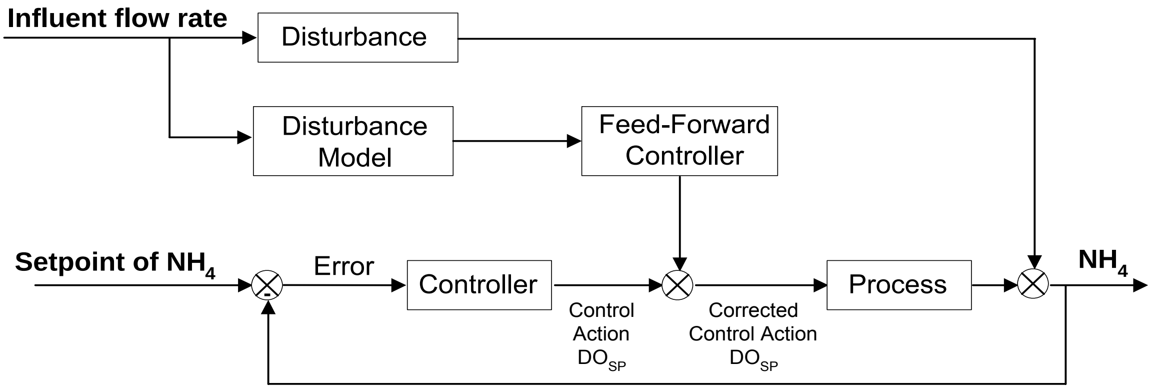


Figure 1.11: Representation of combined feedback/feed-forward ammonium control loop. The symbol DO_{SP} in means setpoint of dissolved oxygen.

In the case of Figure 1.11, the influent flow rate was considered as the main disturbance of the effluent ammonium control. The disturbance model, in this case, is the relationship between the influent flow and the ammonium concentration in the effluent when the control loops are opened (manual control). In the literature, the aerobic volume of the plant also can be changed and not only the DO concentration works as manipulated variable of the feedback/feed-forward configuration (Brouwer *et al.*, 1998). The use of influent flow rate as main disturbance is the simplest choice for increasing the performance of the ammonium feedback controller. Nevertheless, not always is possible to correlate, in a deterministic manner, influent flow rate values with the DO concentration or even the ammonium concentration. Hence, a better situation to design an ammonium feed-forward control would occur if the ammonium load (volumetric flow rate multiplied by ammonium inlet concentration) were known. Such knowledge is restricted to the plants which have an ammonium sensor in the inlet part of the plant (head of the plant) or in which oxygen uptake rate (OUR) experiments are performed (Baeza *et al.*, 2002). In an ultimate case, off-line measurements of influent ammonium concentration would be used to calibrate a phenomenological model to predict the inlet ammonium concentration. Naturally, other variables should be monitored and the model will use them to make the calculations (Krause *et al.*, 2002).

While ammonium disappears of the system, nitrate is brought from the aerobic zone to the anoxic zone to be denitrified. In theory, the control objective of improving the effluent quality also comprises reducing the nitrate effluent concentration. This reduction is done by the anoxic reactors. As explained in previous sections, to perform denitrification, soluble BOD is necessary. Unfortunately, in many plants there is a lack of BOD content and an amount of nitrate passes through the anoxic zone without denitrifying. Due to the limited denitrification, nitrate accumulates in the system. This fact motivates operational staff of AS plants to make use of feedback controller to control nitrate at the end of anoxic stages, by means of changing the mixed liquor recycle flow rate (Ekman *et al.*, 2003; Baeza *et al.*, 2004). Some works make reference to plants in which an external carbon source flow rate (usually acetic acid or ethanol) is used as an extra manipulated variable to obtain complete denitrification (Samuelsson and Carlsson, 2001; Carlsson and Rehnström, 2002; Lindberg and Carlsson, 2002).

Although contributions of process control theory in AS plants commented before have improved the effluent and inventory control, some external perturbations provoked by storm and rain events are not completely refused by those strategies. In addition, the knowledge of plant operators and process engineers is not so easily incorporated into the control architecture. Thereby, in some plants and in literature works, the fuzzy logic and expert based control system have been applied in AS plants (Kalker *et al.*, 1999; Meyer and Pöpel, 2003).

Fuzzy logic controllers calculate control actions based on the classification of plant states. Depending on the plant state, the aeration in some reactor is turned on or off, for instance. Some rules like "*If-Then*" and weight functions determine the control action amplitude. The key point to obtain success with this kind of controller is to recognize the different plant states investigating historical data of operation. Tools to perform this quest have been designed (Rosen and Yuan, 2001).

Expert based control works as a supervisor layer which operates sending set-points to the effluent quality controllers and inventory control. Plant behaviour is studied through some important variables and recorded not only during normal operation conditions but also when an undesired event occurs. By comparison, the controllers know which control actions should be taken to bring the system to the normality (Baeza *et al.*, 1999, 2000).

Although several control strategies have been developed along the time to improve the effluent quality and to reduce operational costs in WWTP, they usually did not take into account the multivariable behaviour of the process (Suescun *et al.*, 2001; Copp *et al.*, 2002; Ayesa *et al.*, 2005; Ingildsen *et al.*, 2005). Historically, the majority of such control strategies employed in WWTP took into account just the organic matter and nitrogen removal. In such applications, control structure design (CSD) is the first step to attain good performance of the controllers. To design a control structure is necessary to define if the controllers will be independent each other or centralized like a Model Predictive Controller (MPC) for instance, if just feedforward or a combined feedback/feedforward actions will be employed or if decouplers are suitable or not, amongst other details. The kind of controllers, that is, if the controllers will be PID controllers, predictive controller or adaptive one also needs to be defined (Maciejowski, 2002; Skogestad, 2004). Comparisons between decentralized and centralized controllers are found in literature of WWTP control (Steffens and Lant, 1999; Zarrad *et al.*, 2004; Stare *et al.*, 2006).

The CSD has been reported in some works in simultaneous COD and N removal process but they usually do not include or do not pay too much attention to P removal, and do not systematically check all points commented before when they build a control structure (Suescun *et al.*, 2001; Copp *et al.*, 2002; Baeza *et al.*, 2004; Ayesa *et al.*, 2005; Samuelsson *et al.*, 2005). Such apparent lack of interest to include P removal can probably be explained by the novelty of the phosphorus removal and because of operational difficulties in real facilities added by P removal processes. However, recent developments of the theory of P removal and progressive constraints in the environmental regulations have been the driven forces for developing control structures considering simultaneous removal of COD, N and P (Ingildsen *et al.*, 2005). Having got designed, a control structure should be tested in pilot plant or full scale plant to proof its stability and performance with real external disturbances. Usually, process controller setpoints used in these tests are the values of the controlled variables under open loop operation and probably these values are not the optimal ones regarding the effluent quality and cost operation. Some strategies move the control structure forward to more profitable operating conditions as presented in the literature, even though P removal has not been considered (Cadet *et al.*, 2004). Another way to determine the best process controller setpoints is performing an off-line or on-line optimization using an accurate process model (in general non-linear models) or experimental data. So, a hierarchy in the plant operation is depicted. There is an optimization layer (supervisor) that commands the process control layer. The control layer is divided into two parts according to the importance of process control variables: a master layer, containing ammonium, nitrate and so on and another one, called slave layer, including DO control for instance.

As observed, WWTP processes had to be modified along the time. Process modifications were added to the classic COD removal, first to include nitrogen removal and recently to include phosphorus removal. Each change was made thinking in the benefits of a process able to remove more pollutants, but each new control variable added, decreased the capacity of the manipulated variables to keep the process working stably at a certain operating point since the degree of freedom of control decreases. For instance, when process removes only COD and nitrogen (A/O configuration, for example), the most common control manipulated variables are biomass recycle, internal recycle and DO, while control variables are effluent nitrate and ammonium concentrations. When phosphorus removal is added as a control objective simultaneously to COD and N removal (A^2/O configuration, for instance), effluent phosphate concentration enter in the set of control variables. The number of manipulated variables continues being the same as in the latter configuration but now one more variable need to be controlled.

Considering the reasons for converting existent plants which cannot biologically remove P into WWTP that are able to perform such process, this work proposes a model-based strategy to retrofit existent WWTP to perform EBPR considering also the controllability of the system.

1.3 Structure of the text

This work is divided into six chapters and one appendix. Chapter 2 presents the motivations and objectives of this work. Chapter 3 presents the proposed methodology for systematically retrofitting an A/O WWTP into a WWTP for removing COD, N and P in a biological way. Chapter 4 shows the application of the methodology of the chapter 3 in a full scale WWTP (Manresa WWTP, Manresa, Catalonia, Spain). Chapter 5 and 6 bring the conclusions of the present work and future works that could be based on this work, respectively. Appendix completes the written part of the thesis.

Chapter 2: Objectives

The main objective of this work is to present a systematic way to modify an existent WWTP that biologically removes only organic matter and nitrogen into a WWTP that removes organic matter, nitrogen and phosphorus, also biologically. This necessity arises from the great number of WWTP that are not ready to biologically remove simultaneously COD, N and P and, according to the strict regulations, phosphorus removal is an absolute pre-requisite in new WWTP facilities. The upgrading process will be based on a deep study of the existent facility, including the influent composition characterization, the first principles modelling of biological processes, the current process control strategy and current performance of the overall treatment evaluations. Such study will provide enough information about the kinetic parameters of the autotroph, nitrifying and denitrifying biomasses in order to create alternatives which will partially preserve the plant identity concerning to N-removal with new characteristic introduced by the EBPR processes. An input-output model for process control will be obtained of the current facility data in order to evaluate the best decentralized control structure and for further comparisons with the control model of the plant with the EBPR processes already incorporated.

A set of new plant configurations (retrofitting alternatives) will be proposed, based on the plant model of the current facility. The reference model will be calibrated using the available plant data in order to capture the main dynamic characteristics of the system. . The proposed alternatives will be tested with special influent profiles (with strong N and P shock loadings) to evaluate the achievable overall treatment performance of each plant configuration under stressing conditions. Besides the pollutant removal capacity, all the alternatives will be confronted concerning the investment costs, the operating costs and the process stability. Once determined the new plant layout, a new transfer function will be obtained and compared to the previous one, to allow the analysis of the influence of the PAO into the whole process control performance. The best control structure will be designed using the chosen plant configuration for introducing the EBPR processes.

The usage of chemical products for P-removal and the amounts of produced sludge will be compared amongst all the tested alternatives and the current plant. It is expected that the retrofitted plant will produce less sludge and demand much less chemicals for P-removal.

The proposed methodology will state for taking the maximal advantage of the process data of the current plant (historical data) in order to obtain a process model. Also, in the creation of possible alternatives for implementing the EBPR the following premises will be defended:

- To give preference to solutions that impact as less as possible the operation of the current WWTP (minimum number of changes).

- To keep the main reactors characteristics (do not change from CSTR to SBR reactors, for instance or from CSTR to membrane reactors).

- To keep the same performance of the existent current plant in the COD and N removal processes (not to lose the acquired benefits of old retrofittings, like to change from only COD removal to COD + N removal, for instance).

- To build a control structure with standard process controllers (PIDs) that will be able to refuse external disturbances of N and P better than the existent plant.

Other important objective of this work is also to test the proposed retrofitting methodology with data from real full-scale WWTP plants. Fortunately, the proposed methodology could be tested in a full A/O WWTP located at Manresa city (Province of Barcelona, Catalonia, Spain).

The software Matlab/Simulink® will be used for plant modelling tasks and for model simulations.

Chapter 3: The Proposed WWTP Retrofitting Methodology for EBPR implementation

The proposed retrofitting methodology begins with an exhaustive search for plant information through data mining. Laboratory and sensor data are employed to determine operating points and influent patterns, and to calibrate a plant model. At this stage, the methodology of the "*seeds*" using FIM (*Fisher Information Matrix*) helps to find and optimise the most useful model parameters with the lowest possible uncertainty (Machado *et al.*, 2009). Once a model is developed and fitted, new plant configurations or alternatives are proposed for improving COD, N and P removal. After that, cost and process controllers are designed for the new alternatives which are developed to have the ability of refusing as fast as possible the external disturbances (rain events, increase of pollutant inlet concentrations). Finally, all the alternatives are compared, following pre-defined criteria and the most economic and useful for treating the wastewater, are presented to the WWTP managers. These criteria for choosing the best alternative is defined based on the investment costs, the capacity of treatment and the robustness of the process controllers in order to keep the plant around the operating point. Figure 3.1 presents a schematic flowchart of the proposed retrofitting methodology.

Plant data of the existent configuration is extremely useful for determining how the plant is far from the maximum treatment capacity. It helps to determine influent concentration patterns and when the aeration system will be more demanded. With plant data, it is possible to correlate variables as the internal and external recycle rates with the nitrate and phosphate in the effluent and along the plant, for instance. Plant data (and lab data) also allow determining DO transfer coefficients.

Extra experiments could be necessary to determine the amount of active biomass inside the basins, DO dispersion in aerobic basins and influent characterization according to the state variables of a plant model, necessary in the proposed methodology.

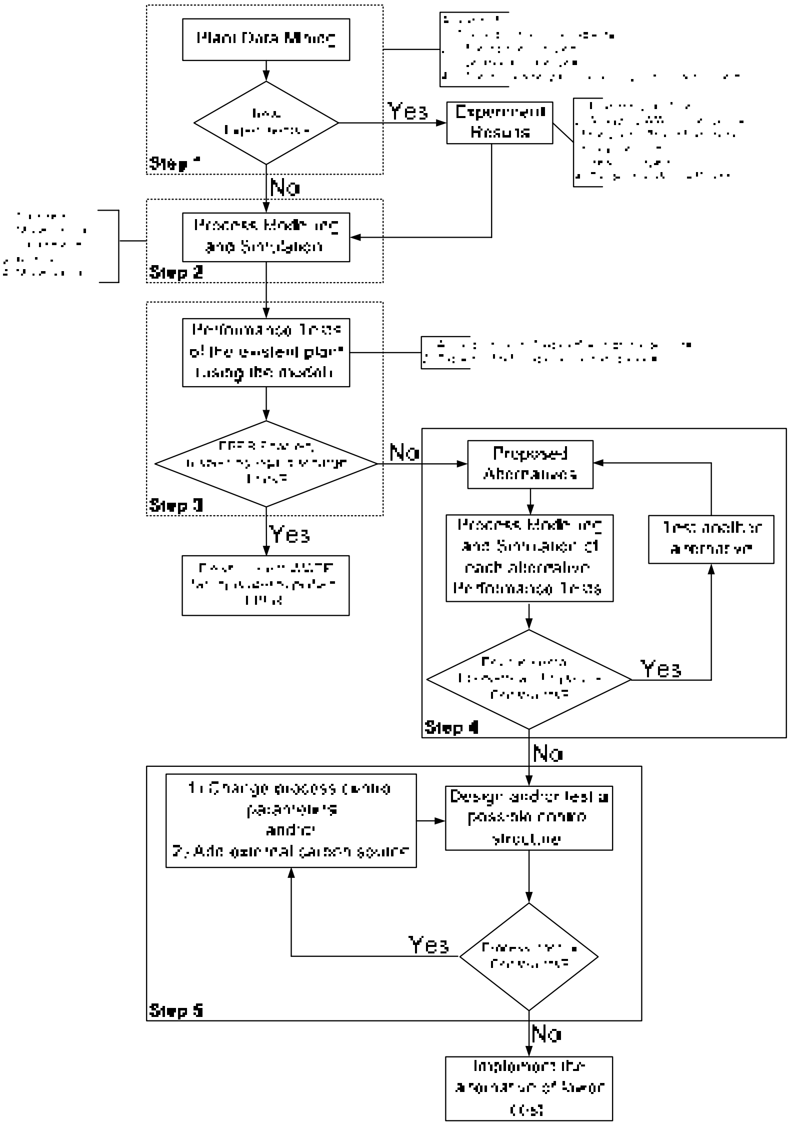


Figure 3.1: Flowchart of the proposed methodology for retrofitting WWTP including EBPR.

Process modelling and simulation are also very important in the proposed methodology since a plant model converts the physical-chemical and biological behaviour of the system and also the operation team's knowledge (practical knowledge) into an easy interface for obtaining predictions of the plant variables, even in extreme situations or in unusual operation. Here, the plant data also plays an important role: influent and effluent pollutant concentrations, flowrates and temperature are used as inputs of the simulations of the current plant and possible alternatives of the new plant. It is important to select datasets when the current plant is operating in a stable manner to create a fair basis of comparison amongst all the proposed new configurations which are the products of the methodology. Understanding how the plants will work in other operating conditions than the common ones, it is possible to change in a safely way the manipulated variables in order to reduce cost without losing the quality of the effluent. Hence, plant limitations will arise and will be possible to study them without running the existent plant under these undesired conditions. Another function of the modelling step is to generate a common starting point for testing other plant configurations, keeping the same values of the kinetic parameter (and other ones) of those biomasses that will be present for testing the new proposed configurations. At this step, kinetic and stoichiometric parameters and the behaviour, limitations and qualities of the existent plant are known. Thereby, a set of solutions for improving the wastewater quality, decrease costs and improve the control structure are selected. The proposed methodology uses standard solutions of type of WWTP, like A^2/O, Bardenpho, UCT, combined to more advanced control structures than those ones used to be found in practice (*feedforward* for $NH4^+$ control, cascade control for NH_4^+ and NO_3^-, model predictive controller…).

After the model of the current plant and a set of proposed new plant configurations have been developed, expert knowledge related to the site specificities should be taken into account and used for filtering the great number of retrofitting solutions of revamping an A/O WWTP, producing a concise subset of alternatives. This step is also necessary not to test infeasible solutions regarding to the plant constructability, maintainability and operability, for instance, try to build a great anaerobic basin that probably would promote high phosphorus elimination but never would be constructed because there are a small community near the plant that would complaint about the odours generated by the fermentation processes or even if there are no space to build such a basin. Applying the criteria of low investment costs, low operating costs and maximal effluent quality and robustness of the control structure, the best proposed solution for improving the existent WWTP is recognized.

At this point, the methodology of retrofitting produces its final result: the new plant configuration with the most robust process control structure as possible with the existent resources, with the lowest operating cost and delivering a treated wastewater according to the legal pollutant limits.

3.1 Available information in a WWTP

Each day hundred of data is collected from a WWTP: influent and effluent lab analysis (BOD, COD, Kjeldahl nitrogen, ammonium, nitrate, phosphate, pH, inlet and outlet flowrates, purge, internal and external recycles (if applied), total suspended solids in settlers and basins, DO measurements, air flow rates, electrical consumption, and so forth. These data, when used only to control the process in a daily time basis, are poorly used to improve the system operability, to find the best operating point and to understand what really is behind the physical measurements. Nevertheless, if specific variables are forced to be correlated amongst them and an historical of all the variables are studied, interesting information could be generated, like nitrification and fermentations rates, the best value of internal and external recycling flow rates or what should be the biomass concentration inside plant reactors and settlers. Plant data could be used to feed mass balances in reactors and in subsystems, providing a relationship among different parts of the treatment process, and also providing relationships amongst manipulated variables and controlled variables for better tuning process controllers. Influent patterns could be arisen from plant data along the years, which helps to pre-setting what will be the manipulated variables that will help to control the process, like the setpoint of DO, or the internal and external flowrate setpoints. Plant data is also extremely useful to help to obtain a process model, which has a representative set of equations that describes the biomasses behaviour (van Veldhuizen *et al.*, 1999; Hao *et al.*, 2001; Hulsbeek *et al.*, 2002; Gernaey *et al.*, 2004b;.Makinia *et al.*, 2005; Nuhoglu *et al.*, 2005; Ingildsen *et al.*, 2006; Fall *et al.*, 2010).

As WWTP are becoming more and more automated, too much data can be stored, providing a source of experimental knowledge very useful for predicting the behaviour in other operating points. In terms of retrofitting, model calibration allows to determine specific values of biomass parameters to employ in improved plant configurations, like full WWTP for biologically removing COD, N and P.

3.2 Model calibration and validation

The model calibration procedure is based on the sensitivity analysis, the FIM calculations (RDE criteria) and the parameter estimation through minimizing a calibration cost function (CCF) that represents the difference amongst effluent data and the predicted effluent concentration (see appendix for details). Figure 3.2 shows a flowchart illustrating the proposed methodology. A pre-selection of the most influential parameters is recommended in the literature (de Pauw, 2005) to prevent the combinatorial explosion of the number of parameter subsets in later steps of the procedure. Therefore, the sensitivity analysis (see appendix for details) is employed for the initial classification of the parameters studied. The first twenty parameters of the ranking are selected as candidates to be evaluated. They are called "*seeds*" because each one will originate a parameter subset for model calibration. The RDE criteria for all the possible pairs between the first seed and the other parameters of the sensitivity ranking are calculated around the model (ASM models for example) default parameter values. The pair with a maximum RDE value is chosen to continue building a new parameter subset. Next step is to calibrate the model minimising the CCF using the pair of parameters selected. Once the CCF is optimized, the RDE criteria is recalculated with the optimized parameter values (RDE_C, RDE corrected). Note that each new RDE calculation implies the evaluation of a new FIM matrix with the updated set of parameters (see appendix for details).

Next step is to calculate the RDE for all combinations between the pair previously selected and one of the remaining parameters of the sensitivity ranking. Then, the three-parameter subset with a maximum RDE value is selected for calibration. The CCF is optimized and the RDE_C is calculated with the new optimized values for the three parameters. The whole procedure of parameter subset extension is repeated until the current RDE_C is lower than the RDE_C of the previous step. Note that the procedure adds only one parameter at each step. At this point, the subset of the previous step, which has the maximum RDE_C value among all the optimized subsets along the iterations, is taken as the final subset produced by the seed that is being investigated. Then, the subset of the next seed is generated (second parameter of the sensitivity ranking). This procedure is repeated until each one of the 20 seeds has been investigated.

During the calibration step, if the tested subset has any optimized value out of the physical range defined in the model (e.g. negative values of any parameter or yield parameters higher than 1.00) the subset is considered not identifiable and discarded. Then, the next extended subset with a higher RDE index is chosen for calibration instead of the subset that generated inappropriate optimized values. It is important to highlight that the initial guess of the optimization of pairs for each seed is the default model value of each parameter. Optimizations with three or more parameters have their initial guesses obtained from the values of optimized parameters in the previous iteration and the default value of the new parameter. Next step is to choose the best subset among all produced subsets by all seeds. The RDE criterion is also used for this purpose, as it indicates how much a subset is able to explain the experimental process behaviour producing lower estimation parameter errors. Therefore, the subset with the higher RDE can be considered the best subset.

Finally, potential bias problem is studied to evaluate the influence of parameters that do not belong to the calibration subset over the optimized values of the own calibration parameters (Brun *et al.*, 2002; de Pauw, 2005). To perform a simple study, three parameters that could not enter the selected subset during its construction but presented high values of RDE are chosen. These parameters are modified around their default values, the subset is re-calibrated and the parameter confidence intervals are calculated.

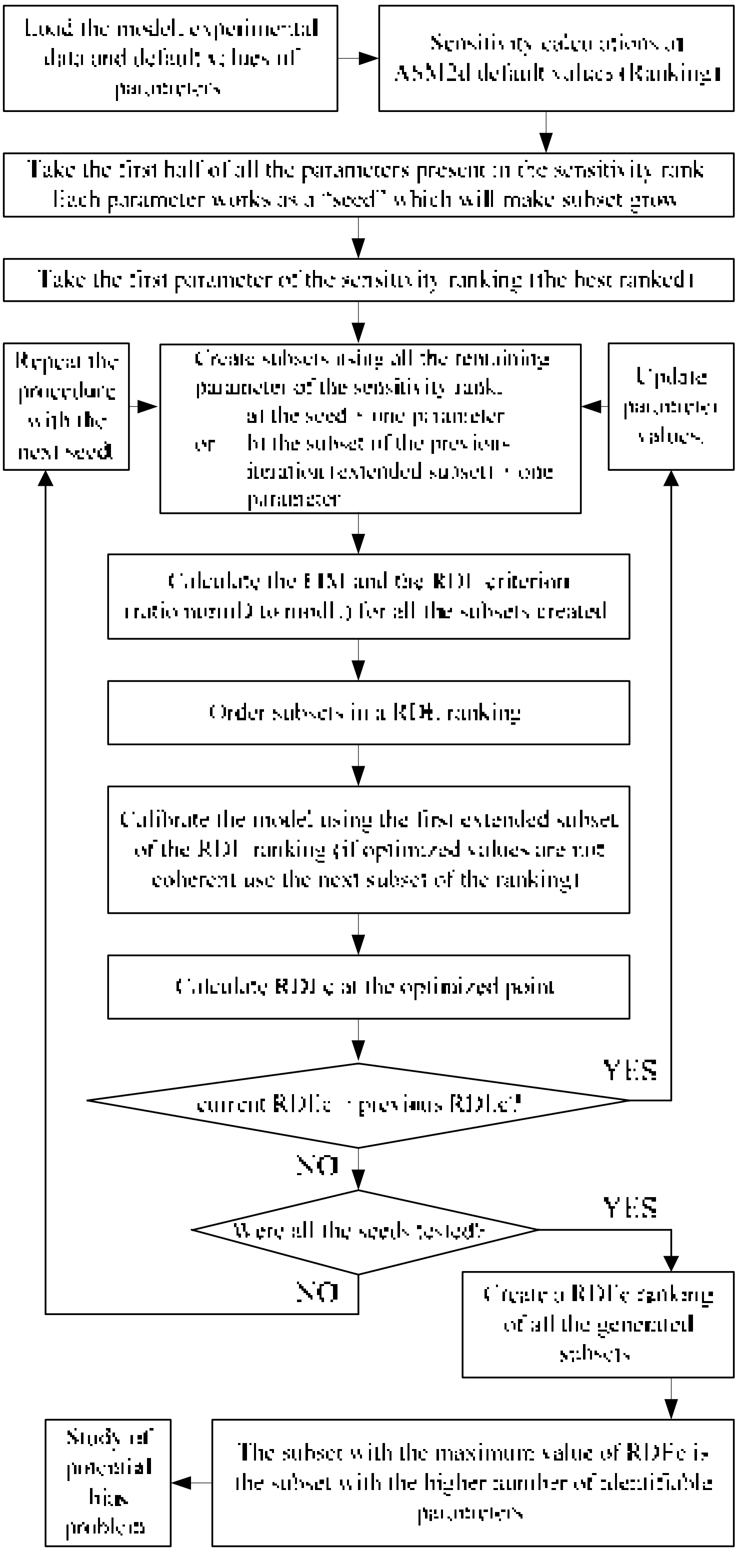


Figure 3.2: Flowchart of the model calibration and validation of the proposed retrofitting methodology.

3.3 Legal, economical and physical constraints

Retrofitting methodology should overcome physical and process control constraints, respecting effluent discharge limits and budget restrictions (for implementing new process, build new basins, etc). The main physical and process control constraints in WWTP operation are: oxygen distribution constraint, poor denitrifying rates, excess of biomass, insufficient instrumentation for automated process control, insufficient reactor volume and poor mixing of the WW in anoxic basins. Considering these restrictions, it is important to determine how much the existent plant is limited by each one of these factors (legal limits, physical constraints, process control constraints and economical constraints). It is important to remember that a part of the WWTP budget should be invested in integrity inspections (and maintenance) of pipes, vases, pumps, valves, blowers, etc, but all these kind of limitations will not be treated by the proposed methodology.

In order to determine the degree of plant limitation, performance tests are proposed for the current plant, since the plant model was calibrated and validated and there are extra experiments that could be carried out in any simulation environment. An example of these tests is the simulation of the plant model with an influent with strong peaks of ammonium and phosphate concentrations to verify how much the current plant is able to refuse external disturbances and how long the effluent will be unspecified according to the discharge legislation (Sintic *et al.*, 1998).

3.3.1. Legal restrictions

All the WWTP should be designed and managed to produce an effluent with a quality equal or superior than the current discharge limits (EC Directive of 1991), as previously cited in the introduction section (Sintic *et al.*, 1998). Plant data (lab data) are obtained in order to monitor the effluent quality (COD, BOD_5, total N, total P, ammonium, nitrate, total suspended solids). Comparing plant data and legal limits, it is possible to infer which is the main problem of the plant: lack of anoxic volume or lack of biodegradable organic matter (when nitrate at the end of the anoxic zone is observed), lower internal recycling rates (when the nitrate concentration in the anoxic zone is low and high nitrate concentration is observed in the effluent stream), lack of aerobic volume or mixing problems (high concentrations of ammonium in the effluent), lack of chemical agent for P precipitation and so on.

3.3.2. Economical evaluation

Investment costs and operating costs are fundamental issues for a retrofitting process. Some literature researches indicated the most relevant operating costs: aeration costs, pumping costs, costs of chemical additions, sludge production costs and effluent costs (in some countries, WWTP manager is rewarded with bonuses for delivering an effluent with a higher quality than the specified by the law) (Copp *et al.*, 2002; Stare *et al.*, 2007). The daily operating cost of the secondary treatment of a WWTP can be depicted by the equation 3.1. It does not include the cost of addition of an external carbon source(s).

$$OC\left[€\ d^{-1}\right]=\gamma_E\left(AE+PE\right)+\gamma_{SP}SP+EF \qquad \text{Eq. 3.1}$$

where *AE* and *PE* are aeration energy and pumping energy [kWh d^{-1}] respectively, *SP* is the sludge production [kg d^{-1}] and *EF* are effluent fines [€ d^{-1}]. The conversion factors γ_E and γ_{SP}, are 0.1 € kWh^{-1} and 0.5 € d^{-1} (Stare *et al.*, 2007). Aeration energy is calculated by equation 3.2, for *r* aerobic reactors (Copp *et al.*, 2002).

$$AE\left[kWh\ d^{-1}\right]=24\left[\sum_{i=1}^{r}0.0007\left(k_La_i\right)^2+0.3267\,k_La_i\right] \qquad \text{Eq. 3.2}$$

where k_La_i is the oxygen transfer rate [d^{-1}] of each aerobic reactor. Nevertheless, k_La values are not available in most of the cases, and then the daily aeration energy is easily obtained multiplying the power of each blower by the operation time during the day, as states Eq. 3.2a.

$$AE\left[kWh\ d^{-1}\right]=\sum_{i=1}^{r}P_i\left(kW\right)\cdot t_{oper,i}\left(h\,d^{-1}\right) \qquad \text{Eq. 3.2a}$$

By its turn, pumping energy is calculated by equation 3.3, where P_F is a pump factor to convert flow rate in energy, with suggested value 0.04 kWh m^{-3} (Copp *et al.*, 2002).

$$PE\,[kWh\ d^{-1}] = P_F\,(Q_{RINT} + Q_{RAS} + Q_W) \qquad \text{Eq. 3.3}$$

Unknowing P_F, it is possible to use the equation 3.3a, where it is needed to know the daily time of operation of each pump, similar to the equation 3.2a for computing the aeration energy.

$$PE\left[kWh\ d^{-1}\right] = \sum_{i=1}^{r} P_i(kW) \cdot t_{oper,i}\left(h\, d^{-1}\right) \qquad \text{Eq. 3.3a}$$

Nominal power of blowers and pumps can be found in the equipment datasheets or at the sites of manufacturers.

Instantaneous sludge production is calculated by the relationship written in equation 3.4,

$$SP\,[kg\ d^{-1}] = X_{TSS}^{Q_W} \cdot Q_W \qquad \text{Eq. 3.4}$$

As the solids content in the purge flow is not on-line measured, an estimative could be made based on the solids balance around the settler. Supposing that solids concentration in the effluent flow stream is equal to zero and the biomass hold up in the settler is approximately constant, the following relationship can be written:

$$X_{TSS}^{Q_W}[g\,TSS\,m^{-3}] = \left(\frac{Q_{IN} + Q_{RAS}}{Q_W + Q_{RAS}}\right) X_{TSS}LR \qquad \text{Eq. 3.5}$$

where $X_{TSS}LR$ is the solids concentration in the stream that comes from the reactors to the settler. So, using equation 3.5 and 3.4, it is possible to estimate the sludge production and multiplying by the γ_{SP} (to convert kg into monetary units), the costs of the produced sludge.

Finally, effluent fines are calculated by equation 3.6 (Stare *et al.*, 2007). Equation 3.6 was calculated for ammonium, total nitrogen (TN) and phosphate.

$$EF\,[€\,d^{-1}] = \sum_{j=NH_4,TN,PO_4} Q_{EFF}\,\Delta\alpha_j\,C_j^{EFF} + \left(Q_{EFF}\left[\beta_{0,j} + \left(C_j^{EFF} - C_{L,j}\right)\left(\Delta\beta_j - \Delta\alpha_j\right)\right]\right)\left(Heaviside\left(C_j^{EFF} - C_{L,j}\right)\right) \qquad \text{Eq. 3.6}$$

where:

- $\Delta\alpha_j$ is the slope of the curve *EF* versus effluent concentration when the latter variable was lower than or equal to the effluent discharge limit;

- $\Delta\beta_j$ is the slope of the same curve when the effluent concentration is higher than the effluent discharge limit;

- $\beta_{0,j}$ is the increment of fines when the effluent concentration is higher than the effluent discharge limit;

- C_j^{EFF} is the effluent concentration of the pollutant "*j*";

- $C_{L,j}$ is the discharge limit of the pollutant "*j*".

The *Heaviside* function is defined, in this work, being equal to the unit (equal to one) when C_j^{EFF} is greater than $C_{L,j}$. Otherwise, its value is equal to zero. The values of all parameters involved in the *EF* calculation are given in Table 3.1.

Table 3.1: Parameters to evaluate the effluent fines.

Effluent variable	$\Delta\alpha_j$[€ kg^{-1}]	$\Delta\beta_j$[€ kg^{-1}]	$\beta_{0,j}$[€ m^{-3}]	$C_{L,j}$[kg m^{-3}]
Ammonium	4.00	12.00	2.70 10^{-3}	4.00 10^{-3}
Total nitrogen	2.70	8.10	1.40 10^{-3}	1.80 10^{-2}
Phosphate	4.00	12.00	2.70 10^{-3}	1.50 10^{-3}

It is worth noticing that ammonium, nitrate and phosphate effluent concentrations are estimated by a model or using lab data. The parameter values for *EF* calculation concerning ammonium and TN were obtained from literature (Stare *et al.*, 2007). Phosphate parameters for effluent fines calculations were assumed, in the present work, to be the same to the ammonium parameters but with different effluent discharge limit. Such limits used in the present work were the same found in the work of Gernaey and Jørgensen (2004). Figure 3.3 shows the three effluent fine curves (ammonium, total nitrogen and phosphate).

The most part of the investment cost in retrofitting process of A/O to A^2/O plant is basically represented by the construction of an anaerobic tank upstream the conventional A/O process. Hence, land, concrete, steel, earth moving services, modifications in the biomass recycle line and the exit line of the primary settler should be provided to perform this task. The cost of these materials and services are summarized in Table 3.2 (US-EPA, 2000).

Table 3.2: Investment cost associated to the retrofitting process from an A/O plant to an A^2/O plant.

Item	Costs
Earth moving services	50.00 €/m^3
Piping (material)	~15.00 €/m
Piping (services)	~15.00 €/m
Concrete	~300.00 €/m^3
Civil project and documentation	~15000.00 €

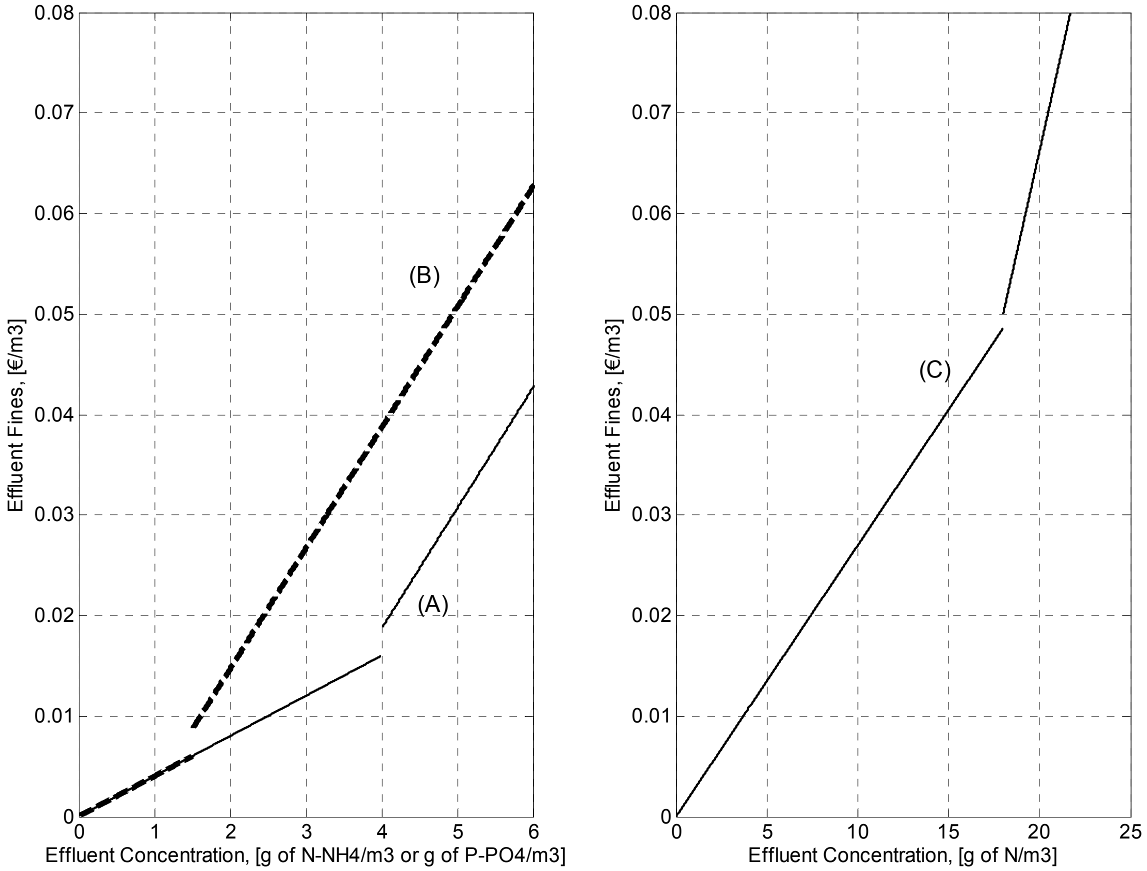


Figure 3.3: Effluent fines for each cubic meter discharged depending on the effluent concentration of ammonium, total nitrogen and phosphate. (A) Ammonium. (B) Phosphate. (C) Total nitrogen.

One alternative not to build new basins is to use part of the anoxic volume as anaerobic volume, just modifying the point where the internal recycle (nitrate recycle) is connected to the process. In this case, only earth moving services and piping services would be necessary. Investment costs and operating costs are variables that are taken into account in order to choose the best alternative for the solutions pointed out by the proposed retrofitting methodology.

3.3.3. Physical limitations

Physical limitations are straight forwarded linked to wrong design premises which, in most cases, did not take into account the population growth rate or used an incorrect prediction. As a result, an important set of physical constraints to the WWTP performance, not only in the effluent quality but in higher operating costs, is commonly realized by the plant managers and technical staff during the operation of some existent WWTPs, as follows:

-“Bottleneck” in the air supply system (few blowers, an inefficient/short air distribution system, etc);

-Systematic increase of the nutrient load (ammonium and phosphate);

-Need for more carbon source for denitrification processes;

-Low capacity of the pumping system (internal recycles and biomass recycles in the case of A/O WWTP);

-Few area for revamping the plant (to increase the useful volume of the tanks). Other public/private building and facilities have taken the neighbours areas, not allowing future expansions of the current WWTP.

-Need for expanding electrical energy network (more transformers, cables, lines, speed control drivers) to append more fluid motion / mixing equipments.

-Need for building more settlers or to install the cleaning system of membranes (fixed biomass).

3.4 Proposal and evaluation of new plant configurations

Once developed a process model of the current facility and identified the physical, economical, legal and process control limitations, a set of alternatives for improving the benefits of the WWTP should be posed. In case of an A/O configuration, the classical alternative to improve plant performance is to add an anaerobic step previously to the anoxic one. The following advantages are expected with this modification:

- Decreasing or even eliminating the amount of chemical agent for phosphorus precipitation (reduction of the operating cost).

- Improving sludge settleability, since fermentation processes that occur in the anaerobic zone increase the concentration of readily biodegradable organic matter which allow to floc-forming bacteria growing up faster than filamentous bacteria, being the later responsible of bulking sludge problems.

- Improving the nitrogen removal, specifically the denitrification process, since the anaerobic zone could produce more readily biodegradable matter (fermentation products) when complex COD is available, reducing the necessity of external carbon sources.

Two ways are idealized to add an anaerobic volume to an existent A/O WWTP and at the same time keeping the process in a continuous operation:

- Decreasing the existent anoxic volume, changing the connection of the internal recycle.

- Building a new basin with suitable changes in the connections of the external recycle.

In case of decreasing the existent anoxic volume, the addition of external organic matter should be evaluated in order to keep the denitrification rate, if the simulation step (current model) indicated lack of anoxic volume or carbon source. Moreover, the addition of external organic matter could occur in different points of the anoxic zone. Also, the outlet stream of the primary clarifier (influent of the secondary treatment) should be connected to distinct zones of the plant (step feed), being it another manipulated variable to be evaluated during the conversion of the A/O WWTP to A^2/O configuration. Another point to be checked out is the control structure, from the most elemental control scheme for DO control (different alternatives) and the way process controllers will refuse external disturbances (implementation of feedfoward action for cancelling the effect of influent NH_4^+ peaks, for instance).

All the proposed alternatives should be evaluated using the following criteria:

a) Investment costs

b) Operating costs

c) Plant controllability

Investment and operating costs are easily identified in all the tasks involved in the implementation of the proposed alternatives. Nevertheless, the controllability involves the knowledge of the external disturbances frequency or the fines established for the out of range effluent quality and it depends on the capacity of the control structure.

One way to determine the plant controllability in terms of costs is to measure the period of time that plant effluent are not in accordance to the legal discharge limits, the same manner already posed in the literature (Copp, 2002).

For testing all these possibilities and to calculate all the appropriate costs, process model of the new plant layout, one for each scenario, should be also developed. Note that the kinetic parameters of the model will be taken from the calibration step with the A/O experimental data.

It should be let clear that one of the design premises of the whole methodology is not to change abruptly all the current plant configuration, process technology (suspend growth to attached growth biomasses for instance), nor increasing costs, nor interfere in the current operation of the plant, since the existent plant should be working simultaneously to the changes. Besides, the operators should be trained in the new way of operating and this is another reason why extreme changes at the same time are not welcome. The main idea is to make use of all the existent plant to save the labour expend to build the plant as it already is. Other premise of the proposed retrofitting methodology is to keep working all the process, without possibility of accumulating incoming wastewater. With these premises, the WWTP becomes easy to be operated during the implementation of the proposed (and approved by the WWTP manager) configuration, avoiding sequential and mechanical daily operations prone to error.

3.5 Process control issues

Basically, WWTP have regulatory type controllers since no change in setpoints of its variables is usually performed and there are some legal limits that pollutant concentrations must not reach. This situation is exactly the opposite of a petrochemical plant which, depending on the clients' necessities, all the process variables setpoints are adjusted for a new production campaign. Hence, the most important characteristic of WWTP process controllers is to refuse external disturbances, like changes in the influent flowrate or composition, as an abrupt increasing of ammonium in the influent or a problem with the air diffusers in the aerobic basins (abrupt decreasing in the DO concentration). To develop this characteristic in the WWTP process control system, it is necessary to know the relationship amongst input and output variables (like the DO setpoint and the ammonium concentration in the effluent, for instance). Such a knowledge is bring back by a process control model (composed by black-box sub-models for instance, Ljung, 1999 and Machado 2007) that could be derived from the available data (section 3.1) or by the linearization of the full model (phenomenological model) developed and calibrated as described in section 3.1 and 3.2.

All input-output models should be grouped into a transfer function matrix and the best input-output pairing should be studied. Also, the transfer function matrix is useful for fast tuning and testing the process in events when hard control actions should be taken, such as raining events or peaks of pollutants (ammonium in the influent). The transfer function matrix is also important for performing performance tests in the process controllers, submitting the process models to external disturbances and checking how long the process will be out of the normal operating point. Such experiments help to better tune process controllers to deal with undesirable external disturbances and to keep strategic variables for the wastewater treatment processes under interesting levels.

It is worth noticing that the way the plant variables are organized and the position to install sensors (or sample points) is a very important issue in the process control design of WWTP and during its retrofitting process for improving plant capacities. For example, is it better to control the ammonium concentration in the effluent using the speed of the air blower or using the DO setpoint (cascade control)? Or, is it better to control nitrate in the effluent or in the middle of the treatment (at the end of the anoxic zone)? These questions will be answered by the control structure design, starting from the analysis of the existent control structure for improving performance and evaluating the system controllability of the new proposed plant configuration.

3.5.1. Analysing the current control structure

The plant model obtained in previous steps should also be used for determining control limitations of the current WWTP. An exhaustive batch of tests should be performed with simulations using the current process controllers, from the lowest control level (inventory control loops) until the most refined control loop in higher levels (cost control or pollutant control using other cascaded variables). The observed deviation from the simulation outputs and the legal limits determined in the EC Directive of 1991 should be measured to establish a starting point (reference basis) to compare each control solution developed by the retrofitting methodology.

The inventory control loops should be developing their primal task: to guarantee that wastewater treatment processes at least work, even if they work in a sub-optimal operating point. In WWTP, (excepting SBR and attached biomass plants) there are generally two continuous inventory control loops: the suspended solids concentration loop, controlled by the purge flow rate (to purge the excess of biomass) and the DO control, basic loop for eliminating COD and for keeping a proper nitrification rate. The latter loop is usually composed by a bundle of air blowers, air flowmeters, pressure sensors, control valves and an air distribution system with diffusers.

Once inventory control loops are checked and tuned, the control of strategic variables (higher level process variables) for improving the performance of the whole WWTP in reducing the pollutant concentrations in the effluent should be studied. Usually, ammonium, nitrate and phosphate are controlled in the effluent, using, respectively, air flowrates, internal recycle flowrates and external recycle flowrates as manipulated variables. The best point to control the pollutants not always is in the effluent, considering the capacity of refusing plant disturbances (Machado *et al*., 2009b). Also, it is recommended to use cascade controllers for controlling ammonium, using a slave controller of DO (Suescun *et al*., 2001).

It is important to pay attention to the current process controller settings and the current type of the controllers of the higher level process variables. The way such variables are interconnected inside the control structure, improvements on the pollutant capacity and external refusing disturbances could be obtained (Ingildsen *et al*., 2002; Ekman *et al*., 2006; Machado *et al*., 2009b). The most practical, cheap and useful controllers are the linear feedback controllers, like PI and PID controllers. Other alternatives were presented for controlling WWTPs in literature like the fuzzy logic and model predictive controllers which could be applied during the retrofitting process (Steffens and Lant, 1999; Rosen and Yuan, 2001).

3.5.2. Control structure design for a new plant configuration

The proposed retrofitting methodology takes into account the necessity to implement an automatic control system for the new plant configuration. In literature, it is proved that implementing SRT and DO feedback control is an action for reducing operating costs, since the process will work in the same conditions and will be capable to answer to external disturbances, in comparison to plants without any automatic control system (Brouwer *et al*., 1998; Galuzzo *et al*., 2001; Ekman *et al*., 2006; Vrecko *et al*., 2006). It is known that to implement an automatic control system is an investment (expensive but less expensive since the end of the 90's (Olsson, 2006)). Although the benefits of the automation program of WWTPs are visible when the operating costs (energy) decrease and the quality of the effluent is monotonically higher, instrumentation for on-line nutrient measurements are not still present in some WWTP. This lack of proper on-line instrumentation makes difficult the execution of control actions for keeping the effluent quality and to refuse undesired plant disturbances (Olsson, 2006).

In the proposed retrofitting methodology, it is necessary to quantify how much the WWTP modifications will affect the existent process controllers. The developed phenomenological model cited in sections 3.1 and 3.2 and the transfer function matrix for control purposes, should be updated with the new part of the process. In case of WWTP that only perform COD removal and nitrification of ammonium, it is important to understand how the nitrate controller will affect the COD elimination process in an eventual plant upgrade to a predenitrifier configuration (upgrading a COD WWTP to an A/O WWTP). The same analysis should be performed for determining how much the phosphate processes will affect the N and COD removal processes (upgrading an A/O WWTP to an A^2/O WWTP for instance).

A useful way to perform these quantifications is to obtain the Relative Gain Array (RGA), proposed by Bristol (1966). Although RGA is not a recent tool, its information for control structure design is extremely powerful, as registered in recent scientific works (Machado *et al.*, 2009; Araújo *et al.*, 2011). If availability of the WWTP model in an operating point is supposed, the first step for designing control structures is pairing correctly the manipulated variables with the controlled variables (Skogestad, 2004). A correct pairing means to use the manipulated variable which presents the major influence over a controlled variable, avoiding interactions with other output variables. This task is performed by the RGA. By definition, the relative gain λ_{ij} between the jth manipulated variable and the ith controlled variable is $\lambda_{ij} = K_{ij}/K_{ij}^{C}$, where K_{ij} is the open loop gain between the jth manipulated variable and the ith controlled variable. The K_{ij}^{C} is the closed-loop gain between the jth manipulated variable and the ith controlled variable. In practice, both gains can be determined performing variations in the jth manipulated variable and observing the effect in the ith controlled variable. The main difference between both situations is the presence of the controller, which could affect the value of the ith controlled variable under a variation in the jth manipulated. Such difference is due to the interactions amongst the different control loops. However, if the steady-state gain matrix $K(0)$ is available, the static RGA could be calculated, in an easier manner, by:

$$RGA(0) = K(0) \cdot \left(K(0)^{-1}\right)^{T} \qquad \text{Eq. 3.7}$$

Therefore, the RGA represents the influence of the other control loops in a certain output. If the value of an λ_{ij} is close to one and the other λ_{ij} of the same row are close to zero, this means the output "*i*" in the pair "*ij*" is not affected by the other control loops. Then, ideally it is important that the variables involved in the control structure present a RGA diagonally dominant, in order to design a control structure with low-order and decentralized controllers, such as PI or PID controllers.

Calculating that the WWTP during the retrofitting process will have the number of its controlled and manipulated variables increased and new processes will be incorporated into the system (EBPR), the existent process controllers must be retuned and the RGA information will give the right extend how deep will be the changes in the parameter values.

To complement the RGA calculations, the minimized condition number (Boyd *et al.*, 1994) could be computed. Such a tool is defined by:

$$\gamma^{*}(G(\omega)) = \min_{L,R} \gamma(LG(\omega)R) \qquad \text{Eq. 3.8}$$

where L and R are scaling matrices, $G(\omega)$ is the frequency response of the system and γ is the condition number, defined by:

$$\gamma(G(\omega)) = \frac{\overline{\sigma}(G(\omega))}{\underline{\sigma}(G(\omega))} \qquad \text{Eq. 3.9}$$

The variables $\overline{\sigma}(G(\omega))$ and $\underline{\sigma}(G(\omega))$ are the maximum and the minimum singular values of the system, at the frequency ω (Skogestad *et al.*, 1998). Since the singular values of $G(\omega)$ are the eigenvalues of the product $G(\omega)(G^{H}(\omega))$, where $G^{H}(\omega)$ is the complex-conjugate transpose matrix of $G(\omega)$, equation 3.9 can be expressed as:

$$\gamma(G(\omega)) = \left(\frac{\lambda_{MAX}\left(G(\omega)\cdot G^{H}(\omega)\right)}{\lambda_{MIN}\left(G(\omega)\cdot G^{H}(\omega)\right)} \right)^{1/2} \qquad \text{Eq. 3.10}$$

where λ_{MAX} and λ_{MIN} are, respectively, the largest and the smallest eigenvalue of $G(\omega)(G^{H}(\omega))$.

As the condition number depends on the system units, it is more convenient to calculate the minimized condition number, determining the best L and R matrices to meet the minimum value of γ. Matrices L and R can be viewed as matrices of conversion factors amongst all the control variables units. There are L and R matrices that minimize the condition number for each frequency. The calculation of L and R starts from building the following LMI (linear matrix inequality):

$$\mu I \leq \left(LG(\omega)R\right)\cdot(LG(\omega)R)^{T} \leq \gamma^{2} I \qquad \text{Eq. 3.11}$$

where *I* is the identity matrix and the symbol "*T*" stands for transpose. Such LMI is the same as:

$$\left(RR^T\right)^{-1} \leq G^H(\omega)(L^T L)G(\omega) \leq \gamma^2 \left(RR^T\right)^{-1} \qquad \text{Eq. 3.12}$$

This is equivalent to the existence of diagonal P and Q with $P > 0$ and $Q > 0$ (P and Q are positive definite matrices) that the following LMI can be written:

$$Q \leq G^H(\omega) P G(\omega) \leq \gamma^2 Q \qquad \text{Eq. 3.13}$$

It is possible to see that $L = P^{1/2}$ and $R = Q^{-1/2}$. Hence, matrices P and Q, can be determined if the following optimization problem is solved for each frequency ω:

Minimize γ^2 Eq. 3.14
subject to P and Q, with $P > 0$ and $Q > 0$
and subject to $Q \leq G^H(\omega) P G(\omega) \leq \gamma^2 Q$

The optimization problem abovementioned is a type of "*Generalized Eigenvalue Problem*", and can be solved through interior point methods (Boyd *et al.*, 1994). In MATLAB®, one implementation of these algorithms is available in the file *gevp.m*.

The minimized condition number gives an idea on how difficult is to invert the process model, since it is based on the condition number of ordinary matrices. If γ^* is higher than the unit, then the system is considered to be ill-conditioned because two or more rows or lines of the gain matrix are quite similar, indicating dynamic or steady-state coupling. As many techniques for designing controllers are based on model inversion, the minimized condition number is an essential measure, together with the RGA, for controllability analysis of a system. So, both indexes are employed to determine, in many cases, suitable decentralized control structures.

3.5.2.1 Centralized Control Structure

Differently from the PI and PID controllers, which commonly belongs to a decentralized control structure, each one taking care of its own controlled variable with movements in its own manipulated variables, which could bring undesired consequences like internal conflicts since manipulated variables affect more than one output variable, centralized control structures watch all the relationships amongst input and output variables, including naturally the effect of measured disturbances on the controlled variables (influent flowrate on the ammonium effluent, for instance) (Maciejowski, 2002; Stare, 2006).

Conversely, if a more complex type of controllers is desired, one possible alterative is a Model Predictive Controllers, where all the interrelationships amongst all the manipulated and controlled variables are used in the calculation of the control actions (centralized controller) (Maciejowski, 2002). The Predictive Controller minimizes the objective function *F* (equations 3.15 and 3.16) to find the optimum control movements (deltas) in a control horizon *m*. Such controller uses an internal model (model for process control, like state space model or a transfer function model) to predict the future behaviour of the outputs (*y*, controlled variable) starting from the measured variable *y*|*k* (*k* is the current sampling time). The simulation runs until the prediction horizon *p*. After a step of calculation, only the first movement is physically applied and the optimization problem runs again at the new *k* instant.

$$\min_{\Delta u(k\mid k),\ldots\Delta u(m-1+k\mid k)} F \qquad \text{Eq. 3.15}$$

$$F=\sum_{i=0}^{p-1}\left(\sum_{j=1}^{n_y}\left|\omega_{i+1,j}^{y}\left(y_j(k+i+1\mid k)-r_j(k+i+1)\right)\right|^2+\sum_{j=1}^{n_u}\left|\omega_{i,j}^{\Delta u}\cdot\Delta u_j(k+i\mid k)\right|^2+\sum_{j=1}^{n_u}\left|\omega_{i,j}^{u}\left(u_j(k+i\mid k)-u_{jTARGET}(k+i)\right)\right|^2\right) \qquad \text{Eq. 3.16}$$

The variables in equations 3.14 and 3.15 are explained as follows:

Δu(k|k), …, *Δu(m-1+k|k)*	Such variables are the control actions to be taken by the controller, in the current sampling time *k* to the *m*-1 sampling time, which is the last period before the end of the control horizon. In the optimization problem formulation, such variables are the decision variables

p	Prediction horizon (in multiple of sampling times)
m	Control horizon (in multiple of sampling times)
y_i	Control variable "*i*"
u_j	Manipulated variable "*j*"
r_j	Reference signal to the control variable "*j*" (setpoint or a specified trajectory)
ω_i^y	Weight of the error (difference between the control variable and its setpoint or reference signal) of the control variable "*i*"
$\omega_j^{\Delta u}$	Penalty factor in the rate of variation of the manipulated variable "*j*".
$\omega_{i,j}^u$	Penalty factor in the usage of the manipulated variable "*j*".
$u_{jTARGET}$	Nominal value of the manipulated variable "*j*", when the controller does not use it to control the plant.
n_y	Number of controlled variables.
n_u	Number of manipulated variables.

The first term of equation 3.16, $\sum_{j=1}^{n_y} \left| \omega_{i+1,j}^{y} \left(y_j(k+i+1|k) - r_j(k+i+1) \right) \right|^2$, is related to the weight that each error in controlled variables contributes to the value of *F*. The second term $\sum_{j=1}^{n_u} \left| \omega_{i,j}^{\Delta u} \cdot \Delta u_j(k+i|k) \right|^2$ adds to F a set of penalties caused by abrupt movements in the manipulated variables. And finally, the third term $\sum_{j=1}^{n_u} \left| \omega_{i,j}^{u} \left(u_j(k+i|k) - u_{jTARGET}(k+i) \right) \right|^2$ can be seen as a penalty to *F* if there are manipulated variables that should not be changed far from their nominal value not to increase operation costs or to mitigate other operational risks (Maciejowski, 2002).

3.5.3. Robustness tests

The current process control structure should be tested to the operation limits, considering that the developed model also indicated possible limitations in the wastewater treatment. Since the current plant is passing through a retrofitting analysis, its control system should be tested to predict its modifications and include them in the revamp budget. The tests include:

- To saturate manipulated variables to its lower and upper bounds and watch out what will be the behaviour in all the basins of the biological treatment (Ex: to maximize the DO until the maximum capacity of the blowers or to maximize the internal or external recycle flowrates to observe the impact of these extreme conditions in the WWTP performance);

- Increase the concentration of ammonium and phosphate in the WWTP influent. This stressing condition will test how fast the process controllers will refuse external disturbances.

Naturally, the tests cited before should be performed with the developed model in the previous steps not to affect the operation of the full-scale WWTP (to avoid bills in case of fails and producing unspecified effluent). Once the tests had been performed, probably, control system limitations will be identified and should be corrected in the new plant configuration. Note that these tests should be performed in the new configuration plant also, to really check that all the limitations (or a good part of them) were truly removed.

Chapter 4: Case Study – Redesign of the Manresa WWTP

The proposed methodology for WWTP redesign was applied to a full scale WWTP that removes COD and N of a wastewater produced by 130000 inhabitants (Manresa WWTP). A WWTP model was calibrated and then a feasible alternative for biologically removing phosphorus was developed using this model. Process control aspects were taken into account for optimising the amount of recycling flow rates as well as the effect of transforming anoxic volume into anaerobic one. DO, ammonium and nitrate controls were improved in order to maintain the quality specification of the plant product (plant effluent).

The model was calibrated using the seed methodology (Machado *et al.*, 2009), based on the sensitivity analysis and the FIM (Fisher Information Matrix) criteria.

The redesign methodology applied to the Manresa WWTP intends to reduce operating costs and to help the facility to continue to respect the legal limits of effluent discharges.

4.1 Brief description of the Manresa WWTP

The average flowrate of Manresa WWTP is around 25.000 m^3/d. This WWTP (Figure 4.1) is made of a pre-treatment (gross and grit removal), primary treatment with a clarifier, a secondary stage (biological removal) and a tertiary stage (chlorination). There are two main treatment lines in the secondary stage (Figure 4.2). Each line has three anoxic reactors (1460 m^3) and one aerobic reactor (3391 m^3). Each reactor has approximately 7 m of depth. After passing through the anoxic zone, the bulk liquid is mixed and is again divided to enter in the aerobic zone. Along the influent path inside the aerobic reactors, air is bubbled from the bottom of the tank, rising up until the tank level, allowing biological oxidation of the organic material and the oxidation of ammonium to nitrate. A system of holes helps to divide the air bubbles in smaller ones and provides mixing between the influent components, the microorganisms and the air. At the end of the secondary stage there is a settler to separate the biomass content from the treated effluent. The excess of sludge is anaerobically digested and sent to the composting plant in which fertilizing material will be produced. The effluent, after leaving the secondary settler, can be chlorinated and is disposed to the environment at the Cardener River. Settled biomass returns to the entrance of the anoxic reactor by an Archimedes screw. An internal recycle pipe connects the aerobic zone to the anoxic one in order to bring the nitrate to be denitrified in the anoxic zone.

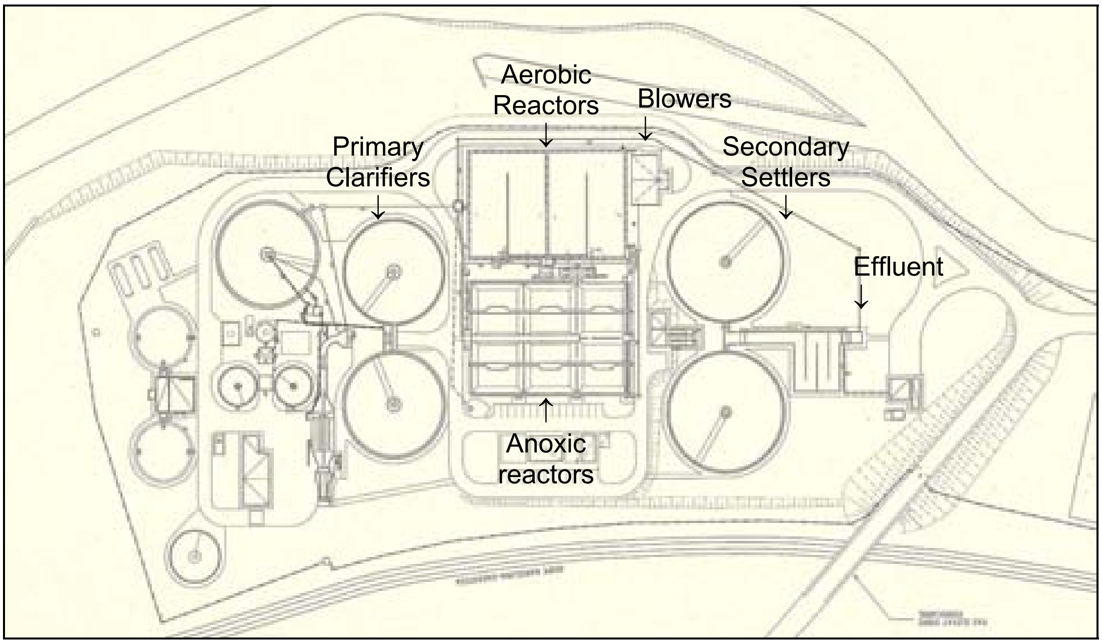


Figure 4.1: Scheme of the Manresa WWTP.

It is worth noticing that experimentally is observed preferential flux of the inlet mass stream to one of the main treatment lines. Also, a non-homogeneous spatial distribution of DO was observed along the aerobic reactors, not only along the influent path but also in depth. The presence of DO (0.5-1.0 mg/L) at the end of the anoxic reactors indicates that the denitrification is not occurring at the maximum intensity because it is possible that there is a lack of readily biodegradable matter to improve the nitrate reduction or a poor mixing is taking place.

Daily analyses of COD, BOD_5, TSS, NH_4^+, NO_3^-, PO_4^{3-}, Kjeldahl Nitrogen and Total Nitrogen at the effluent are performed. DO is continuously monitored by sensors installed in two points of each aerobic reactor. These analyses are performed also to the stream that leaves the primary clarifier (the entrance of the secondary treatment). The only system variable measured in each reactor of the secondary treatment is the total suspended solids concentration.

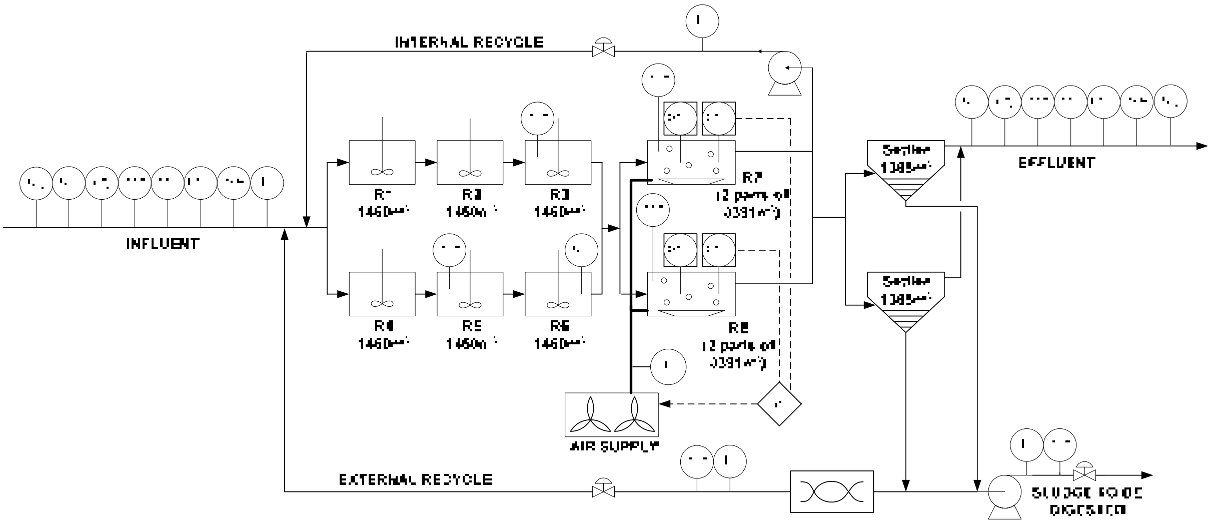


Figure 4.2: Monitored variables of the Manresa WWTP.

The air supply system is composed by 4 air blowers with 100,000 Nm^3/d of capacity, whose motor speed are controlled by a single DO feedback controller in the aerobic basins. The aerobic zone of each water line has two DO sensors, one of them placed at the 25% of the path along the zone and the other one placed at 75% of the aerobic zone. The DO PI controller uses a weighted average of the four DO concentrations as the measured variable, and compares it to a DO setpoint, usually equal to 2.0 mg/L. Once computed the error between the setpoint and the averaged DO, the new setpoint speed of the blowers is calculated by the PI algorithm and sent to the devices. Physically, the air is moved to a primary header after being discharged by the blowers. Then, the air flow rate is divided into two lines, called right and left branches. The right branch feeds the middle part of the two aerobic zones while the left branch feeds the entrance and the end of the two aerobic zones. Such configuration of the air supply system brings some difficulties to control the process, and will be discussed latter.

The main operation costs are electrical energy for aeration and pumping, sludge treatment (anaerobic digestion and composting) and chemical products for flocculation of the suspended solids.

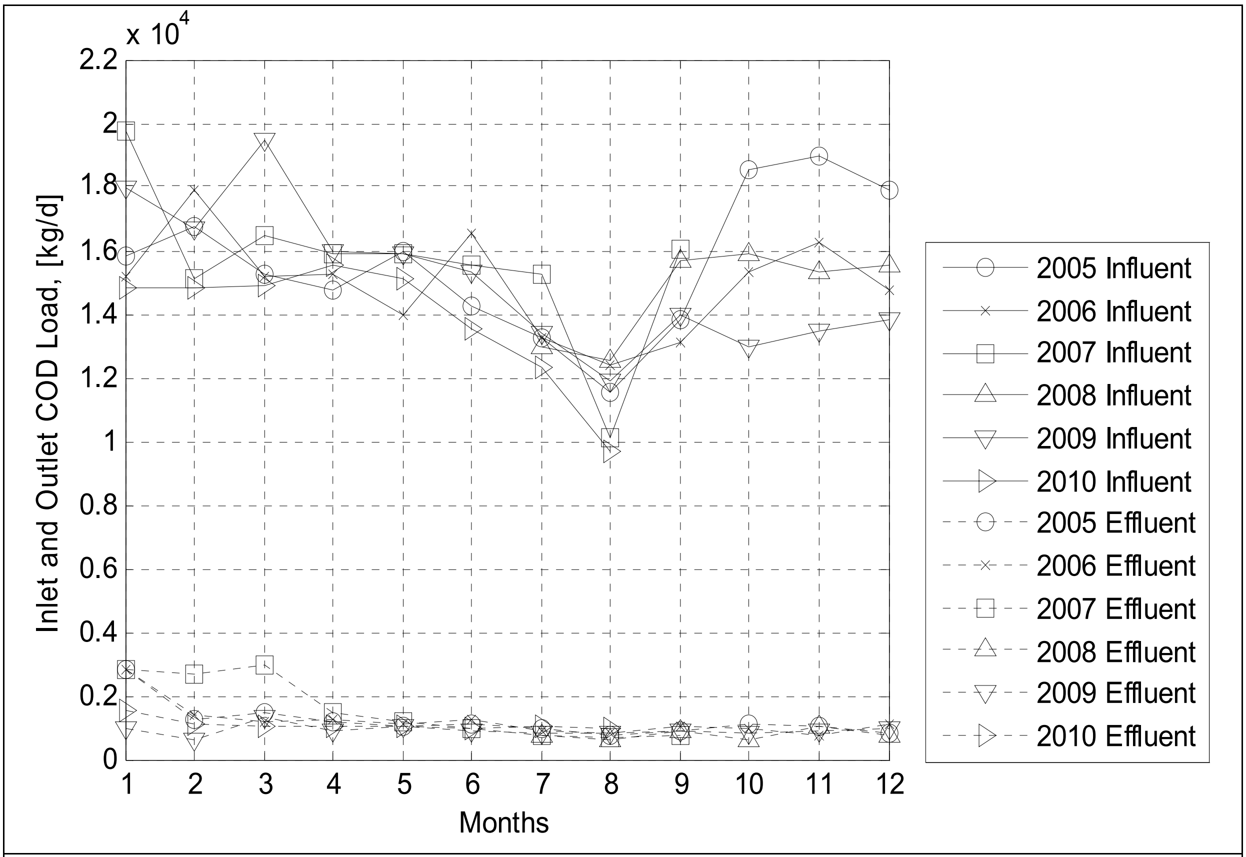
4.2 Influent composition and patterns

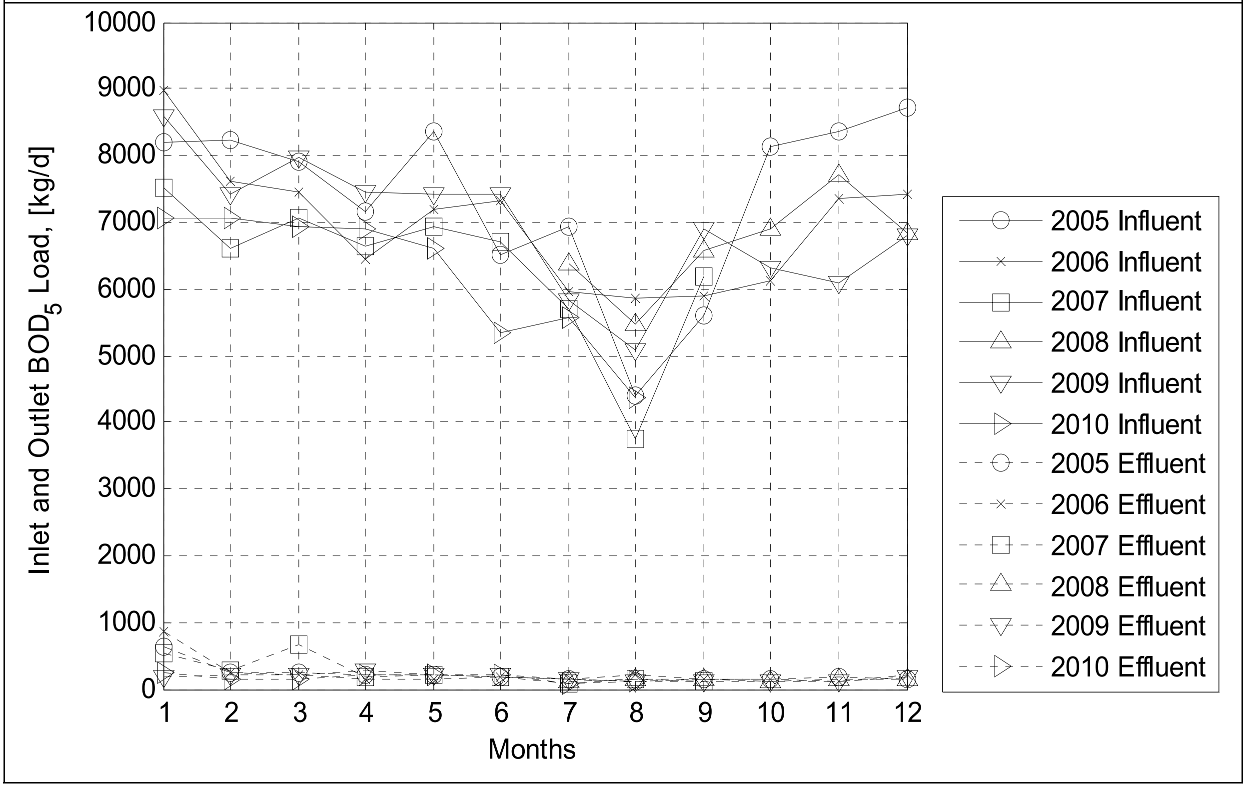
Influent composition, as commented in chapter 3, is key information for reactor designing. These data is required to obtain a correct estimation of the model parameters for the model-based test of different plant configurations and to choose the configuration that will improve effluent quality and will reduce operating costs. As occurs with many WWTP, influent composition changes along the year, not only because the temperature changes but also because people moves among towns. Table 4.1 shows influent properties (averages) straightforward linked to the wastewater composition in winter and summer months for the Manresa WWTP.

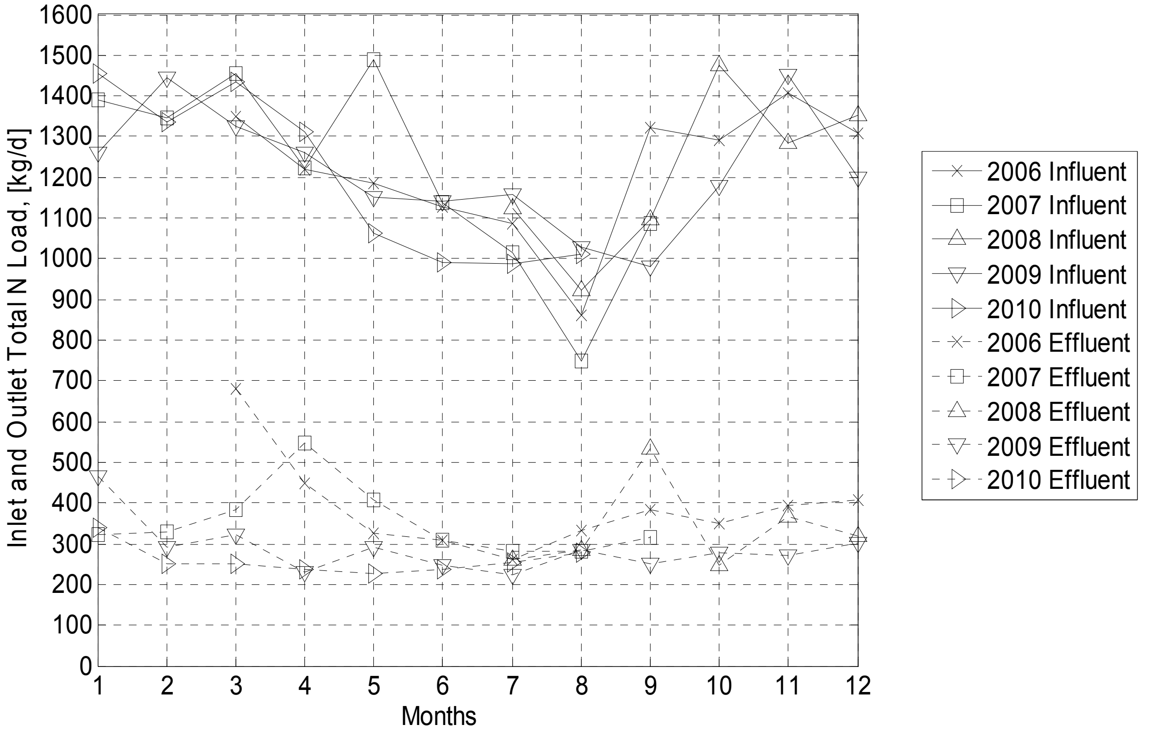
Table 4.1: Average influent composition.

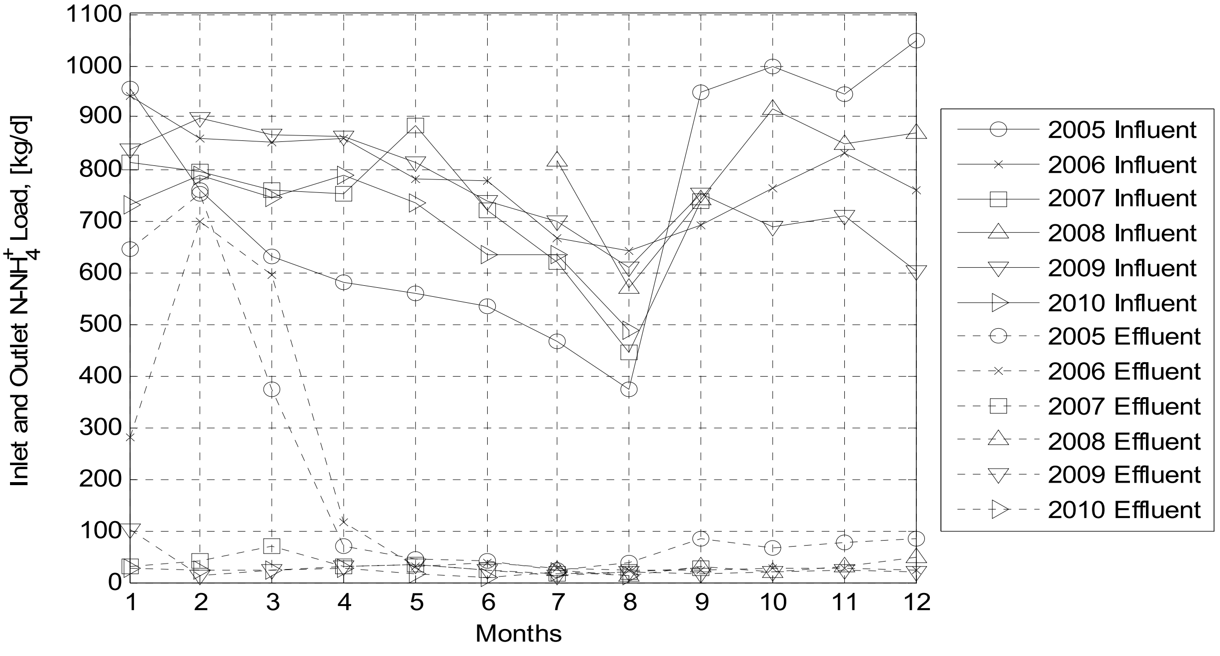
Property	Winter (Average Temperature = 13°C)	Summer (Average Temperature = 27°C)
pH	7.9	7.6
NH_4^+ [mg N/L]	33	20
BOD5 [mg/L]	290	170
COD [mg/L]	600	460
Total N [mg N/L]	53	33
NO_3^- [mg N/L]	3.5	2.0
Total P, [mg P/L]	8.0	5.5
NTK [mg N/L] (Kjeldahl nitrogen)	48	33
Zn [mg Zn/L]	0.8	0.5

Figure 4.3, shows average values of COD, BOD5, total nitrogen, ammonium and total phosphorus loads at the influent (wastewater that leaves the primary clarifier) and at the effluent along the months for the years of 2005 to 2010.






Inlet and Outlet Total N Load, [kg/d]
0
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1
2
3
4
5
6
7
8
9
10
11
12
Months
2006 Influent
2007 Influent
2008 Influent
2009 Influent
2010 Influent
2006 Effluent
2007 Effluent
2008 Effluent
2009 Effluent
2010 Effluent


Inlet and Outlet N-NH$_4^+$ Load, [kg/d]
0
100
200
300
400
500
600
700
800
900
1000
1100
1
2
3
4
5
6
7
8
9
10
11
12
Months
2005 Influent
2006 Influent
2007 Influent
2008 Influent
2009 Influent
2010 Influent
2005 Effluent
2006 Effluent
2007 Effluent
2008 Effluent
2009 Effluent
2010 Effluent

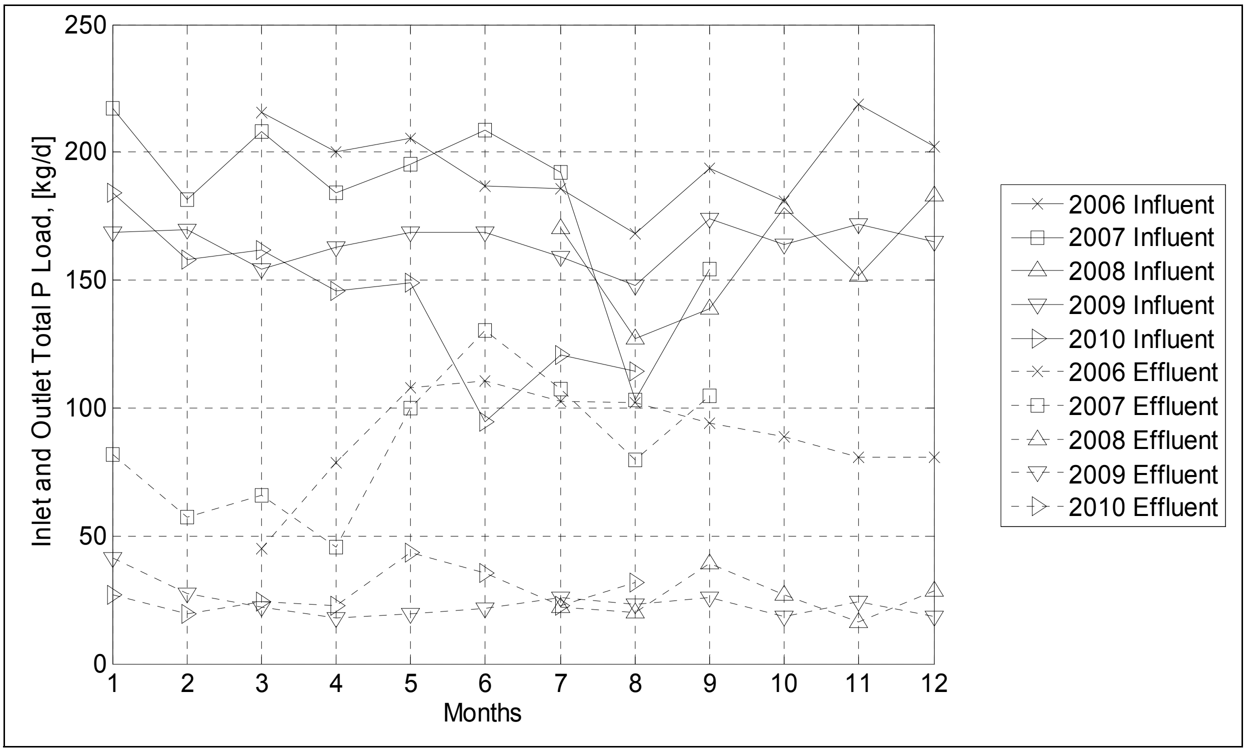


Figure 4.3: Average values of COD, BOD5, Total N, NH_4^+ and Total P loads along the months of 2005, 2006 and 2007, 2008, 2009 and 2010.

Considering the effluent limits of COD (125 mg O_2/L), BOD5 (25 mg O_2/L), total N (10 mg/L), ammonium (4 mg/L) and total P (1 mg/L), defined by the local water agency (ACA), the Manresa WWTP, with average effluent flowrate of 27,000 m^3/day, could deliver an effluent load of 3375 kg/d, 675 kg/d, 270 kg/d, 108 kg/d and 27 kg/d, respectively for these pollutants. In the case of COD, BOD5 and Total N, the graphics of Figure 4.3 clearly show lower nitrification rates on winter months, especially from January until March and from 2005 to 2006. Ammonium removal is significantly improved after April 2006. The nitrate produced could not be denitrified at the same rate than the ammonium is oxidized. The total P levels were kept at the limit of 27 kg/d, which means an average value of 1 mg/L of P, with large usage of $FeCl_3$ in 2008, 2009 and 2010. Such chemical precipitation represents an annual cost around of € 50.000. The current performance of the Manresa WWTP regarding the chemical P removal process is on the legal limit determined by the EC directive (Table 1.1).

On summer months, contaminant loads are considerably lower than in winter months, probably also due to the people moves from Manresa to vacation locations. These recognized patterns could help to improve the tuning of feed-forward controllers, for refusing external variations whose pure feedback controllers do not deal easily, as well as, to promote a timescheduling load profile for dosing extra COD source for denitrification and $FeCl_3$ for chemical P removal.

4.3 Plant modelling

4.3.1. Model structure and premises

The kinetic model implemented for modelling COD, N and P removal was the IWA ASM2d model (Henze *et al.*, 1999). This model is being used in many researches concerning WWTP due to including the most important biological processes of ordinary heterotrophic biomass, heterotrophic PAO biomass and ordinary autotrophs. ASM2d model has 19 state variables and 21 processes, which include nitrification and denitrification and the PHA (poly-hydroxyalkanoates) accumulation process, the latter fundamental for biological phosphorus removal. See appendix for more details about the ASM2d model.

The kinetic model does not consider effects of cannibalism amongst the different species of microorganisms as reported in literature (Moussa *et al.*, 2005). The GAO (Glycogen Accumulating Organisms), which compete with PAO but do not provide phosphorus removal, neither are considered in the ASM2d model. These limitations of the ASM2d model can be attenuated changing the values of decay and YPO_4 parameters.

All the reactors of the anoxic zone were grouped in one CSTR reactor, keeping constant the total volume of the zone (m^3/wastewater treatment line). Although the aerobic reactor of the plant seem to be a Carrousel (plug-flow reactor), only one CSTR reactor was considered per treatment line. These considerations were taken because model response in different hydraulic configurations did not bring relevant changes in the steady-state values of all the variables of interest.

The settler model adopted was the 10 layer Tákacs model (Tákacs *et al*, 1991). The wastewater entrance is at the fifth layer. At the end of the process, the effluent leaves the settler from the upper part (the collector, layer 1) and the settler biomass is recycled from the bottom of the settler (layer 10) to the feed of the biological treatment. The recycled biomass is reincorporated to the process, being mixed to new influent of the biological treatment. This recirculation is called “external recycle” (Q_{RAS}). The soluble components of the wastewater leave the settler with a concentration calculated considering CSTR behaviour for these compounds. The settleability of particulate states is linked to the settling velocity which is calculated by a double exponential function (Equation 4.1).

$$v_s = v_0 \cdot e^{-r_h (X_i - f_{ns} \cdot X_{IN})} - v_0 \cdot e^{-r_p (X_i - f_{ns} \cdot X_{IN})}$$ Eq. 4.1

Where:
v_0 is the settling velocity if the *Stokes' Law* could be applied to the wastewater, [m/h];
f_{ns} is the non-settleable solids, [%];
X_{IN} is the inlet solid concentration, [g TSS/m^3];
X_i is the solid concentration of the layer *i*, [g TSS/m^3];
r_h and r_p are weights for modelling the effect of the size of the particles in the settling velocity.
Parameter v_s is compared to a maximum settling velocity, $v_{s,max}$, which is experimentally determined. *Xt* is a threshold value that indicates an upper limit in the settler capacity not to occur an overflow of solids in the equipment. The default values of the adopted model are:

v_0: 500 m/h
v_{smax}: 250 m/h
r_p: 0.00286
r_h: 0.000576
f_{ns}: 0.228%
X_t: 3000 g TSS/m^3

4.3.2. Influent characterization according to the model states

Although daily analysis of the influent are performed to know the COD, BOD5, Kjeldahl nitrogen and so on, for model calibration and to predict the plant behaviour under different operating conditions, additional experimental data is needed to obtain the specific characterization required for ASM2d (see appendix A.1). Therefore, some experiments were use for characterising the biological treatment influent (wastewater that leaves the primary clarifier) as detailed in (Montpart, 2010), following the methodology described in (Orhon, 1994; Orhon *et al*., 1994). Using these data, it was possible to determine next influent stream characteristics:

SI = 0.080 COD
XI = 0.055 COD
X_S = 0.450 COD

$S_F = 0.410$ COD

The values of the influent variables X_{TSS}, SNH_4, SNO_3, SPO_4 were assumed to be equal to the experimental observations (daily analysis). The variables S_A, X_{PHA}, X_{PAO}, X_{PP}, S_{N2}, S_{O2}, X_A, X_{MEP} were assumed to be zero. Hence, the inlet heterotrophic biomass was calculated by the equation 4.2:

$$X_H = COD - (S_I + S_A + S_F + X_I + X_S + X_A) \qquad \text{Eq. 4.2}$$

The variable X_{MEOH} was not considered zero due to the presence of chemical phosphorus precipitant agent and its value along the time was defined in the steady state calibration, when the phosphorus behaviour in the effluent was evaluated. Finally, S_{ALK} (the plant influent alkalinity) was considered to be 7 moles of HCO_3^-/m^3. See appendix A.2 for details of the experiment for influent characterization to determine unobservable ASM2d model states.

4.3.3. Model Calibration

Model calibration was performed in two steps: a steady-state calibration and a dynamic calibration. The former step was useful to minimize structural discrepancies between the plant model and plant data, like as Vanrolleghem (2001). By its turn, the dynamic calibration involves not only the determination of kinetic and stoichiometric parameters, but also an estimative of the useful volumes of reactors and settlers and the necessities of P chemical precipitant agent and extra load of biodegradable COD for denitrification.

Data from seven influent variables were available for model calibration of Manresa WWTP: ammonium, nitrate, phosphorus, total suspended solids, COD, BOD5 and Kjeldahl nitrogen. These variables are considered the output variables or interest variables. Data period used for model calibration was from October 2007 to May 2008. Due to daily oscillation in the COD and BOD5, these variables were used only for model validation. In all the steps used for model calibration, the following cost function was used:

$$CCF = \sum_{i=1}^{5} w_i \sqrt{\cdot \sum_{j=1}^{251} \left(y_{EXP,i,j} - y_{Model\,i,j} \right)^2} \qquad \text{Eq. 4.3}$$

Where:

- w_i is the weight to normalize all the output variables. The basis used was ammonium (w = 1). The weights were calculated as the ratio of the average of ammonium concentration to the average of the other output variable, shown in equation 4.4.The weights for nitrate, phosphorus, total suspended solids and nitrogen Kjeldahl were, respectively, 0.235, 1.124, 0.091 and 0.532.
- i is related to each output variable
- j is related to each experimental data (each day). The whole period studied had 251 days.
- $y_{EXPi,,j}$ is the experimental data of variable i at day j.
- $y_{Model,i,,j}$ is the model output of variable i at day j.

$$w_i = \frac{\frac{1}{251} \sum_{j=1}^{251} y_{j,NH4}}{\frac{1}{251} \sum_{j=1}^{251} y_{i,j}} \qquad \text{Eq. 4.4}$$

Where $y_{i,j}$ is the data of the other output variables (i = NO_3, X_{TSS}, $N_{Kjeldahl}$ or PO_4^{3-}).

The same equation for calculating CCF was used for calculating a VCF (validation cost function), using validation data (data from 2008 until 2010). Due to their associated uncertainties, operational variables, as the plant flowrates and the DO in the aerobic basins could be also used as calibrating parameters. The internal recycle, external recycle and purge flowrates data observed by the WWTP personnel probably contained uncertainties (no reliable mass flowmeters were available) and hence, some multiplying factors were created to consider these uncertainties. These factors were f_{QW} for the purge flowrate; f_{QRINT} for the internal recycle flowrate and f_{QRAS} for the external flowrate. In the case of the uncertainties of the DO sensors, the multiplying factor was the DO_Gain.

As the influent concentrations of each model state also are not perfectly determined, additional influent factors were adopted for further adjustments in the inlet concentration of each state of the model.

4.3.3.1 Preliminary calibration

Experimental data were averaged (influent values and operational parameters like DO and flowrates) and the resultant values were used as inputs to the simulation model (constant inputs). A period of 1200 days was simulated with the default ASM2d parameters and the steady state values were used as initial values for all the simulations performed afterwards.

Preliminary calibration aims to reduce structural discrepancies between the model and the experimental variables, especially to reduce the main differences between experimental TSS and the TSS predictions. TSS concentrations (in aerobic reactors, wastage purge and effluent) and the external recycling flowrate were used as output variables to calibrate the following parameters:

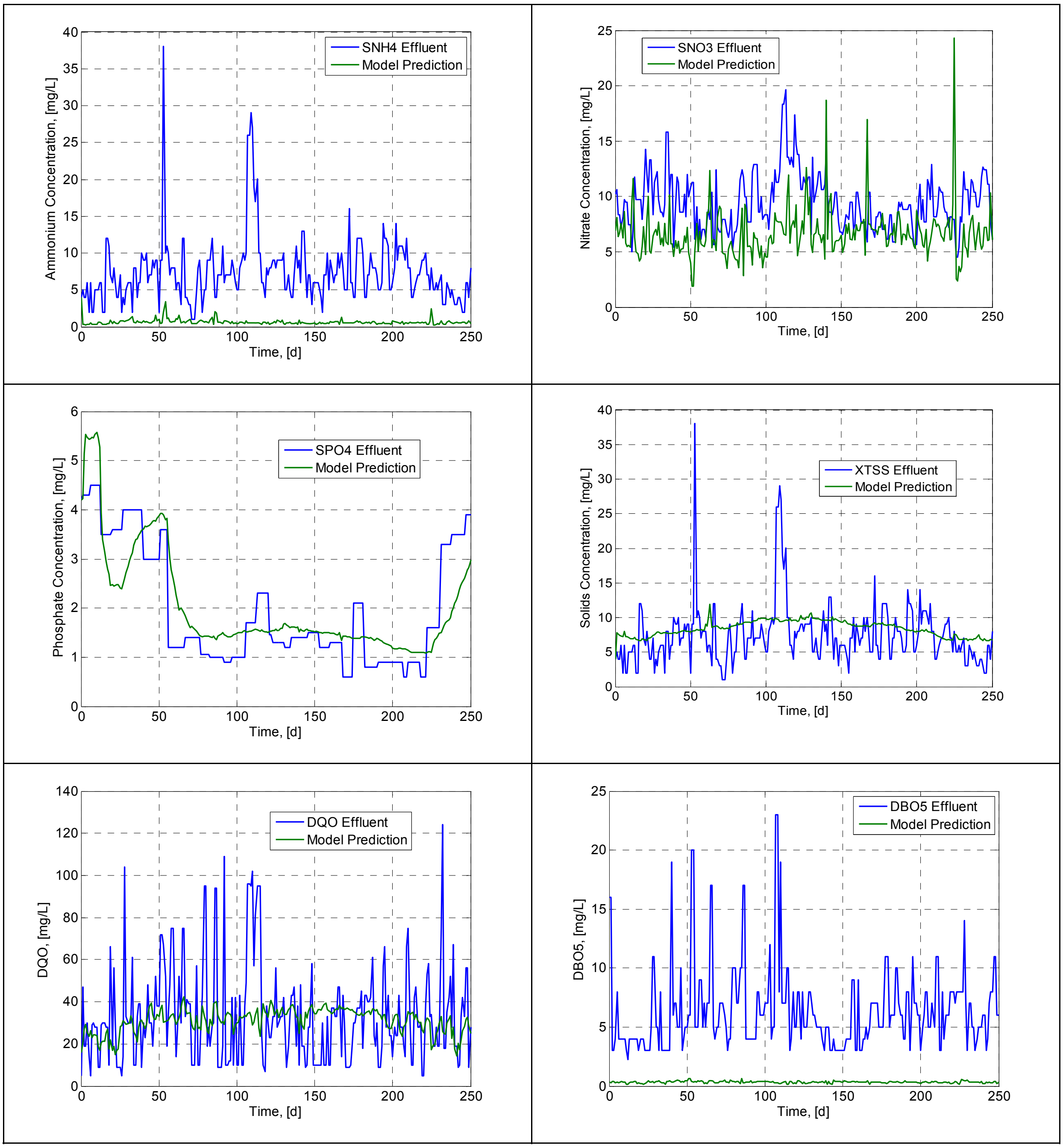
a) r_p and f_{ns} (settling model parameters), to decrease the differences between TSS in the effluent and the model predictions for this output.
b) f_{Qw} and f_{QRAS}, in order to adjust the model TSS in the external recycle/purge flowrates and in the solids inside the aerobic reactors.

In addition, X_{MeOH} in the influent was manipulated to adjust the phosphate concentrations in the effluent. The cost function used was the same presented in Eq. 4.3 and the calibrated values of the parameters were:

$r_P = 0.010359$
$f_{ns} = 0.002566$
$f_{Qw} = 0.17362$
$f_{QRAS} = 1.91077$
$f_{XMeOH} = 1.23658$

The weights used for the objective function to fit the TSS in the reactors and in the external recycle / purge flowrates were calculated by the Eq. 4.4, and their values were respectively:

3.637 10^{-4} and 2.404 10^{-4}. Figure 4.4 shows the experimental data and the model predictions for the main output variables after the preliminary calibration step. The calibration cost function value (CCF) after preliminary calibration step was **67.68**, which means a reduction of 18.9% from the CCF calculated with the original model prediction (83.46).



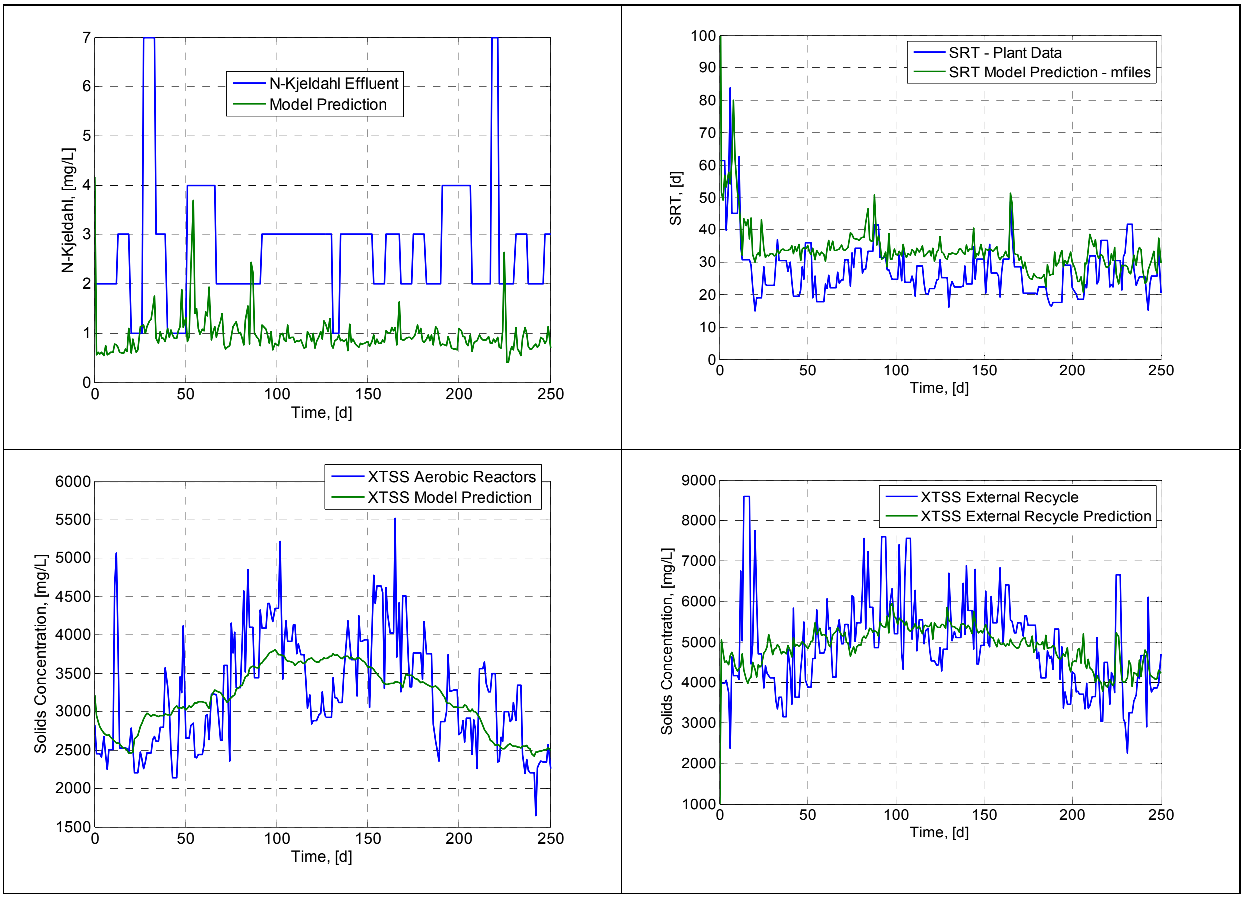


Figure 4.4: Plant data for calibration and model predictions after the preliminary calibration step.

4.3.3.2 Dynamic calibration

Dynamic calibration was performed following the methodology of the "*seeds*" (Machado *et* al, 2009) and starting from the results obtained by the preliminary calibration. Initially, a set of 90 parameters was selected to be analyzed. This set was divided into three subsets (groups presented in table 4.2): the kinetic/stoichiometric parameters (group K), the influent parameters (group I) and the operational parameters (group O). In fact, only parameters of the kinetic/stoichiometric macro-group will serve for model calibrating parameters. The macro-groups I and O were used only to obtain additional information for process control and data quality. Using extra data sets as model validation data (years of 2008, 2009 and 2010), the most suitable parameters to be used as calibration parameters were shown. The subset of kinetic/stoichiometric parameters was made up of the growth and decay parameters, yields and saturation constants of all the involved biomasses (autotrophic, heterotrophic and PAO). When calibrating the model with this group, it was considered that the influent composition during all the calibration period was completely known, as well as the operational parameters. This assumption was not strictly correct since on-line measurements of all the ASM2d states were not available. On the other hand, using the subset of influent parameters, it was considered that all the default kinetic/stoichiometric ASM2d parameters were perfectly correct, as well as the operational parameters. As determining on-line all the ASM2d variables in the influent stream is a hard and very expensive task, the group I calibration was used for obtaining additional information about the influent data quality and to determine which variables in the influent could be easily modified in order to adjust the model. At last, using the group of operational parameters, both kinetic/stoichiometric parameters and the influent composition were considered perfectly fitting the biological processes rates and the incoming pollutant loads, respectively. Amongst all the parameters, group O was used for process control in the normal plant operation. So, it was determined the parameters of this group that more easily provided fast plant response to refuse external disturbances to the control system. This knowledge was obtained using the same calibration methodology of the group K to the group O.

Table 4.2 presents the relative sensitivity of the weighted sum of the ammonium, phosphate, nitrate, Kjeldahl nitrogen and total suspended solids in the effluent (see the used equation in Appendix A.4). The parameters of each macro-group that most affect the model outputs were ranked in descending order in Table 4.2. In the case of the K group, the heterotrophic biomass growth yield, the nitrification and the phosphorus chemical precipitation are well represented by the ranked parameters. K_{PRE} and K_{RED} have almost the same impact on the model outputs, but their impacts are less important than N removal processes.

In case of the influent group, the inlet X_S, P-related processes and the inlet ammonium concentration were the most important calibrating parameters. It is possible to observe that PO_4^{3-} or MeOH inlet concentrations are more important that the own kinetic precipitation parameters K_{PRE} and K_{RED}. As P-precipitation and P-redissolution processes depend on the phosphate concentration in the biological reactors, which are pretty lower than the influent phosphate concentration, the parameters K_{PRE} and K_{RED} affect less the outputs than the influent PO_4^{3-} and MeOH concentrations. Table 4.2 also shows that inlet MeOH concentration, which could be used to control P chemical precipitation, produces more impact on the outputs that the process control variables considered in group O. Regarding S_F inlet concentration, which could be used for controlling denitrification, it would affect the outputs in the same extent of the best parameter of the group O, the purge flowrate.

In the case of the operational parameters, the purge flowrate and the DO have the most influence on the model outputs. Nevertheless, all the parameters of this group would have to change considerably to affect the outputs in the same quantity than the kinetic/stoichiometric or the influent parameters.

Tables 4.3, 4.4 and 4.5 present the results of applying a systematic procedure for model calibration using parameters of groups K, I and O, respectively. Figure 4.5 shows the calibration data of the Manresa WWTP before starting the dynamic calibrations using all the parameter groups.

Table 4.2: Relative sensitivity of the weighted sum of ammonium, phosphate, nitrate, Kjeldahl nitrogen and total suspended solids in the effluent, for all the three groups of parameters.

Kinetic / Stoichiometric Group (K group)

Order	Parameter	Short Description	Related biomass or process	Sensitivity
1	Y_H	Yield coefficient for X_H.	Heterotrophic	756
2	μ_A	Maximum growth rate of X_A	Autotrophic	678
3	b_A	Rate for lysis of X_A	Autotrophic	634
4	$K_{NH4,A}$	Saturation coefficient of substrate NH_4^+ for nitrification on S_{NH4}	Autotrophic	412
5	K_{PRE}	Precipitation constant	Chemical phosphate precipitation	150
6	$K_{O2,A}$	Saturation coefficient of O_2 for nitrification on S_{NH4}	Autotrophic	149
7	K_{RED}	Solubilisation constant	Chemical phosphate precipitation	148
8	b_H	Rate for lysis of X_H	Heterotrophic	97
9	$K_{ALK,A}$	Saturation coefficient of alkalinity for nitrification on S_{NH4}	Autotrophic	73
10	$\eta_{NO3,D}$	Reduction factor for denitrification	Heterotrophic	51

Influent Group (I group)

Order	Parameter	Short Description	Related biomass or process	Sensitivity
1	f_{XS}	Multiplying factor of X_S representing an uncertainty on the estimated inlet X_S fraction	Influent characterization	670
2	f_{XTSS}	Multiplying factor of the inlet X_{TSS} vector.	Influent characterization	555
3	f_{XMeOH}	Multiplying factor of the inlet X_{MeOH} vector.	Influent characterization	439
4	f_{SPO4}	Multiplying factor of the inlet S_{PO4} vector.	Influent characterization	429
5	f_{SNH4}	Multiplying factor of the inlet S_{NH4} vector.	Influent characterization	393
6	f_{SF}	Multiplying factor of the inlet S_F vector.	Influent characterization	247
7	f_{SALK}	Multiplying factor of the inlet S_{ALK} vector.	Influent characterization	169
8	f_{SI}	Multiplying factor of the inlet S_I vector.	Influent characterization	160
9	f_{SNO3}	Multiplying factor of the inlet S_{NO3} vector.	Influent characterization	87
10	f_{SA}	Multiplying factor of the inlet S_A vector.	Influent characterization	0

Operational Group (O group)

Order	Parameter	Short Description	Related biomass or process	Sensitivity
1	f_{QW}	Multiplying factor of Q_W representing an uncertainty on the measured value of Q_W.	Process control	297
2	DO_Gain	Multiplying factor of DO concentration on the aerobic basins representing an uncertainty on the measured value of DO.	Process control	180
3	f_{QRINT}	Multiplying factor of Q_{RINT} representing an uncertainty on the measured value of Q_{RINT}.	Process control	135
4	f_{QRAS}	Multiplying factor of Q_{RAS} representing an uncertainty on the measured value of Q_{RAS}.	Process control	116

Table 4.3: Results of the calibration methodology for the Group K.

Items	**Seeds**									
	Y_H	μ_A	b_A	$K_{NH4,A}$	K_{PRE}	$K_{O2,A}$	K_{RED}	b_H	$K_{ALK,A}$	$\eta_{NO3,D}$
Parameters	Y_H b_A K_{PRE} b_H	μ_A Y_H K_{PRE} b_H	b_A Y_H K_{PRE} b_H	$K_{NH4,A}$ K_{PRE} Y_H b_H	K_{PRE} μ_A Y_H b_H	$K_{O2,A}$ K_{PRE} Y_H b_H b_A	K_{RED} μ_A Y_H b_H	b_H K_{RED} μ_A Y_H	$K_{ALK,A}$ K_{PRE} Y_H b_H	$\eta_{NO3,D}$ K_{PRE} b_A Y_H $K_{O2,A}$ b_H
Optimized Values	0.452 0.168 1.045 0.104	0.908 0.448 1.013 0.102	0.168 0.452 1.045 0.104	1.616 1.011 0.457 0.108	1.013 0.908 0.448 0.102	0.089 1.008 0.4105 0.0786 0.2277	0.593 0.908 0.448 0.101	0.101 0.593 0.908 0.448	0.895 1.011 0.449 0.103	0.0296 1.005 0.2203 0.4181 0.1130 0.0829
Parameter Confidence Interval (%)	22 3 9 59	3 26 9 64	3 22 9 59	6 9 21 48	9 3 26 64	68 9 30 71 5	9 3 27 66	66 9 3 27	16 9 25 61	52 9 9 22 114 52
Norm of Parameter Confidence Interval (%)	64	70	64	53	70	103	72	72	68	138
normD	$1.58.10^{14}$	$4.72.10^{12}$	$1.58.10^{14}$	$5.46.10^{11}$	$4.72.10^{12}$	$1.81.10^{16}$	$1.02.10^{13}$	$1.02.10^{13}$	$1.45.10^{11}$	$9.40.10^{21}$
modE	393.41	62.61	393.41	46.37	62.61	491.80	69.09	69.09	69.56	1420.93
RDEc	$4.03.10^{11}$	$7.55.10^{10}$	$4.03.10^{11}$	$1.18.10^{10}$	$7.55.10^{10}$	$3.68.10^{13}$	$1.47.10^{11}$	$1.47.10^{11}$	$2.09.10^{9}$	$6.61.10^{18}$
CCF	66.275	66.359	66.275	65.075	66.359	65.479	66.359	66.359	66.434	63.55
VCF	172.155	172.154	172.155	170.417	172.154	171.250	172.130	172.130	172.360	167.700
Janus	1.288	1.288	1.288	1.294	1.288	1.292	1.288	1.288	1.288	1.295

As visible in Table 4.3, the subset of $\eta_{NO3,D}$ presents the highest RDEc, the lowest CCF and VCF, which convert it in the most suitable subset for model calibration. As the current plant is an A/O WWTP, no parameters related to the biological P-removal appear in the 10 most impacting seeds. On the other hand, in all the subsets appears K_{PRE} or K_{RED}, parameters linked to the P-chemical precipitation. Y_H and b_H are present in all the subsets, with high values of parameter confidence interval, which indicate less reliable calibrating values. Parameter $\eta_{NO3,D}$ is the parameter that provides more information about the plant behaviour (lowest CCF and VCF when this parameter is inside the calibration set), despite its lower value (0.0296) and more than 50% of confidence interval (default ASM2d value is 0.80). Such value indicates that a poor denitrification process is occurring in the plant, caused by, probably two factors: a lack of easily biodegradable carbon source and some amount of DO transported from the aerobic zone to the anoxic one. It would be recommendable to add extra carbon source to the influent stream to increase the efficiency of the nitrogen removal processes.

Table 4.4: Results of the calibration methodology for the Group I.

Items	**Seeds**									
	f_{XS}	f_{XTSS}	f_{XMeOH}	f_{SPO4}	f_{SNH4}	f_{SF}	f_{SALK}	f_{SI}	f_{SNO3}	f_{SA}
Parameters	f_{XS} f_{SNH4} f_{SPO4} f_{SALK} f_{XMeOH}	f_{XTSS} f_{SF} f_{SNH4} f_{SALK} f_{SPO4} f_{XMeOH}	f_{XMeOH} f_{SNH4} f_{SALK} f_{XS} f_{SPO4}	f_{SPO4} f_{SNH4} f_{SALK} f_{XS} f_{XMeOH}	f_{SNH4} f_{SPO4} f_{SALK} f_{XS} f_{XMeOH}	f_{SF} f_{XTSS} f_{SNH4} f_{SALK} f_{SPO4} f_{XMeOH}	f_{SALK} f_{SF} f_{XTSS} f_{SNH4} f_{SPO4} f_{XMeOH}	f_{SI} f_{SPO4} f_{SNH4} f_{SALK} f_{XS} f_{XMeOH} f_{SF} f_{SNO3}	f_{SNO3} f_{SF}	-
Optimized Values	1.038 1.116 0.758 0.949 0.936	0.537 2.861 1.433 1.126 0.708 1.223	0.936 1.116 0.949 1.038 0.758	0.758 1.116 0.949 1.038 0.936	1.116 0.758 0.949 1.038 0.936	2.861 0.537 1.433 1.126 0.708 1.223	1.126 2.861 0.537 1.433 0.708 1.223	6.835 0.706 1.414 1.266 1.361 1.229 2.472 0.144	1.009 0.929	-
Parameter Confidence Interval (%)	9 4 10 6 10	26 16 5 6 12 11	10 4 6 9 10	10 4 6 9 10	4 10 6 9 10	16 26 5 6 12 11	6 16 26 5 12 11	7 12 5 13 912 18 96	35 9	-
Norm of Parameter Confidence Interval (%)	18	35	18	18	18	35	35	101	36	-
normD	$1.336.10^{16}$	$2.635.10^{16}$	$1.336.10^{16}$	$1.336.10^{16}$	$1.336.10^{16}$	$2.635.10^{16}$	$2.635.10^{16}$	$9.148.10^{18}$	16598	-
modE	99.320	1480.73	99.320	99.320	99.320	1480.73	1480.73	1138.80	18.66	-
RDEc	$1.345.10^{14}$	$1.779.10^{13}$	$1.345.10^{14}$	$1.345.10^{14}$	$1.345.10^{14}$	$1.779.10^{13}$	$1.779.10^{13}$	$8.033.10^{15}$	889	-
CCF	66.129	63.609	66.129	66.129	66.129	63.609	63.609	55.847	67.663	-
VCF	170.89	168.47	170.89	170.89	170.89	168.47	168.47	162.30	172.37	-
Janus	1.289	1.311	1.289	1.289	1.289	1.311	1.311	1.371	1.278	-

Although the influent group was not used to calibrate the model, Table 4.4 brings some interesting remarks, as follows:

- The optimized values of parameters are factors that multiply the influent vectors for each variable of the influent. Therefore, a value of 1.414 of f_{SNH4} of the S_I seed means that the ammonium vector of original plant data increased 41.4% in order to minimize the cost function.
- From the 10 tested seeds, only 4 different calibrating subsets were created, which means that the influent variables participate in the same processes with almost the same importance. It is not possible to affirm that one part of the variables is much important that other one of this group.
- Comparing the results of f_{XTSS} and f_{XS} seeds it is possible to observe that the result of f_{XTSS} seed explains better the outputs than the result of f_{XS} seed, although the inclusion of S_F in the former subset increases correlation among parameters. In addition, the

calibrating methodology did not allow the simultaneous presence of X_S and X_{TSS} in any calibration subset, probably due to the high correlation between these variables.

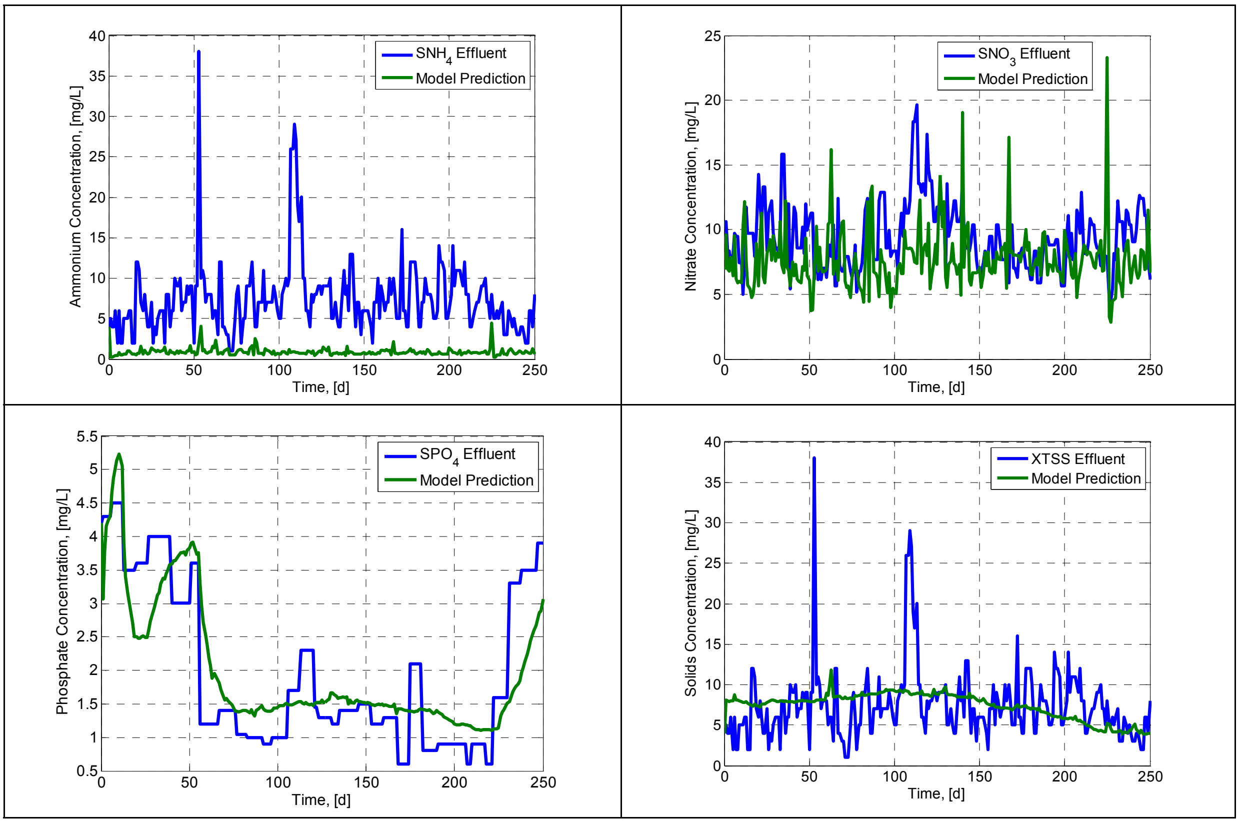
- Nitrate data are correlated to the S_F data, since in both created subsets where f_{SNO3} appears (seeds f_{SNO3} and f_{SI}), high parameter confidence interval values are reported. The existence of such a correlation is unmistakeable realized in the subset created by the f_{SNO3} seed, which is made up only by f_{SNO3} and f_{SF}.

Table 4.5: Results of the calibration methodology for the Group O.

Items	**Seeds**			
	fQ_w	DO_Gain	fQ_{rint}	fQ_{RAS}
Parameters	fQ_w fQ_{rint} DO_Gain	DO_Gain fQ_w fQ_{rint}	fQ_{rint} fQ_w DO_Gain	fQ_{RAS} DO_Gain fQ_{rint} fQ_w
Optimized Values	0.344 0.389 0.931	0.931 0.344 0.389	0.389 0.344 0.931	2.781 0.925 0.122 0.388
Parameter Confidence Interval (%)	8 18 11	11 8 18	18 8 11	15 11 97 9
Norm of Parameter Confidence Interval (%)	23	22	22	99
normD	$1.61.10^{9}$	$1.61.10^{9}$	$1.61.10^{9}$	$3.26.10^{10}$
modE	13.78	13.78	13.78	193.77
RDEc	$1.17.10^{8}$	$1.17.10^{8}$	$1.17.10^{8}$	$1.680.10^{8}$
CCF	62.348	62.348	62.348	62.284
VCF	168.91	168.91	168.91	168.95
Janus	1.322	1.322	1.322	1.323

Table 4.5 clearly shows that inserting the biomass recycle flowrate, a strong correlation to the purge flowrate is added. It indicates that in a possible control structure for controlling simultaneously N, P and COD removal, the purge flowrate and the biomass recycle flowrate could not be changed at the same time or their modifications should be done in different magnitudes. As occurred with the group I parameters, only about 50% of different subsets were created from all the initial possibilities, which again indicates that all the operational variables participate in the same processes (N, P and COD removal processes).

Considering that the influent composition determined by lab test and using plant data is perfectly known along the years of calibration and validation data, the best subset obtained amongst the kinetic group is from the parameter $\eta_{NO3,D}$, following the calibration methodology described in Machado *et al.* (2009). The subset represented by this seed includes the chemical phosphate precipitation phenomenon, as well as the nitrification processes. A calibrated value of 0.4181 for Y_H means that more COD is consumed for maintenance of the heterotrophic biomass than the consumed for promoting the growth of the microorganisms population. It was not expected this low value for this parameter, since the default value of Y_H is 0.625 (Henze *et al.*, 1999).However, similar values for Y_H around 0.45 were obtained in the other subsets from the rest of seeds. Such an unexpected result, probably, is derived from a lack of knowledge on the influent composition. Nevertheless, $\eta_{NO3,D}$ subset showed the best compromise between explaining the plant behaviour and avoiding parameters correlations, with lower CCF and VCF values.



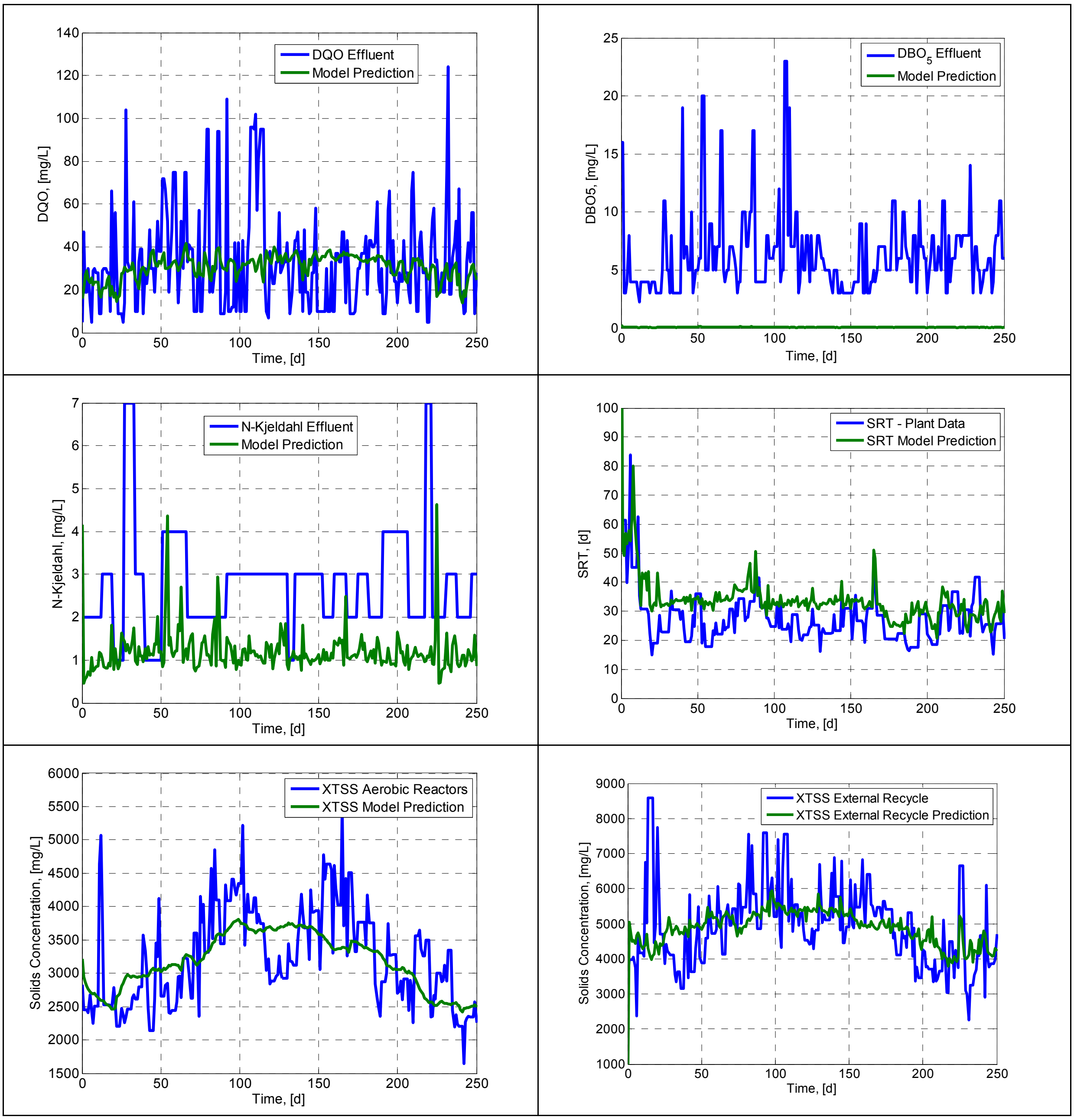
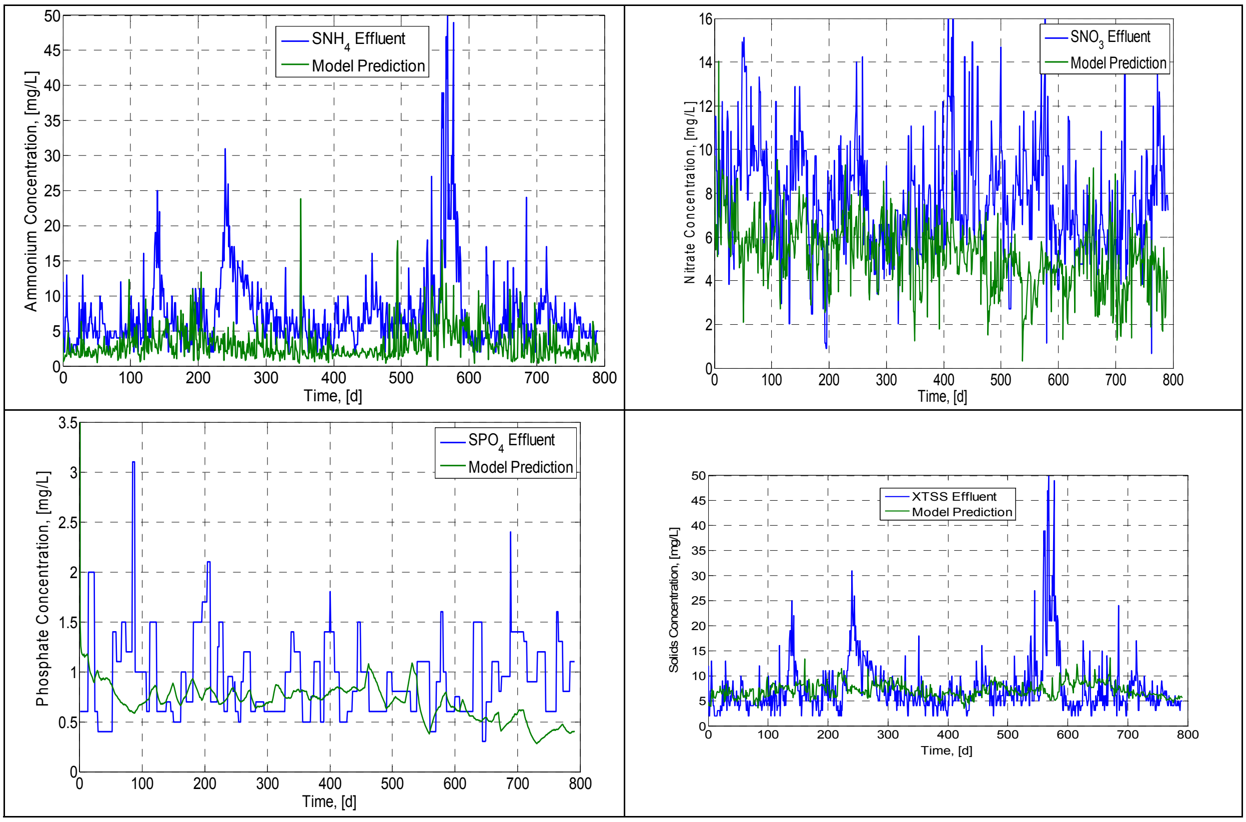


Figure 4.5: Model predictions using the best seed (subset from the seed $\eta_{NO3,D}$) and plant data (calibration data). For checking the parameter values used in this simulation, see Table 4.4.

Figure 4.5 shows the results obtained with the best subset of parameters from the seed $\eta_{NO3,D}$, $\{\eta_{NO3,D}$, K_{PRE}, b_A, Y_H, $K_{O2,A}$, $b_H\}$, which values are respectively, [0.0296, 1.005, 0.2203, 0.4181, 0.1130, 0.0829] obtained during the calibration of group K, using the calibrating data. Considering the results of Table 4.3 and the graphs of Figure 4.5, few changes added the dynamic calibration to the results obtained with the preliminary calibration. Gross modelling errors could be corrected in the preliminary calibration step. Nevertheless, poor BOD5 and ammonium predictions in the effluent could be an indication that a false denitrification rate is occurring, probably because a lack of easily biodegradable COD is not being captured. Figure 4.6 compares the model predictions to the validation data, which is a completely different dataset from the calibration data. In Figure 4.6, the parameters subset of the best seed of Table 4.3 makes the model suitable for predicting correctly nitrate, phosphate, solids, N-Kjeldahl and COD in the effluent stream and the solids in Q_{RAS} stream and inside the basins. Otherwise, poor results were again attained concerned to ammonium and BOD5 in the effluent. Such results also could indicate dead volumes in aerobic basins not modelled as well as a spatial gradient of DO, ignored in the current model. As a consequence, not all the regions of the aerobic basins operate with a reasonable DO concentration (2-3 mg/L). Figures 4.5 and 4.6 clearly show that events with fast dynamics are not well captured, since some plant measurements that made up calibration and validation data subsets have their sample time equal to one day and the samples are integrated (each 2 hours a volume of wastewater is hold to compose a final sample before chemical and biochemical analysis).



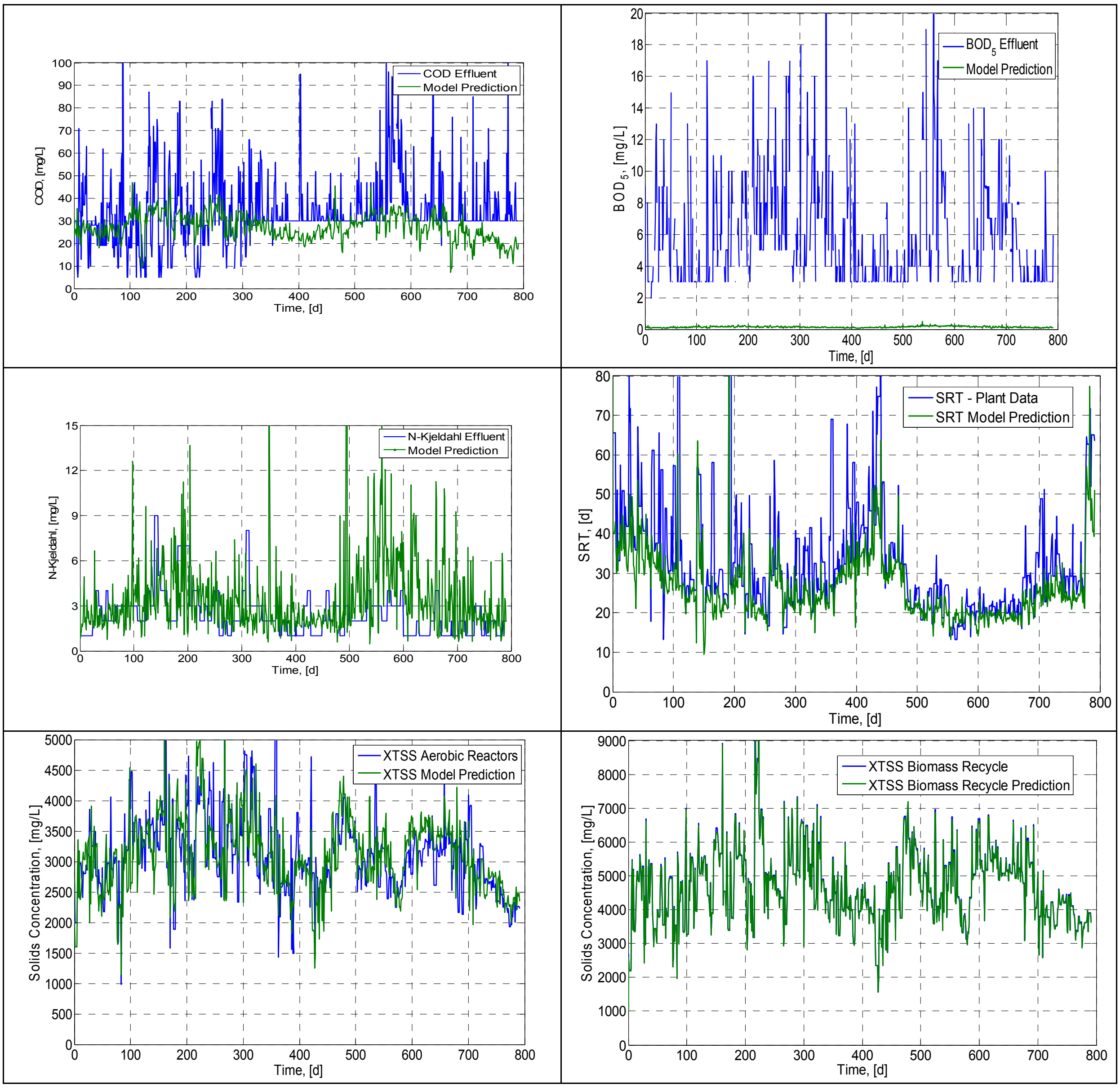


Figure 4.6: Model predictions using the best subset (from seed $\eta_{NO3,D}$) and the validation data (plant data).

4.4 Current control structure

Manresa WWTP has a predominance of proportional-integral feedback controllers. The most important control loop is the DO controller of the aerobic basins. Four blowers are available to send air to the basins. A frequency controller receives the calculated speed from the DO controller and internally changes the engine rotation, providing more or less compressed air to the wastewater. As Manresa WWTP has two treatment lines and each line has two DO probes, the supervisory program takes an average value of the four values and sends it to the DO controllers, closing the control loop. This configuration would be suitable if all the air pipes had the same distance and the same head loss. Experimentally, DO sensors indicate a great difference almost equal to 1 mg of O_2/L, too high to keep a homogeneous DO distribution in all the aerobic reactors volume.

Internal and external recycle flow rates are also automatically controlled. Nevertheless, nitrate, ammonium and phosphate in the effluent are not automatically controlled, since no on-line sensors are available in the plant. Control actions to maintain the effluent composition within the legal limits are performed manually, verifying the results with daily analysis of the effluent quality: i) if the ammonium concentration in the effluent is high, the DO setpoint in the aerobic basins is increased; ii) if the nitrate concentration in the effluent is high, the internal recycle flowrate is increased; iii) if phosphate concentration is high, more chemical agent for P precipitation is added and iv) the purge flowrate is increased when TSS concentration in the settler is high.

For process control analysis, a set of transfer functions were obtained from the non-linear model previously calibrated. A sequence of known perturbations (patterns of the most important input variables) was applied to the non-linear model and a black-box algorithm was used to identify the input-output relationships (Ljung, 1999; Machado, 2007; Machado *et al.*, 2009b). Although only DO control is running nowadays in Manresa WWTP, which can be used as a slave control for controlling the effluent ammonium in a cascade control structure in the future, all the relationships amongst plant inputs (DO, Internal and External Recycling Flowrates) and outputs (Ammonium in the effluent, Nitrate in the effluent and at the end of the anoxic zone and Phosphate in the effluent) were determined. Figure 4.7 shows some important control relationships between controlled variables and manipulated variables in the current A/O plant configuration. It is worth noticing that step tests were applied around a well-known operating point of the WWTP: 2 mg/L of DO concentration, internal recycle flowrate of 75000 m^3/d and external recycle flowrate of 25000 m^3/d.

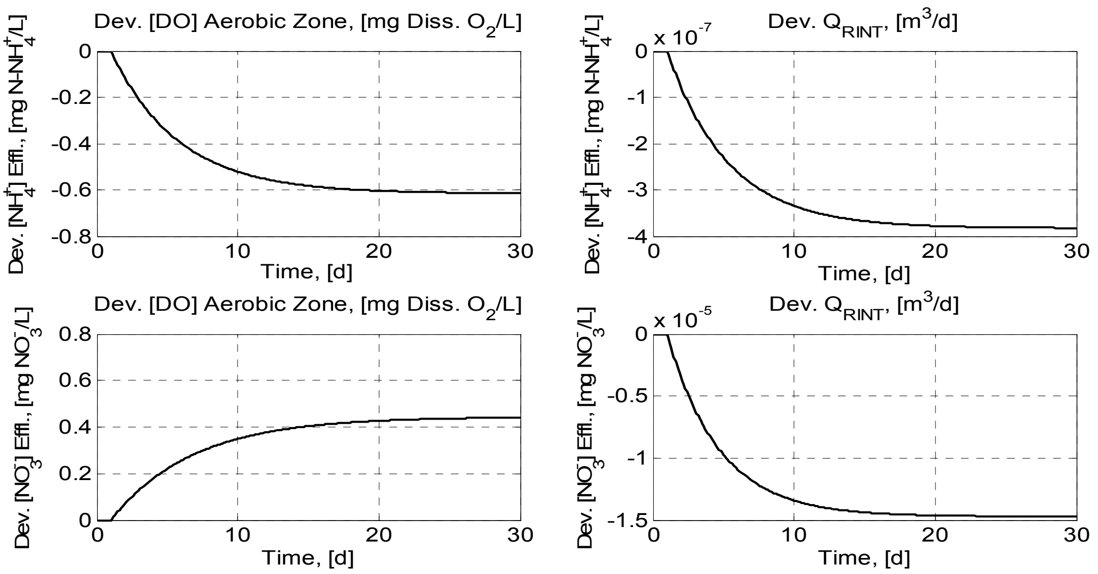


Figure 4.7: Step response of the transfer function model for the A/O configuration (current configuration), using only the main inputs and outputs of the control system.

For each unit of increase in DO concentration in the aerobic basins, ammonium decreases more than 0.5 units in the effluent 10 days after the increase. On the other side, nitrate increases 0.4 units because the intensified nitrification. By the way, model response of Figure 4.7 also shows an unbalanced compromise between nitrification and denitrification in the Manresa WWTP (the ammonium gain due to the increase of DO is greater than the nitrate gain). Considering the internal recycle effects, it is possible to observe that this variable would be better used for nitrate control than for ammonium control (gain almost 38 times greater if nitrate is the controlled variable using internal recycle flowrate instead of ammonium). It is important to note that ammonium and nitrate controllers are not implemented yet in the current plant configuration. On-line sensors should be installed and commissioned for implementing this control structure.

The model that generates the results presented in Figure 4.7, is presented in Table 4.6 and produced the RGA written in Table 4.7 at two different frequencies, ω = 0 rad/min and ω = 1 rad/min, for two different arrangements between inputs and outputs. RGA analysis only indicates the best pairing between inputs and outputs for determined decentralized control structure to make easy the process controllers tuning. In the case of A/O configuration, which is the configuration of the full-scale WWTP of Manresa, two control structures could be implemented with the two available inputs (DO concentration and Q$_{RINT}$ and three outputs, ammonium in the effluent, nitrate at the end of the anoxic zone and nitrate in the effluent).

Table 4.6: Model for process control (transfer functions) of the current input and output variables of Manresa WWTP.

Outputs [g m^{-3}]	Inputs DOSP [g O$_2$ m^{-3}] (DO setpoint in the aerobic zone)	 Q$_{RINT}$ [m^3 d^{-1}]
NH$_4^+$ Eff.	$\frac{-0.1189}{s+0.1932}e^{-s}$	$\frac{-8.816\cdot 10^{-8}}{s+0.2304}e^{-s}$
NO$_3^-$ Eff.	$\frac{0.0537}{s+0.1693}e^{-s}$	$\frac{-1.328\cdot 10^{-5}}{s+0.4631}e^{-s}$
NO$_3^-$ Anox.	$\frac{0.07632}{s+0.1719}e^{-s}$	$\frac{-3.982\cdot 10^{-6}}{s+0.2708}e^{-s}$

Table 4.7: RGA for two different combinations between inputs and outputs for the current plant configuration.

ω = 0 rad/d (steady state RGA)			
Control Structure	**Outputs**	**Inputs** **DO**	 **Q$_{RINT}$**
AO-1	NH$_4^+$ Eff	0.9816	0.0184
	NO$_3^-$ Eff	0.0184	0.9816
AO-2	NH$_4^+$ Eff	1.0069	-0.0069
	NO$_3^-$ Anox.	-0.0069	1.0069
ω = 1 rad/d (dynamic RGA)			
Control Structure	**Outputs**	**Inputs** **DO**	 **Q$_{RINT}$**
AO-1	NH$_4^+$ Eff	0.9869	0.0131
	NO$_3^-$ Eff	0.0131	0.9869
AO-2	NH$_4^+$ Eff	1.0029	-0.0029
	NO$_3^-$ Anox.	-0.0029	1.0029

Both control structures present similar results, not only for steady-state frequencies but also for short times (approximately the operating frequency of the controllers). This behaviour could be an indication that the maximal denitrification capacity of the plant has been reached, since the same nitrate dynamics is observed in two different points of the plant (in the effluent and at the end of the anoxic zone), which means that there is an excess of nitrate leaving the anoxic zone. Thereby, the load of nitrate that is extracted from the aerobic basin is almost the same that the received by the anoxic basin and at the same time, does not matter how the denitrification rate changes since it is slower than the nitrification rate. It is possible to observe that the DO affects much more the ammonium than the nitrate concentration, even in the effluent. This fact corroborates that the anoxic zone has a low performance which does allow the DO in the aerobic zone barely produces a small change in the nitrate concentration in the influent. The internal recycling affects the nitrate more than the ammonium as beforehand was expected.

4.5 Proposed modifications

Based on the particularities of the A/O existent plant and respecting the design premise of minimizing changes and keeping the WWTP processes completely continuous, four retrofitting alternatives were tested for incorporating the EBPR in the Manresa WWTP, as follows:

- A^2/O with two anaerobic reactors (configuration A^2/O-D, of double anaerobic volume)
- A^2/O with one anaerobic reactor (configuration A^2/O-S, of single anaerobic volume)
- BARDENPHO configuration
- University of Cape Town configuration (UCT)

Configuration A^2/O-D can be obtained by converting one of the three anoxic reactors into an anaerobic reactor (one for each treatment line). This configuration is presented in Figure 4.8. The most important change from the current Manresa WWTP to the A^2/O-D configuration is to change the way of the internal recycle, fact that demands new wastewater lines and connections to the forward anoxic basins.

The configuration A^2/O-S, can be obtained using only one anoxic reactor of the current Manresa WWTP to build an anaerobic zone (only in one of the treatment lines), as Figure 4.9 shows. Again, to execute this change, new lines and connections to bring all the internal recycle flowrate after to the first anoxic reactor of today (future anaerobic), is demanded.

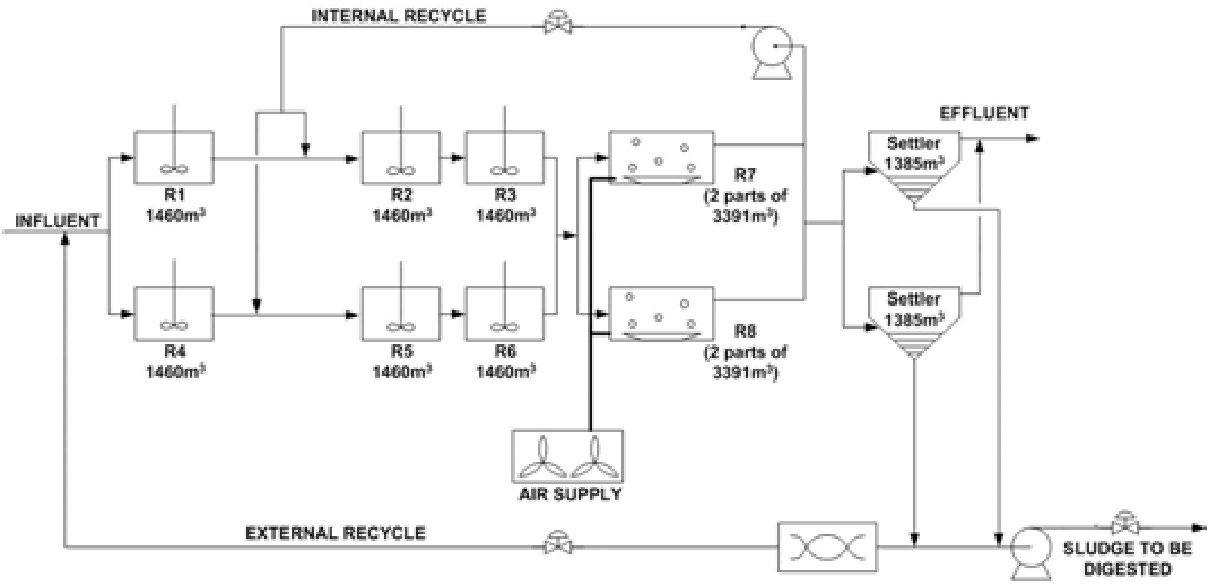


Figure 4.8: Configuration A^2/O-D, where two anoxic tanks of the original A/O WWTP are modified to anaerobic tanks.

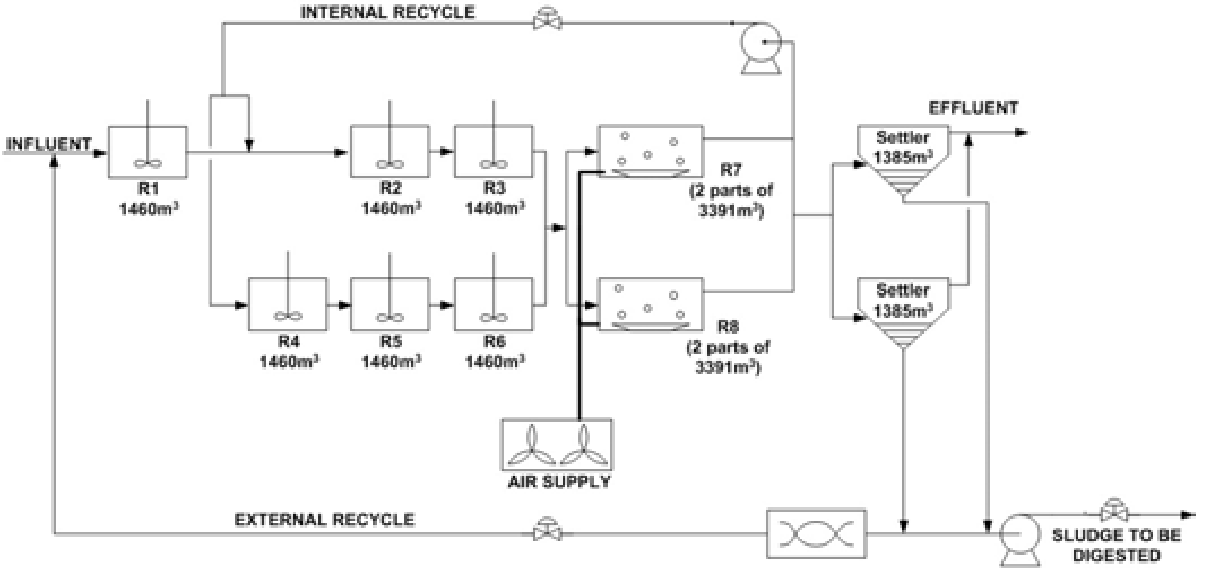


Figure 4.9: Configuration A^2/O-S, made up converting only one anoxic tank of the original A/O WWTP to anaerobic tank.

The third proposed configuration is the BARDENPHO. Figure 4.10 shows this configuration applied to the Manresa WWTP. Such configuration could be implemented not only changing the way of the internal recycle like needed in the A^2/O-D and A^2/O-S configurations, but also building new air pipes to convert the last anoxic reactor into aerobic reactor of each treatment line. Besides, part of the air control valves of the first part of the current aerobic zone should be blocked to create an anoxic zone in the current aerobic zone (in both treatment lines).

At last, UCT configuration is one of the proposed configurations changing the point where the external recycle is added to the main treatment stream. Figure 4.11 shows the proposed UCT configuration for the current Manresa WWTP. In this case, the current internal recycle of Manresa WWTP should be modified: it is needed that the current internal recycle takes wastewater from the end of the current aerobic zone and send it to the upstream of the last current anoxic reactor (for each line). Therefore, the current internal recycle of Manresa WWTP would become the Internal Recycle II of Figure 4.11. Other internal recycle (Internal Recycle I) should be built to discharge the fluid from the downstream of the second current anoxic basin to the upstream of the designed anaerobic zone (which would be made converting one current anoxic reactor into anaerobic one for each treatment line). . No changes are demanded in the current aerobic zone of the Manresa WWTP.

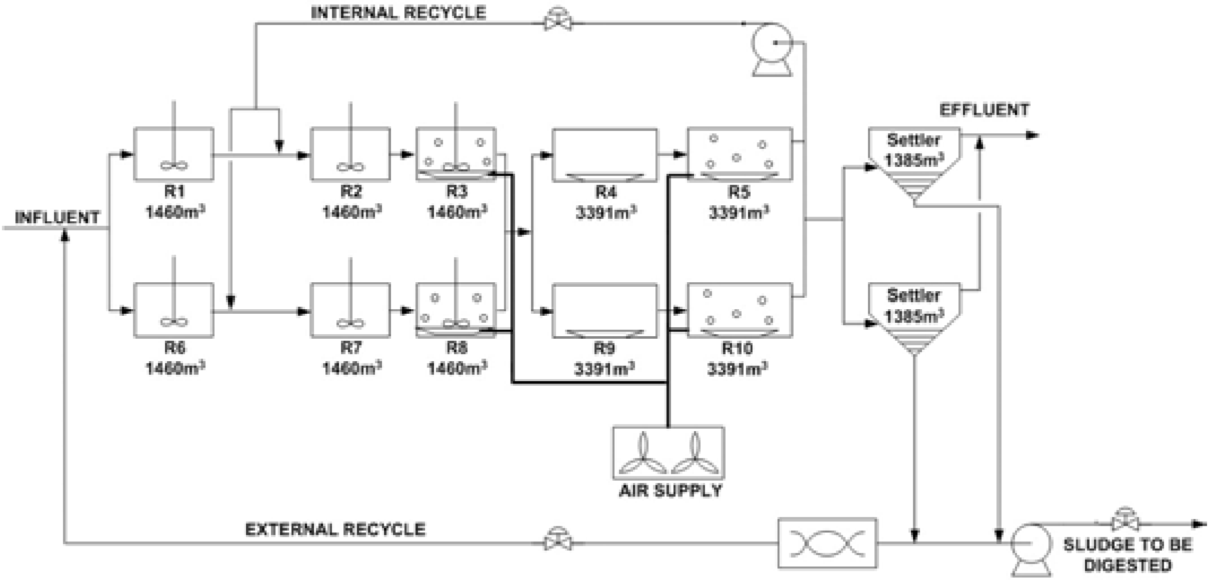


Figure 4.10: Configuration BARDENPHO, made up converting two anoxic tanks of the original A/O WWTP to anaerobic tanks and other modifications detailed in the text.

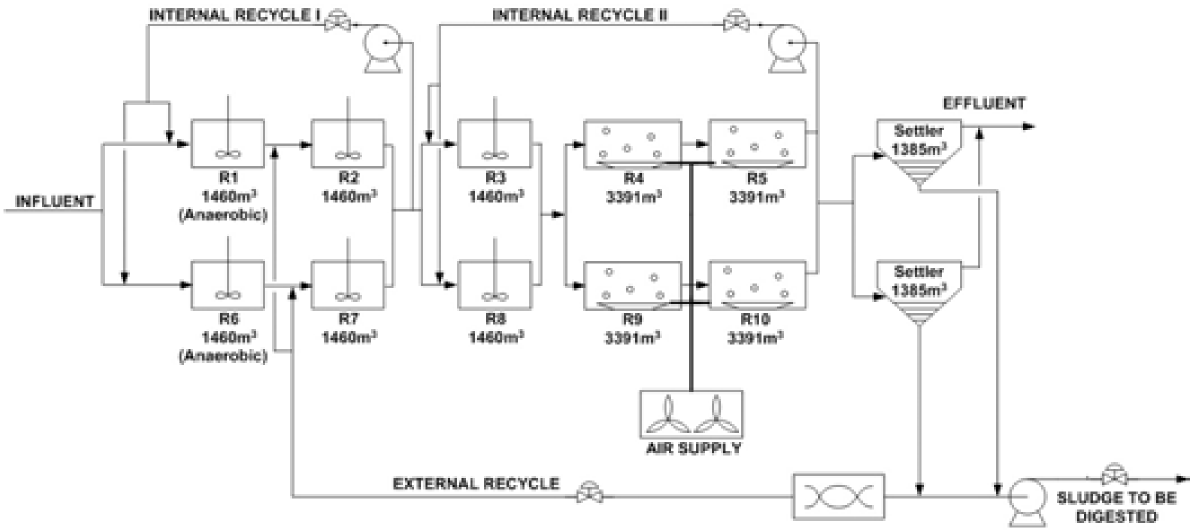


Figure 4.11: Configuration UCT, made up converting two anoxic tanks of the original A/O WWTP to anaerobic tanks and other modifications detailed in the text.

In terms of number of changes, it is clear that the UCT configuration demands at least three changes in the current configuration of Manresa WWTP, while BARDENPHO demands two changes and both A^2/O-S and A^2/O-D only one change. Such a fact certainly weights in the final choice to determine the best alternative of implementing EBPR in the current Manresa WWTP.

4.6 Selecting the best alternative

Once all the developed alternatives have been modelled, simulations using the same input data (influent data) for all the models, which was used also for calibrating the model of the current WWTP, have been performed. Taking into account that the main reason for proposing a new plant configuration is to add biological P removal, Figure 4.12 shows the total P concentration in the effluent of the four alternative configurations tested and the original A/O configuration.

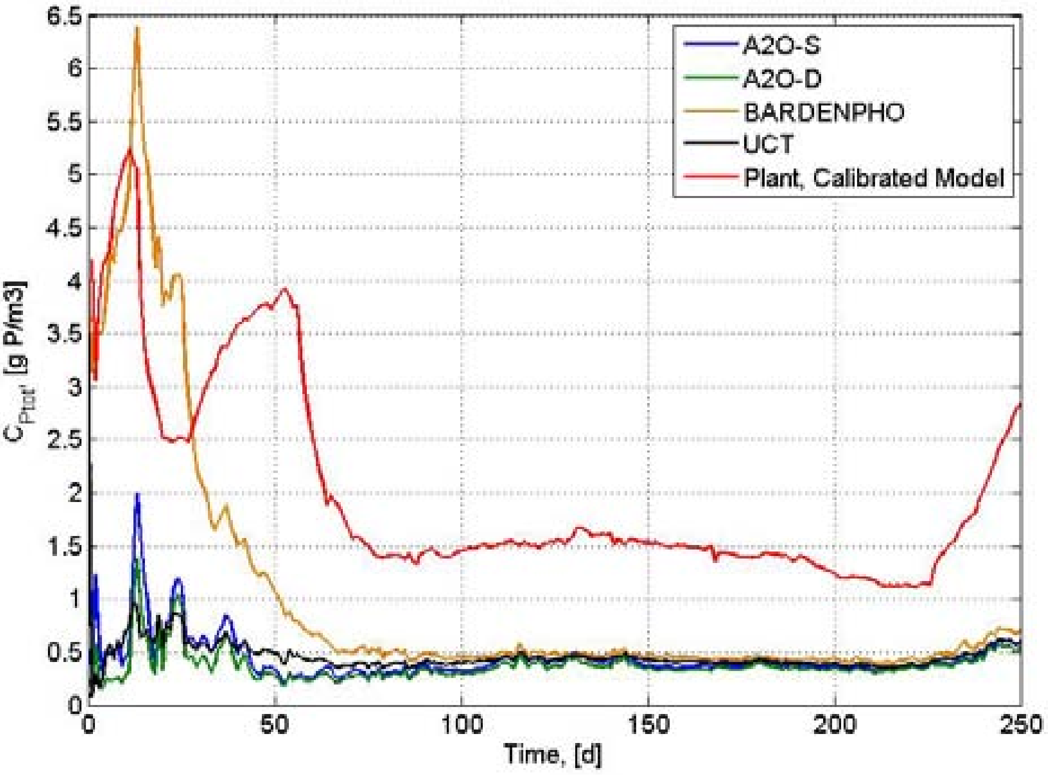


Figure 4.12: Comparison of model predictions for total phosphate effluent concentration for the original configuration and the four alternatives tested.

Clearly, it is easy to show that both A^2/O and UCT proposed plant configurations provide better results in terms of P removal than the A/O plant configuration and BARDENPHO. In fact, at the 50 first days of simulation, which represent strong dynamic changes in the influent, BARDENPHO could not refuse external variations at the same velocity of both A^2/O and UCT configurations. When external disturbances disappear, between times 100 to 200, all the proposed alternatives presented the similar performance. As WWTP scenarios are full of input variations, poor performance of BARDENPHO configuration in the first 50 days decreases the possibilities of such a type of process for being elected as the best alternative for implementing EBPR in Manresa WWTP.

The European Community directive for WWTP discharge limits was applied to the simulation data as a first criterion for measuring the performance of the different configurations. Table 4.8 presents the results.

Table 4.8: Performance of all the tested alternatives according to the EC directive criteria and other current parameters commonly monitored in full-scale WWTP.

Variable computed with Effluent data		Configuration				
		A/O (Current Configuration)	A^2/O-S	A^2/O-D	BARDENPHO	UCT
Average concentration, [mg/L]	**Total P**	1.98	0.79	0.61	1.02	0.47
	$N\text{-}NH_4$	2.93	2.86	2.89	19.42	2.89
	$N\text{-}NO_3$	8.39	8.13	7.95	5.20	10.51
	TSS	7.70	7.42	7.42	7.64	7.70
	TKN	3.96	3.97	4.00	20.56	4.06
	Total N	12.36	12.11	11.96	25.77	14.58
	COD	48.33	52.53	52.83	53.42	54.09
	BOD5	4.36	4.30	4.31	4.45	4.65
Peak. concentration, [mg/L]	**Total P**	4.50	7.65	4.20	6.39	4.20
	$N\text{-}NH_4$	21.02	20.96	21.04	44.12	21.98
	$N\text{-}NO_3$	16.37	15.31	14.94	11.77	17.02
	TSS	24.45	8.64	8.64	24.21	24.45
	TKN	21.91	21.88	21.97	45.40	22.97
	Total N	33.31	33.14	32.93	48.96	35.62
	COD	69.31	63.37	63.75	85.96	87.26
	BOD5	11.30	5.33	5.37	11.26	11.79
Flow Weighted Average. concentration, [mg/L]	**Total P**	2.02	0.81	0.63	1.05	0.47
	$N\text{-}NH_4$	3.00	2.91	2.94	19.19	2.97
	$N\text{-}NO_3$	8.34	8.08	7.91	5.21	10.43
	TSS	7.69	7.40	7.40	7.62	7.68
	TKN	4.02	4.01	4.05	20.32	4.13
	Total N	12.36	12.10	11.96	25.53	14.57
	COD	47.91	52.08	52.38	52.99	53.65
	BOD5	4.32	4.26	4.26	4.41	4.62
Annual reduction of the influent, [%]	**COD**	87.27	86.17	86.09	85.93	85.76
	BOD5	97.52	97.56	97.55	97.47	97.36
	Total N	76.25	76.72	77.00	50.47	71.98
	Total P	42.94	77.10	82.28	70.51	86.46

It is worth noticing that all the tested plant configurations were submitted to the same inputs, as the plant model (A/O configuration) in the model calibration step. This period comprehends more than 8 months of plant data and is characterized by long periods of plant stability. Table 4.8 results point out a better performance of the A^2/O-D and UCT configuration for total nitrogen and total phosphate elimination, respectively. A lack of an anaerobic volume of A^2/O-S configuration does not allow such a configuration to reach the P elimination obtained by the A^2/O-D configuration. Nevertheless, a greater total anoxic volume of the A^2/O-S configuration in comparison to the A^2/O-D configuration does not increase the denitrification capacity of the A^2/O-D configuration. On the contrary, the latter configuration reaches the lowest total nitrogen concentration, slightly lower than the result of A^2/O-S configuration. A greater anaerobic volume promotes a higher yield of fermentation products

(S_A component in the ASM2d model: volatile fatty acids, like acetic, propionic and butyric acids), consuming the readily biodegradable soluble organic substrates (S_F in the ASM2d model), which improves the denitrification process on S_A in the anoxic zone. In the current scenario of Manresa WWTP, the BARDENPHO solution could not reach the best results in any variable. The poor results of BARDENPHO configuration arise from the fact of a reduction of the aerobic zone in comparison to the current A/O configuration and the possible carriage of DO from the first aerobic zone to the second anoxic zone. The UCT configuration presented good performance like the A^2/O-D configuration, especially in the P removal processes. It probably occurs due to the PAO biomass enrichment that occurs because this configuration reduces the amount of nitrate entering the anaerobic reactor in comparison to the A^2/O-D configuration. Figure 4.13 shows the PAO biomass concentration in the first anoxic reactor of the treatment line 1 of both configurations. In fact, simulation results present a greater quantity of PAO biomass inside the UCT configuration than the A^2/O-D one.

In accordance to the discharge limits parameters stated by the EC directive, both A^2/O-D and UCT could overcame almost all the constraints. Only the total nitrogen maximum concentration (annual average) exceeded to 10 mg L^{-1}. Such result implies a possible necessity of adding extra carbon source to promote the required denitrifying process.

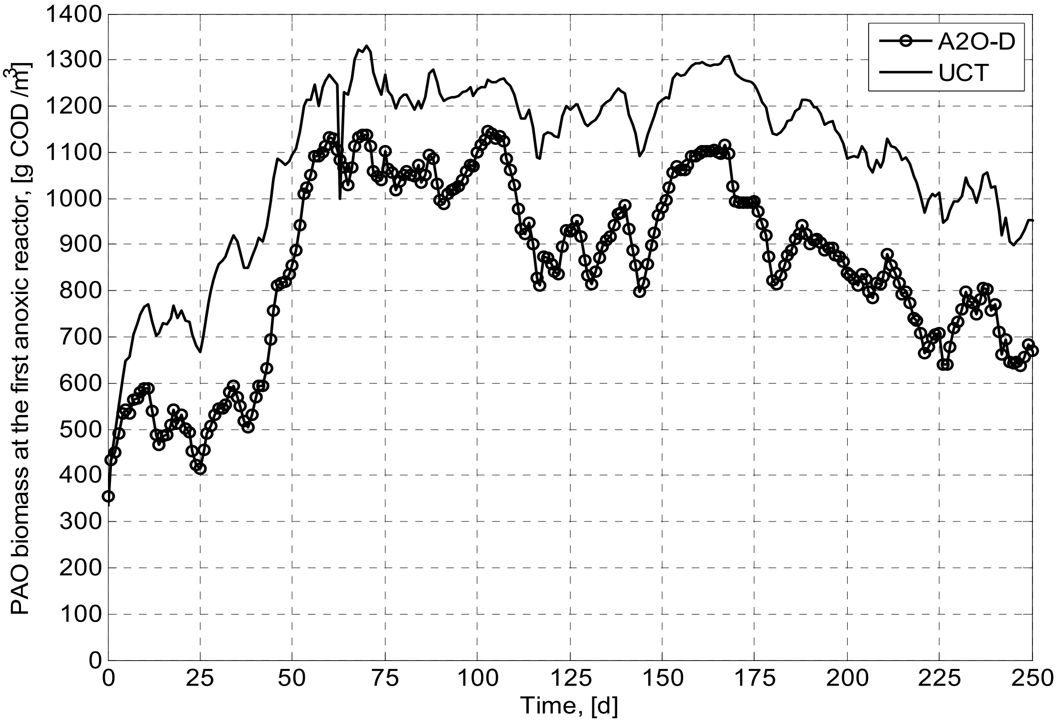


Figure 4.13: PAO biomass in the first anoxic reactor of the treatment line 1 of both UCT and A^2/O-D configurations during the simulations using the original Manresa WWTP data.

The proposed methodology was used for performing robustness tests to evaluate the best retrofitting alternative in case of strong external disturbances, like abrupt increase of pollutants load or extreme lyses of biomass due to toxic agents, for instance. Such tests consist in producing different pulses of ammonium and total phosphate at the influent and observe the effluent quality in all the cases. In both experiments, the pollutant pulse was performed at the day 130 of the input file. The mass of phosphate was integrated during days 131 to 215 for the P-pulse and the mass of N during the days 131 to 150 in the case of the ammonium pulse. The P-pulse had three magnitudes: 2, 5 and 10 times the original total P concentration in the plant data (full-scale profile), while the ammonium pulse had the magnitudes of 1.5, 2 and 3 times the original concentration of ammonium in the original plant data. Figure 4.14 shows the amount of total P released in the effluent during the P-pulse experiments. It is interesting to realize that a pulse of many days as was applied to the proposed retrofit configurations (and to the plant model) could be considered as a permanent increase of plant load in some extent, helping to observe which plant configuration would be able to better respond to an increase of local population.

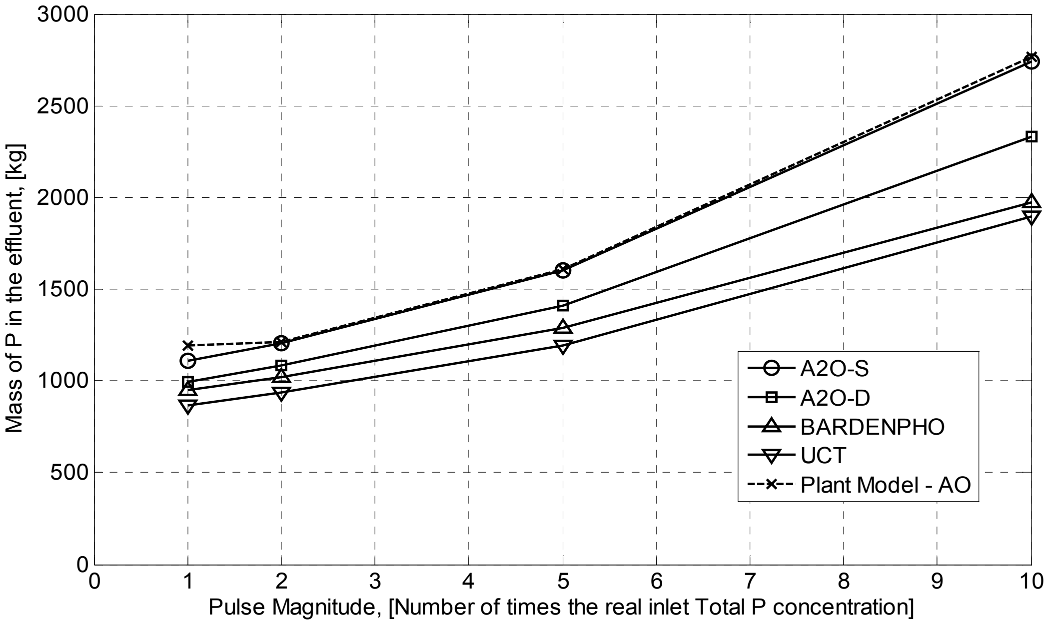


Figure 4.14: Mass of P released in the effluent stream during the pulse-experiment of total P in the influent.

As can be observed in Figure 4.14, the current plant configuration (A/O) and the A^2/O-S configuration present the poorest results. They cannot refuse the external disturbance of inlet

P in the same extent of configurations UCT and BARDENPHO. The configuration A^2/O-D had an intermediate performance. To have an idea about the simulation data during the P-pulse experiment, Figure 4.15 shows the total P concentration in the effluent of all the proposed plant configurations and the input profile of total P in the influent. Both original and modified input profiles are shown.

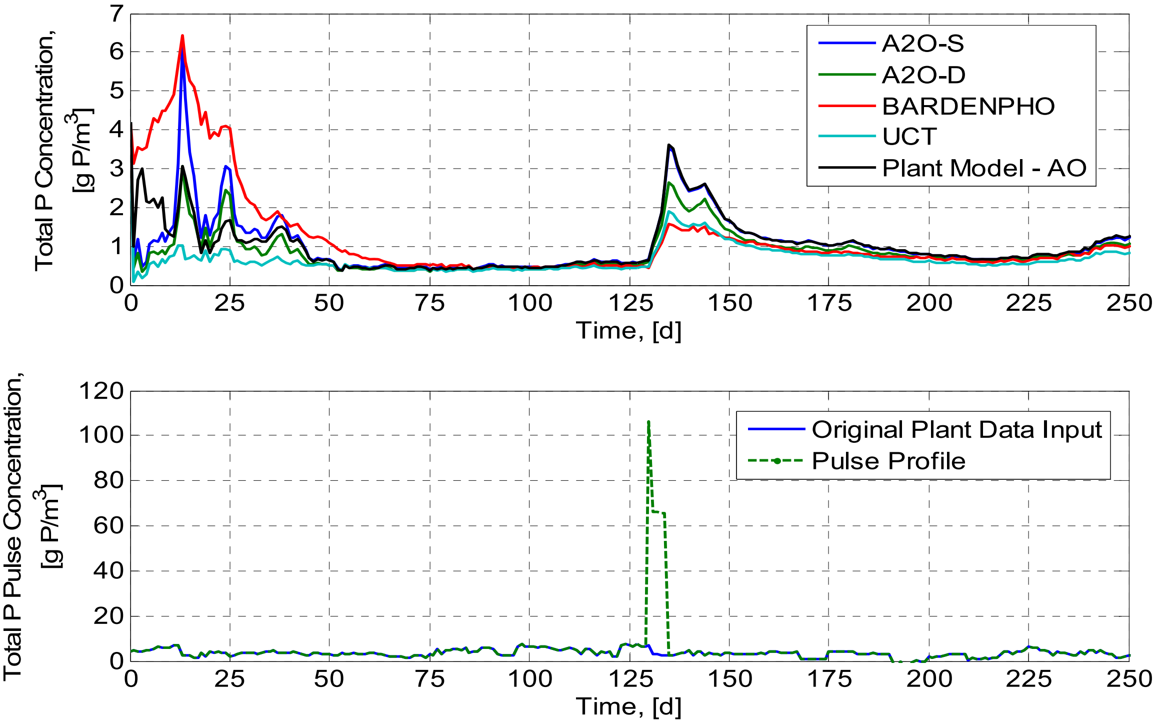


Figure 4.15: Total P concentration in the effluent for all the proposed retrofit configurations and the influent profiles of total P concentration (original and modified profile) during the pulse experiment of 10 times the original profile of total P inlet concentration.

The pulse magnitudes tested deliberately are much higher than the current measurements performed in WWTP of Manresa nowadays, to better visualize the real potential of each proposed configuration for refusing external disturbances. Note that an increase of pollutant concentration at the influent could be the same effect as abrupt biomass decay. Hence, the performance tests also show the plant capacity to have its biomass quantity reposed as soon as possible after an undesirable event.

Regarding the experiment with ammonium pulses, the best results for refusing external disturbances of ammonium nitrogen were achieved by both A^2/O proposed alternatives. The results were slightly better than the current Manresa plant configuration. Figure 4.16 present these results.

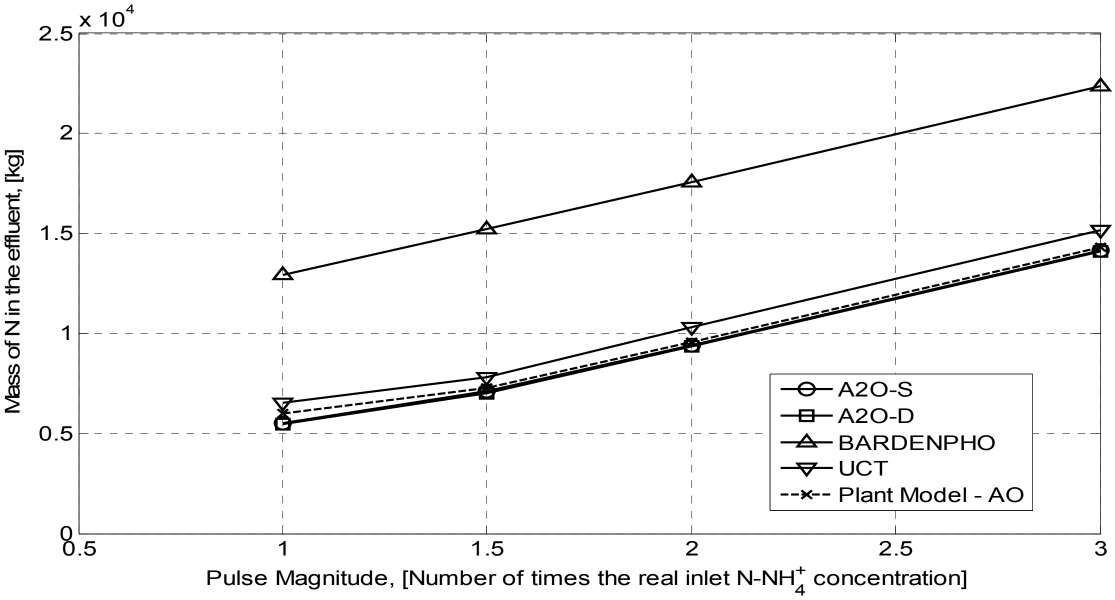


Figure 4.16: Mass of N released in the effluent stream during the pulse-experiment of N-NH_4^+ in the effluent.

The results of Figure 4.16 indicate poor performance of refusing ammonium pulses of BARDENPHO configuration. As commented before, the reduction of aerobic zone to be applicable into the Manresa scenario affects too much the performance of such configuration. On the other hand, A^2/O-D could reach the best performance in this experiment.

Also, the sensibility of the effluent quality to the addition of extra carbon source is measured, simulating all the proposed alternatives. The magnitude of extra amount of carbon was calculated as a percentage of the full-scale COD that enters in the Manresa WWTP. The tested values of this fraction were: 1%, 5%, 10%, 20% and 50%. It is important to remember that, again, the EC directive establishes the main legal objectives that the retrofitting alternatives should attain. Figures 4.17 to 4.20 show important parameters of the EC directive calculated with the results of the simulations of the proposed plant configuration and the current plant model. In advance, there were no exceeds in COD and BOD5 parameters in all the cases for all the plant configurations even though extra biodegradable COD was added to the systems.

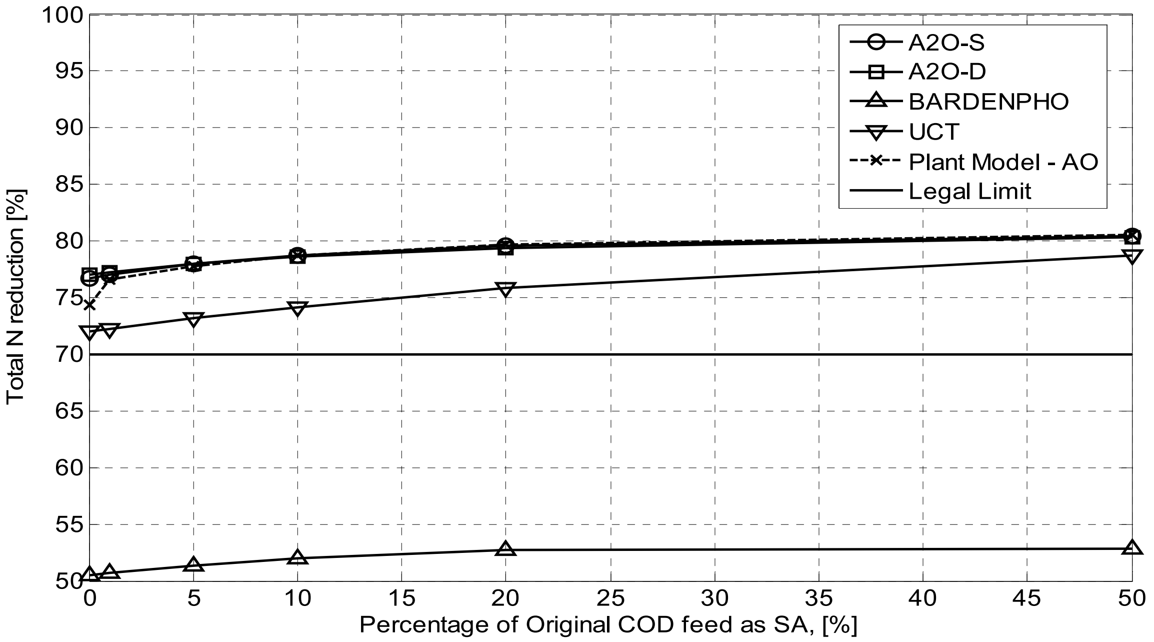


Figure 4.17: Total nitrogen reduction of all the configurations and the calibrated plant model during the experiments of extra carbon source addition.

In the case of total nitrogen removal, the current plant configuration and both A^2/O proposed retrofitting alternatives presented the best results. Nevertheless, an asymptotic behaviour as higher amount of COD as S_A is added occurs. Such effect suggests that the denitrification is not affected by the lack of extra biodegradable COD, but by the own construction way the plant configuration schemes were built, that permits a considerable amount of $N\text{-}NO_3^-$ (ammonium nitrified in the aerobic zone) to be released from the end of the aerobic zone to the secondary settler without a new process step. Such problem would be attenuated increasing the internal recycle flowrate, but pump limits of Manresa and the increase of energy consumption would make a high increase prohibitive. Another possible way to decrease the total N concentration when extra carbon source is added to the wastewater is to maximize nitrification rates somehow. In this case, a work on DO distribution along the aerobic basins and the best DO setpoint determination would be important studies to be performed. The real solution of such problem is presented by the BARDENPHO philosophy, but applied into the Manresa scenario this configuration produces poor results in a general manner.

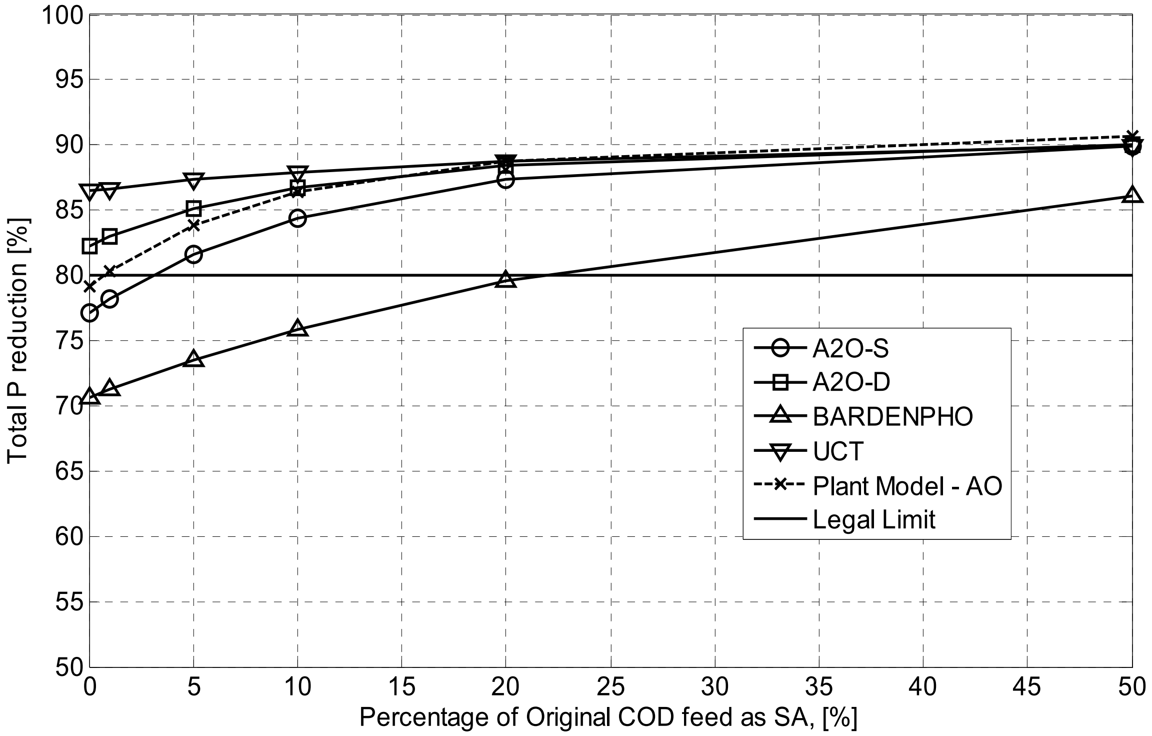


Figure 4.18: Total P reduction of all the configurations and the calibrated plant model during the experiments of addition of extra carbon source.

In the case of total P reduction, the effect of increasing S_A helps the A^2/O-S and BARDENPHO configurations to reach the defined minimum annual reduction determined by the EC directive (80%). The configurations UCT and A^2/O-D are already able to reach the EC directive determination without adding extra carbon source. With some extra carbon source also the current plant configuration is able to reach the minimum P removal. This situation is completely the opposite to the maximum total N concentration admitted by the EC directive. Figure 4.19 shows the results. From the proposed retrofitting alternatives, both the A^2/O configurations and the current plant almost return below to the legal limit but only when 50% percent of the original inlet COD is added as S_A, fact that would increase considerably the operating costs. Again, the present limitations after adding so high amount of extra biodegradable COD lies on the fact that the construction way of the WWTP does not allow to release a null nitrate concentration to the secondary settlers.

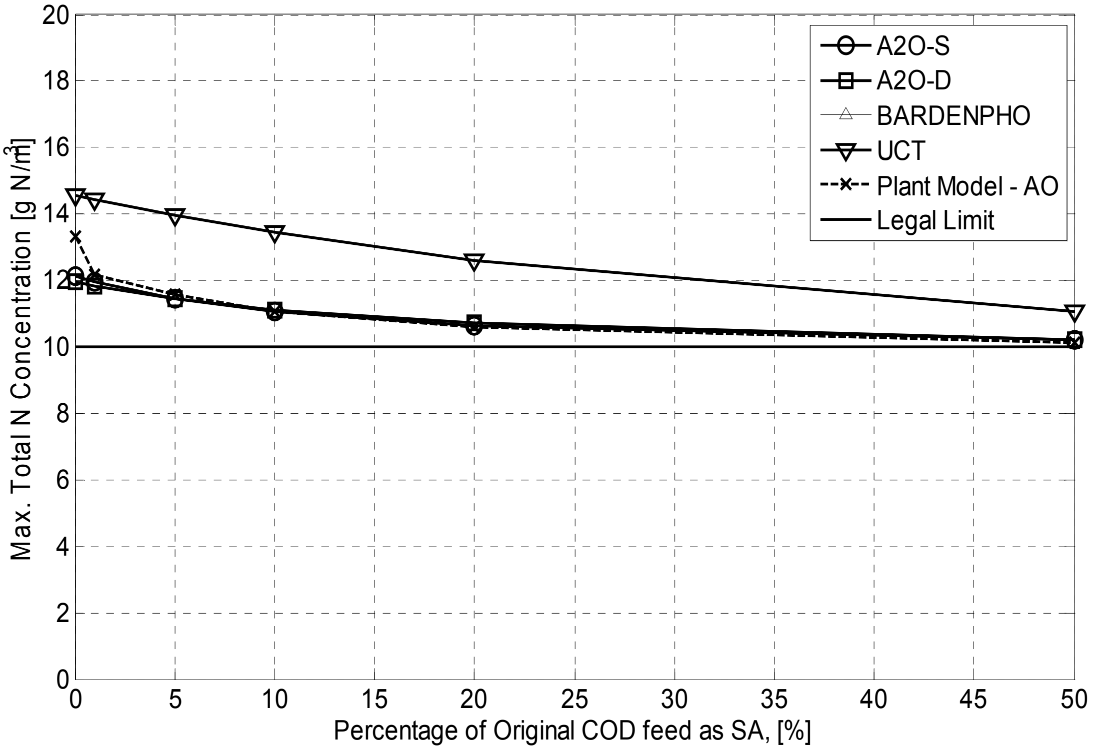


Figure 4.19: Maximum total nitrogen concentration (annual average) for all the configurations and for the calibrated plant model during the experiments of addition of extra carbon source.

Finally, Figure 4.20 presents the behaviour of the maximum total phosphorus concentration in the effluent after the experiments of adding extra carbon source to all the plant configurations and also to the current plant model. No limit was exceeded by any of all the plants. Nevertheless, again, BARDENPHO configuration presented the poorest results.

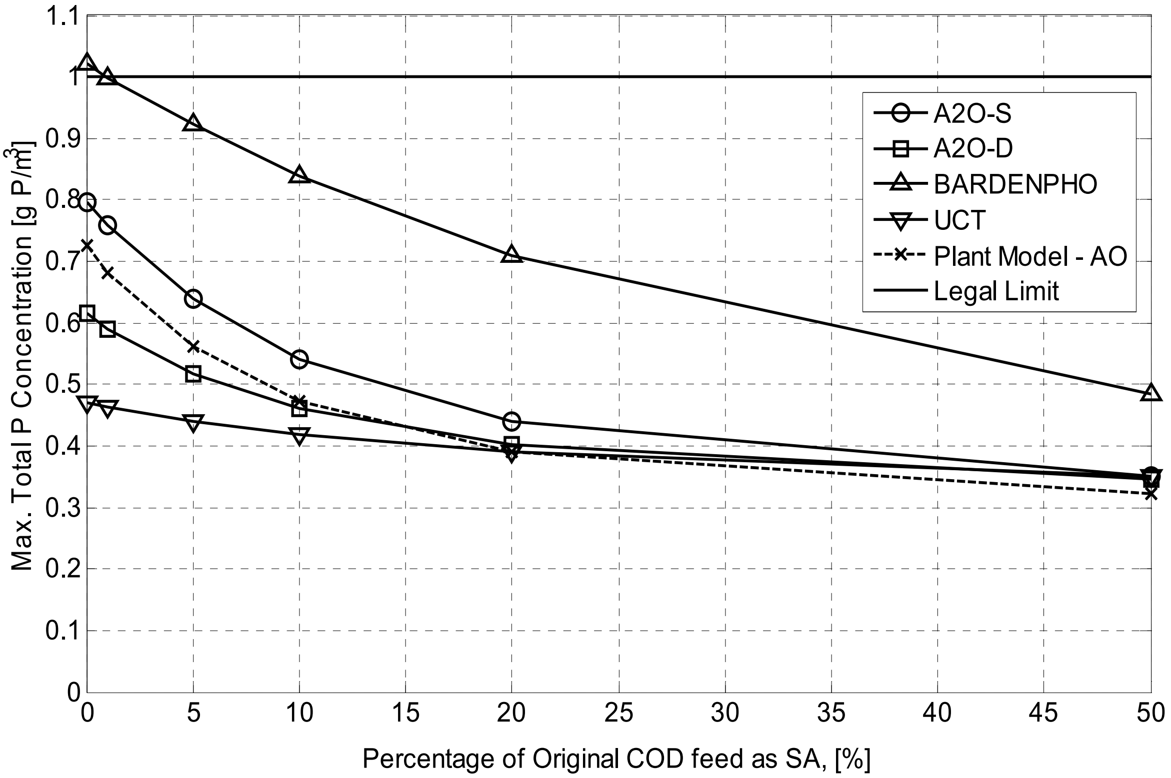


Figure 4.20: Maximum total phosphorus concentration (annual average) for all the configurations and for the calibrated plant model during the experiments of addition of extra carbon source.

The systematic comparison amongst all the proposed alternatives for implementing EBPR includes the cost evaluation, both operating costs and capital/investment costs as stated in chapter 3. Table 4.9 presents the involved costs for aerating, pumping, treating the produced sludge and a measurement of effluent quality. Also, Table 4.9 shows the costs of acquisition of new equipments, of building new pipes and tanks and the cost of the designing itself for the upgrade (US-EPA, 2000). The cost data of the current plant also is presented by Table 9 as a reference.

Table 4.9 data shows a clear advantage of the two A^2/O proposed alternatives considering both kinds of costs. With few modifications which imply less capital costs, A^2/O-D is able to improve the effluent quality compared to the current plant. It is worth noticing that Table 4.9 data are concerned to the WWTP without effluent controllers. The design of a control structure will be discussed afterwards and probably will improve the results of the selected alternative for the retrofitting.

Table 4.9: Capital and Operational costs of all the proposed alternatives.

Operational Costs, [€/d]	**Configurations**				
	A/O (Current)	**A^2/O-S**	**A^2/O-D**	**BARDENPHO**	**UCT**
Aeration Costs, [€/d]	497	500	495	741	502
Pumping Costs, [€/d]	521	521	521	1821	822
Sludge Treatment Costs, [€/d]	312	312	312	309	312
Effluent Quality Costs, [€/d]	1407	1404	1353	9850	1536
Total Operating Costs without Effluent Quality Costs, [€/d]	1330	1333	1328	2871	1636
Total Operating Costs with Effluent Quality Costs, [€/d]	2737	2737	2681	12721	3172
Capital Costs, [€]	**Configurations**				
	A/O (Current)	**A^2/O-S**	**A^2/O-D**	**BARDENPHO**	**UCT**
New Equipments (sensors, pumps)	-	100.000	100.000	100.000	138.564
Air piping	-	-	-	29.940	-
WW Piping	-	42.031	54.640	54.640	120.740
Project and Documentation	-	10.000	10.000	10.000	10.000
Total Capital Cost, [€]	-	152.031	164.640	194.580	269.394

After presenting the results of the main pollutant concentrations, the performance of observing the EC-directive, the performance obtained in the robustness tests and the main operating and capital costs of each proposed alternative to implementing the EBPR, Table 4.10 presents a relative ranking of all the proposed alternatives considering all the criteria pointed out along the retrofitting proposed methodology. The relative ranking is made of five degrees (1 to 5), where the number 1 means the best performance and 5 the worst one amongst the set of proposed alternatives. For each criterion, the results of all the alternatives were divided into 5 linear parts to translate the numerical values of costs, for instance, into the relative 1-to-5 scale. Following this logic, the lowest summation considering all the criteria is the best result amongst all the proposed alternatives.

Table 4.10: Relative performance of all the proposed alternatives considering the criteria evaluated (1= best rating and 5 = worse rating).

Criterion		**Configuration**			
		A^2/O-S	**A^2/O-D**	**BARDENPHO**	**UCT**
Costs	**Capital**	1	2	3	5
	Operating	2	1	5	2
Number of changes from the A/O configuration to the new one.		1	1	3	5
Reduction of	**COD**	3	3	3	3
	BOD5	1	1	1	1
	Total N	4	4	5	5
	Total P	5	4	5	3
Maximum concentration	**COD**	2	2	2	2
	BOD5	1	1	1	1
	Total N	5	5	5	5
	Total P	4	4	5	3
Mass of P in the effluent during the robustness tests	**Pulse Magnitude of 2**	5	3	2	1
	Pulse Magnitude of 5	5	3	2	1
	Pulse Magnitude of 10	5	3	2	1
Mass of N in the effluent during the robustness tests	**Pulse Magnitude of 1.5**	1	1	5	2
	Pulse Magnitude of 2	1	1	5	1
	Pulse Magnitude of 3	1	1	5	1
	Total Rating	47	40	59	42
	Total Number of best results	7	7	2	7

Considering all the exposed results in this section, both A^2/O-D and UCT are the best configurations for implementing the EPBR process in the current WWTP of Manresa. Nevertheless, A^2/O-D configuration is the most prepared plant configuration to keep acceptable nitrogen removal levels without needing strong modifications in the plant like the UCT configuration. Thereby, the next step of the methodology described in Chapter 3, which is the design of a control structure for the retrofitted plant, will be executed for the A^2/O-D configuration.

4.7 Proposed control structure

Although the Manresa WWTP is producing an effluent whose composition respects the legal discharge limits, its current control structure has no capacity to refuse the effect of external disturbances, such as the increasing of inlet flowrate due to population growth (people displacement), rain storms, industrial discharges, and so forth. This limitation arises from the fact that feedback controllers only act if there is an error between the process variable (in this case the influent composition) and the effluent quality setpoint. In the case of Manresa WWTP, it is recommended the adoption of feedforward to better refuse external disturbances of NH_4^+, rising in advance the DO setpoint in the aerobic zone to prepare the plant to faster oxidise the extra inlet ammonium. Nevertheless, to improve the plant capacity of refusing external disturbances, cascade controller of ammonium, for instance, should be also implemented in order to give some intelligence to the DO PID controllers and to avoid linking the main control variable (in this case the NH_4^+, which would belong to the master controller) directly to the final control element (speed of blowers). Avoiding this connection, less noise will be faced by the nutrient control, transferring possible oscillations (process disturbances of blowing and flowing air in pipes) to the DO controller (slave controller) (Oggunaike, 1994).

The implementation of feedforward and cascade controllers would bring improvements in the plant operation. Nevertheless, a centralized controller, like the model predictive controller (MPC), could add more plant stability instead of the decentralized PID controllers since the MPC watch the interrelationships between the manipulated variables (dynamics and gain) and could avoid the internal conflicts amongst all the PID controllers, each one chasing only its own objective but affecting the control variables of the other ones. An example of this conflict would be to try to control both ammonium and nitrate in the effluent at the same time in any A/O plant configuration. On one hand, the ammonium PID controller would raise the DO setpoint to decrease the ammonium concentration and increasing the nitrate. On the other hand, the nitrate controller would increase the internal recycle until the point when the residence time in the aerobic zone could be low to keep nitrifying at good rates. A centralized controller could deal with this problem since it would observe the correlation between the DO setpoint and the internal recycle flowrate setpoint and would become slower the action of the internal recycle flowrate setpoint.

For ammonium control in the effluent, this work proposes a cascade control together with the DO controller. Nitrate control at the end of the anoxic zone, using the internal recycle flowrate would be suitable and the phosphate control at the end of the anaerobic zone is the best proposed choice, using the external recycle flowrate (Machado *et al.*, 2009b). In parallel to the cascade control of the outlet ammonium, a feedforward controller could help to refuse external disturbances of load variations if the inlet ammonium concentration was measured.

An optimizer of the process controller setpoints, taking into account plant operating costs, would be at the highest level in the process control hierarchy (Machado *et al.*, 2009b).

Considering the A^2/O-D configuration, using the calibrated parameters in the A/O model, control relationships were obtained using the three main manipulated variables of this new configuration (DO concentration in the aerobic basins, Q_{RINT} and Q_{RAS}) and three controlled variables in the effluent stream (ammonium, nitrate and phosphate concentrations). The data for developing all the nutrient controllers were obtained performing step tests in the calibrated and validated model. All step tests were performed around a usual operating point of Manresa (DO setpoint of 2.00 mg/L, Q_{RINT} = 75.000 m^3/d and Q_{RAS} = 25.000 m^3/d), with alternating positive and negative values, not to let the non-linear plant characteristics affect the experiment data but higher enough to overcame noise and disturbances in the controlled variables.

Figure 4.21 shows the unit step response of the linear model (model for process control) obtained from the non-linear model of the A^2/O-D configuration.

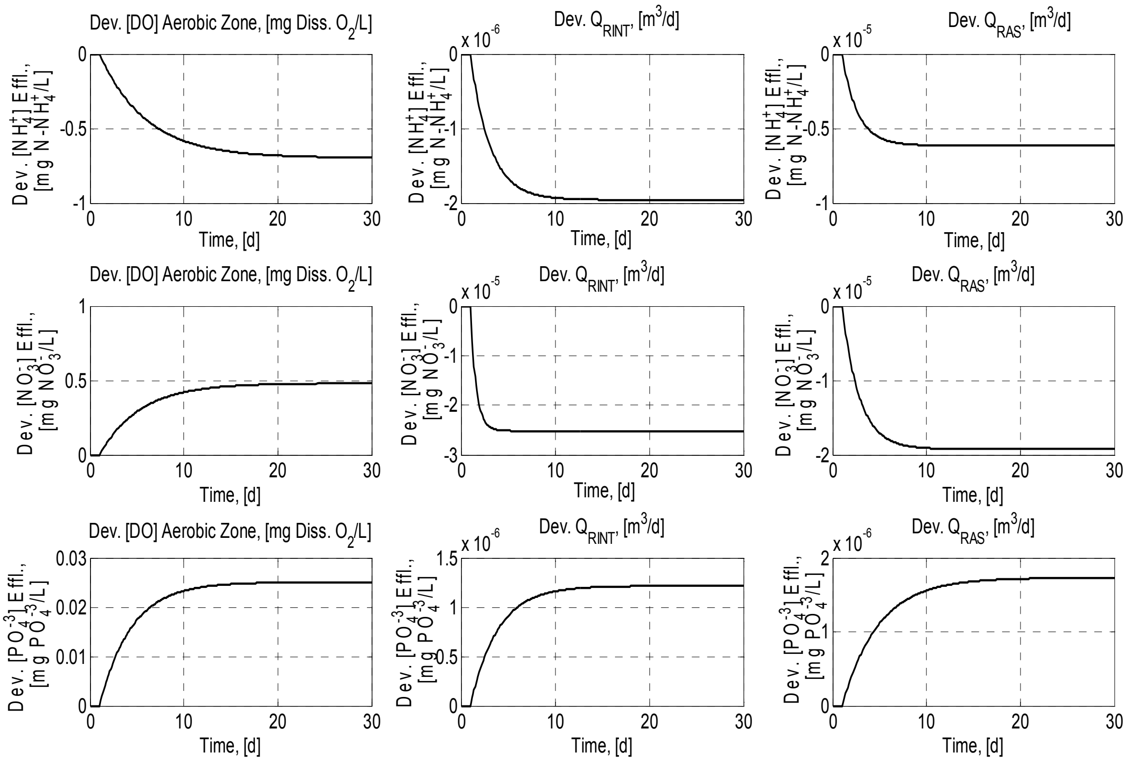


Figure 4.21: Transfer function models for the proposed A^2/O-D configuration (controlled variables observed in the effluent).

Observing the transfer function step response of Figure 4.21, DO concentration produces an expected decrease of the ammonium concentration in a greater extent than in nitrate and phosphate concentrations in the effluent. In fact, DO concentration barely affects the phosphate concentration in the effluent. The internal recycle flowrate affects much more the nitrate in the effluent, knowledge still reported in literature (Machado *et al.*, 2009b). By its turn, the external recycle flowrate is influencing all the three variables at the same time and with considerably magnitude, which will produce undesirable couplings when process controllers are running. The part of the control model which unitary step response is shown by the Figure 4.21 is the full control model that would be studied for decentralized control structure design using the RGA and the minimized condition number, for a centralized control structure with MPC. The identified model also is useful for tuning the PI and PID controller of the decentralized control structures.

4.7.1. Decentralized control structures

The RGA calculations for different combinations amongst possible manipulated and controlled variables provide guidance for choosing the best set for building a decentralized control structure. Four possible sets of control variables were compared for controlling the proposed A^2/O-D plant configuration. Table 4.11 shows the results. All the proposed control structures for the A^2/O-D plant configuration use as manipulated variables the DO setpoint in the aerobic reactors, the internal recycle flowrate setpoint and the external recycle flowrate setpoint.

The first control structure (A^2/O-1) uses the ammonium, nitrate and phosphate concentration measurements at the effluent. The control structure A^2/O-2 switches the nitrate in the effluent by the nitrate at the end of the anoxic zone, which means that one of the control objectives of this control structure will be minimizing the nitrate at the end of the anoxic zone. The control structure A^2/O-3 takes the same control variables of the A^2/O-2 control structure but changing the phosphate at the effluent to the end of the anaerobic zone. This change indicates that the control objective regarding P removal is to maximize the PO_4^{3-} concentration at the end of the anaerobic zone to improve the P-uptaking in the aerobic zone. Finally, the A^2/O-4 control structure takes ammonium and nitrate concentrations at the effluent and the phosphate at the end of the anaerobic zone.

Considering the steady state RGA, controlling all the three pollutant concentrations at the effluent stream is not the best choice since a strong coupling between Q_{RINT} and Q_{RAS} models is observed. The most decentralized control structure would be the third one (A^2/O-3), and the pairing would not be the conventional pairing: Q_{RINT} would be used to control the phosphate concentration in the anaerobic reactor (one anoxic converted reactor) and Q_{RAS} would be used for controlling the nitrate concentration at the end of the anoxic zone. Dynamic RGA shows again the same conclusions of the steady-state RGA. Such result indicates that current value of biomass recycle flowrate (operating point of the process control model) is not the best value for improving denitrification and that nitrate load brought by Q_{RINT} is not being completely denitrified, since changes in Q_{RINT} poorly affect nitrate concentration at the end of the anoxic zone.

Table 4.11: RGA for four different combinations, at two different frequencies (ω = 0 rad/d, ω = 1 rad/d and ω = 2π rad/d) between inputs and outputs for the proposed plant configuration.

ω = 0 rad/d (steady state RGA)				
Control Structure	**Outputs**		**Inputs**	
		DO	**Q_{RINT}**	**Q_{RAS}**
A^2/O-1	NH_4^+ Eff.	**1.5341**	0.2806	-0.8147
	NO_3^- Eff.	-0.2138	**2.8895**	-1.6757
	PO_4^{3-} Eff.	-0.3203	-2.1701	**3.4904**
A^2/O-2	NH_4^+ Eff.	**1.2934**	0.1063	-0.3997
	NO_3^- Anox.	0.2771	**6.1878**	-5.4649
	PO_4^{3-} Eff.	-0.5704	-5.2941	**6.8646**
A^2/O-3	NH_4^+ Eff.	**1.0382**	-0.0309	-0.0073
	NO_3^- Anox.	-0.0848	0.1824	**0.9024**
	PO_4^{3-} Anaer.	0.0465	**0.8486**	0.1049
A^2/O-4	NH_4^+ Eff.	**0.7857**	-0.0133	0.2276
	NO_3^- Eff.	0.1531	0.1993	**0.6476**
	PO_4^{3-} Anaer.	0.0612	**0.8141**	0.1248
ω = 1 rad/d (dynamic RGA)				
Control Structure	**Outputs**		**Inputs**	
		DO	**Q_{RINT}**	**Q_{RAS}**
A^2/O-1	NH_4^+ Eff.	**2.5490**	0.2427	-1.7917
	NO_3^- Eff.	-0.2697	**2.3655**	-1.0959
	PO_4^{3-} Eff.	-1.2793	-1.6082	**3.8875**
A^2/O-2	NH_4^+ Eff.	-0.6982	-0.7603	2.4585
	NO_3^- Anox.	-0.3488	-5.9548	7.3036
	PO_4^{3-} Eff.	**2.0470**	**7.7151**	**-8.7621**
A^2/O-3	NH_4^+ Eff.	**0.9805**	-0.0284	0.0480
	NO_3^- Anox.	-0.0556	0.1080	**0.9475**
	PO_4^{3-} Anaer.	0.0751	**0.9204**	0.0045
A^2/O-4	NH_4^+ Eff.	**0.6814**	-0.0194	0.3381
	NO_3^- Eff.	0.1863	0.1594	**0.6544**
	PO_4^{3-} Anaer.	0.1324	**0.8601**	0.0076
ω = 2π rad/d (dynamic RGA)				
Control Structure	**Outputs**		**Inputs**	
		DO	**Q_{RINT}**	**Q_{RAS}**
A^2/O-1	NH_4^+ Eff.	**2.5763**	0.1558	-1.7321
	NO_3^- Eff.	-0.1702	**1.8849**	-0.7147
	PO_4^{3-} Eff.	-1.4061	-1.0407	**3.4468**
A^2/O-2	NH_4^+ Eff.	**4.8771**	0.5608	-4.4379
	NO_3^- Anox.	0.1516	**5.2590**	-4.4105
	PO_4^{3-} Eff.	-4.0287	-4.8198	**9.8485**
A^2/O-3	NH_4^+ Eff.	**0.9013**	-0.0263	0.1250
	NO_3^- Anox.	-0.0406	0.1716	**0.8690**
	PO_4^{3-} Anaer.	0.1393	**0.8547**	0.0060
A^2/O-4	NH_4^+ Eff.	**0.5894**	-0.0169	0.4274
	NO_3^- Eff.	0.1649	0.2722	**0.5629**
	PO_4^{3-} Anaer.	0.2456	**0.7446**	0.0097

Together with the RGA, the minimized condition number of all the four possible sets of manipulated and controlled variables of the A^2/O alternative was evaluated for a wide range of frequencies. Figure 4.22 shows the results.

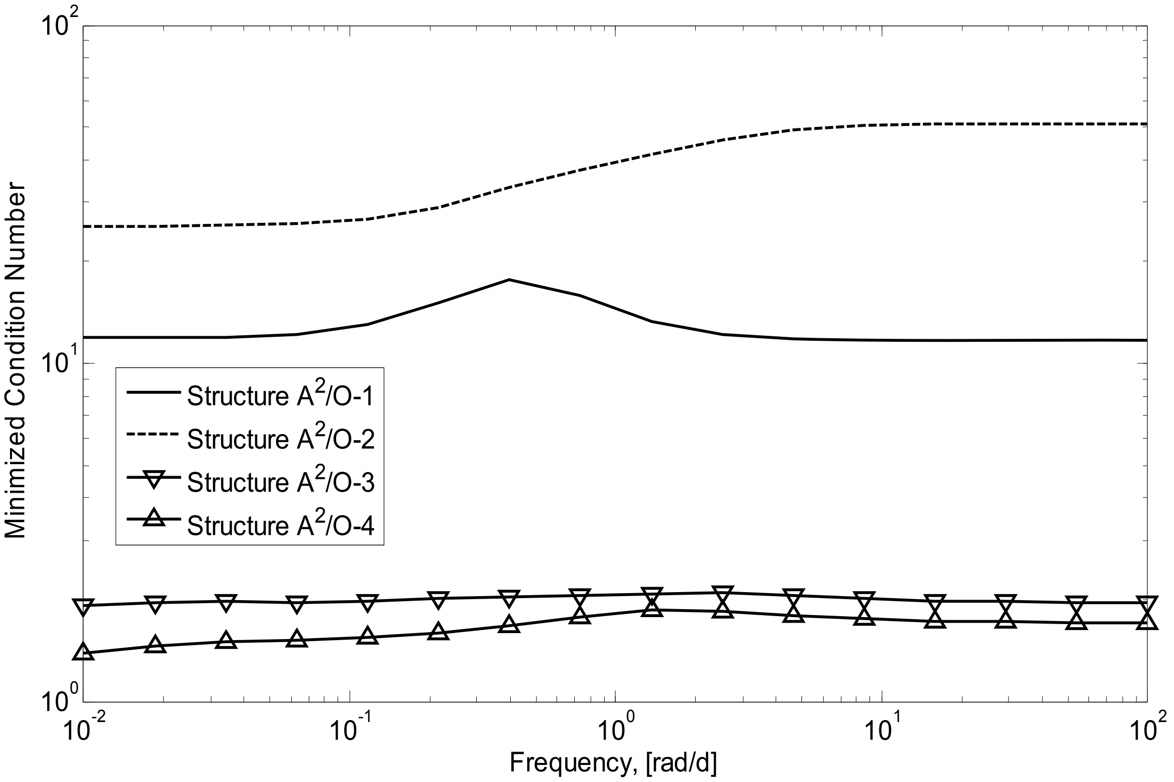


Figure 4.22: Minimized condition number for all the four set of manipulated and controlled variables for the A^2/O-D alternative along a wide range of frequencies.

Figure 4.22 brings interesting information: only two of the four set of variables are not strongly coupled, as they have a lower minimized condition number (close to the unity). They are the structures A^2/O-3 and A^2/O-4. Both control structures do not have the phosphate concentration at the effluent as a control variable, which is strongly correlated to the nitrate concentration both in the effluent and the anoxic zone, according to the identified model. This competition between the phosphate in the effluent and nitrate could be arisen from the fact that external recycling flowrate brings nitrate to the anaerobic zone and affects phosphate removal process in some extent.

The presented minimized condition number of Figure 4.22 also infers that the performance of the control structures A^2/O-3 and A^2/O-4 are less sensitive to the speed of the designed controllers when all the control loops are closed, since their minimized condition number is close to one along all the observed range of frequencies. On the other hand, if the control structure A^2/O-2 was used instead of A^2/O-3 or A^2/O-4, much care should be taken not to tune the process controllers for fast movements. With fast movements, the degree of correlation under the different variables of the control structure would be maximized and the operating costs would certainly increase.

Although the most recommended control structure for the A^2/O-D configuration considering RGA results is the A^2/O-3, the robustness of the most straightforward relationship amongst the manipulated variables and controlled variables (structure A^2/O-1) was tested also. Such control structure is the natural choice for implementing a control structure in full-scale WWTP plants, since the controlled variables are the same commonly monitored to respect the EC directive limits. Therefore, performance tests were also performed with the control structure A^2/O-1, especially the pulse tests of total phosphate and ammonium in the influent, using the same patterns explained in section 4.6.

Process controllers like DO, ammonium, nitrate and phosphorus controllers were designed using the identified model of Figure 4.21 and methods commonly found in control literature (Rivera *et al*., 1986; Ogunnaike and Ray, 1994; Skogestad, 2003). Table 4.12 presents the operating costs of both control structures for the A^2/O-D plant configuration and compare them to the A^2/O-D with only DO control and the current plant A/O (open loop).

As a function of lower non-diagonal interferences in the control matrix, A^2/O-3 control structure is able to maximize the benefits of A^2/O-D plant configuration compared to the A^2/O-1 control structure and the open loop A^2/O-D. Also, A^2/O-3 control structure would reduce around 3.1% the operating costs of the A/O plant configuration (current plant configuration).

Figure 4.23 shows the mass of phosphorus in the effluent during the evaluation period of the A^2/O-D configuration during the P-pulse experiment. Figure 4.23 compares the results of the open loop structure (A/O), he A^2/O-D with only DO controllers and, finally, when all the controllers (DO controllers and the nutrient controllers of the A^2/O-1 and A^2/O-3 control structures) were activated.

The results of Figure 4.23 clearly indicate that a reasonable performance could be obtained when all the controllers are activated in comparison to the only A^2/O-D with only DO control and the current plant configuration (open loop). The attained performance of nutrient controllers is almost 15% better than the capacity of refusing phosphate external disturbances than the proposed A^2/O-D configuration without nutrient controllers. In the case of total nitrogen, the use of process controllers could not increase the A^2/O-D capacity of refusing external ammonium disturbances. Figure 4.24 shows the results of the ammonium pulse experiment for all the tested control model of the A^2/O-D proposed configuration (open loop, only DO, A^2/O-1 and A^2/O-3 control structures). No relevant advantages were observed amongst the tested control modes of the A^2/O-D plant configuration concerning disturbance rejection of inlet N-NH_4^+.

Table 4.12: Operating costs of A^2/O-D configuration (only with DO control) with the designed control structures A^2/O-1 and A^2/O-3. Also, the operating costs of the A/O current plant configuration (open loop) are rewritten for references.

Operational Costs, [€/d]	**Configurations / Control Structures**			
	A/O, current plant (Open Loop)	**A^2/O-D (Only DO control, DOSP 2.00 mg/L)**	**A^2/O-D, closed loop with control structure A^2/O-1. Setpoints:** **NH_4^+ Effl. 1.50 mg/L** **NO_3^- Effl. 6.50 mg/L** **PO_4^{3-} Effl. 0.50 mg/L**	**A^2/O-D, closed loop with control structure A^2/O-3. Setpoints:** **NH_4^+ Effl. 1.50 mg/L** **NO_3^- Anox. 0.50 mg/L** **PO_4^{3-} Anaer. 1.80 mg/L**
Aeration Costs, [€/d]	497	495	479	495
Pumping Costs, [€/d]	521	521	444	277
Sludge Treatment Costs, [€/d]	312	312	312	307
Effluent Quality Costs, [€/d]	1407	1353	1430	1571
Total Operating Costs without Effluent Quality Costs, [€/d]	1330	1328	1235	1079
Total Operating Costs with Effluent Quality Costs, [€/d]	2737	2681	2665	2650

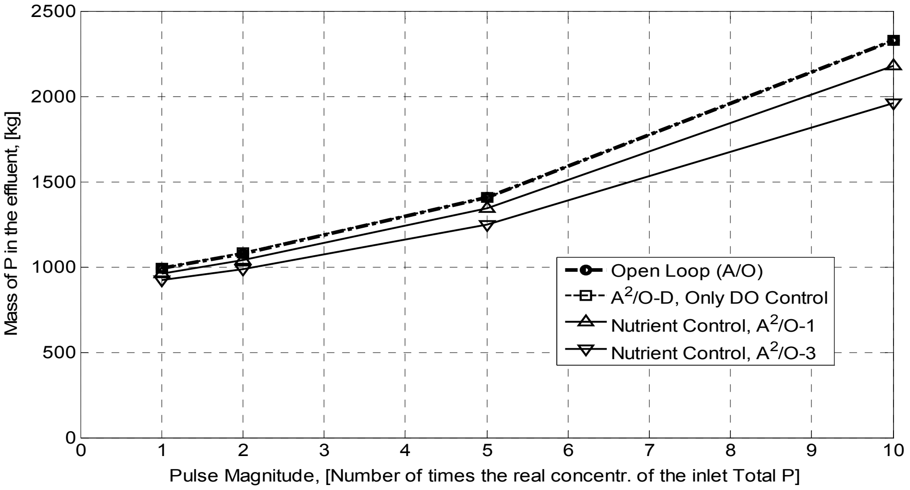


Figure 4.23: Mass of P released in the effluent stream during the pulse-experiment of total P in the influent for the current A/O plant (Open Loop), the A^2/O-D with only DO controllers and the A^2/O-D with nutrient controllers activated (both tested control structures, A^2/O-1 and A^2/O-3).

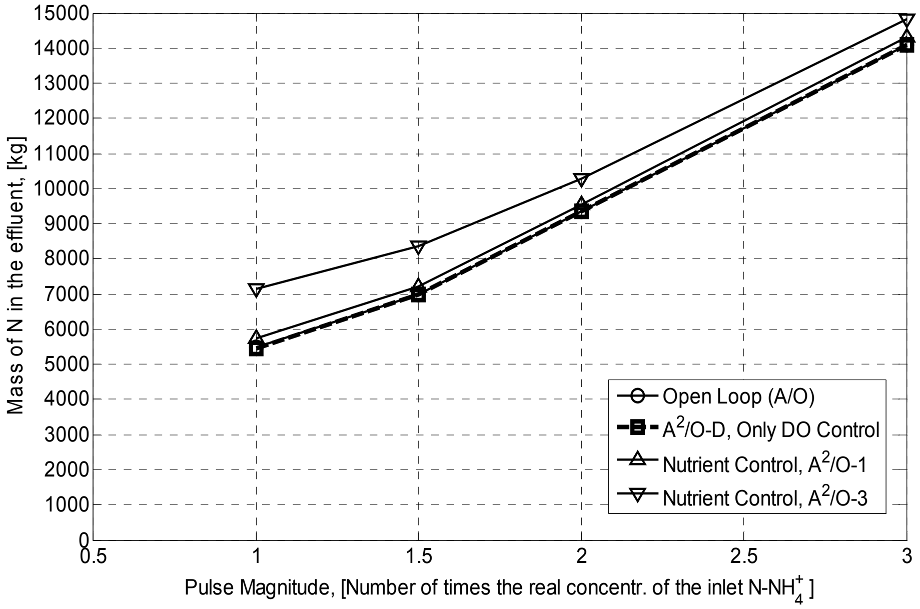


Figure 4.24: Mass of N released in the effluent stream during the pulse-experiment of N-NH_4^+ in the influent for the current A/O plant (Open Loop), the A^2/O-D with only DO controllers and the A^2/O-D with nutrient controllers activated (both tested control structures, A^2/O-1 and A^2/O-3).

4.7.2. Decentralized control structures with setpoint optimization

A simple optimization problem is formulated where the total operating cost is the objective function and the setpoints of the controlled variables are the decision variables, keeping the current PI and PID tuning (Machado et al., 2009b). Such problem mitigates the influence of limitations of the tuning rules for PI and PID (they do not considers sensor noises) and of the considerable degree of uncertainty of the black-box models when the available plant data is far from a local operation point (which is the case in almost all WWTP)..

Minimize OBJF
SPy1, SPy2, SPy3 Eq. 4.5

where OBJF is the average of the daily operating costs along all the period evaluated (calibration data with np points).

$$OBJF = \frac{1}{np} \cdot \sum_{i=1}^{i=np} OC_i \left[€ \ d^{-1} \right] \qquad \text{Eq. 4.6}$$

Table 4.13 shows the summary of costs of the setpoint optimization for the control structures A^2/O-1 and A^2/O-3.

Table 4.13: Results of the setpoint optimization for the control structures A^2/O-1 and A^2/O-3.

Operational Costs, [€/d]	Control Structures	
	A^2/O-1 with setpoint optimization **Setpoints:** **NH_4^+ Effl. 1.67 mg/L** **NO_3^- Effl. 8.94 mg/L** **PO_4^{3-} Effl. 0.50 mg/L**	**A^2/O-3 with setpoint optimization** **Setpoints:** **NH_4^+ Effl. 1.80 mg/L** **NO_3^- Anox. 0.56 mg/L** **PO_4^{3-} Anaer. 1.58 mg/L**
Aeration Costs, [€/d]	473	469
Pumping Costs, [€/d]	363	344
Sludge Treatment Costs, [€/d]	312	319
Effluent Quality Costs, [€/d]	1511	1502
Total Operating Costs without Effluent Quality Costs, [€/d]	1148	1132
Total Operating Costs with Effluent Quality Costs, [€/d]	2659	2634

The setpoint optimization step brings better results of total cost for both control structures compared to the same structures with the original setpoints. Nevertheless, control structure A^2/O-3 still continues to present a slightly better result as a consequence of the lower degree of interaction amongst its variables than the variables of the control structure A^2/O-1.

4.7.3. Centralized control structures

A MPC was implemented and tested using the variables of the A^2/O-1 and A^2/O-3 control structure, generating the control structures A^2/O-1-MPC and A^2/O-3-MPC. Table 4.14 shows the summary of costs of applying the control structures A^2/O-1-MPC and A^2/O-3-MPC.

Table 4.14: Results of the MPC using variables of the A^2/O-1 and A^2/O-3 structures.

Operational Costs, [€/d]	**Control Structures**	
	A^2/O-1-MPC	**A^2/O-3-MPC**
	Setpoints: **NH_4^+ Effl. 1.50 mg/L** **NO_3^- Effl. 6.50 mg/L** **PO_4^{3-} Effl. 0.50 mg/L**	**Setpoints:** **NH_4^+ Effl. 1.50 mg/L** **NO_3^- Anox. 0.50 mg/L** **PO_4^{3-} Anaer. 1.80 mg/L**
Aeration Costs, [€/d]	480	481
Pumping Costs, [€/d]	496	473
Sludge Treatment Costs, [€/d]	312	323
Effluent Quality Costs, [€/d]	1354	1353
Total Operating Costs without Effluent Quality Costs, [€/d]	1288	1277
Total Operating Costs with Effluent Quality Costs, [€/d]	2642	2630

The centralized control structures A^2/O-1-MPC and A^2/O-3-MPC brought better results than the decentralized ones. They provided considerably lower effluent quality costs but also higher total operating costs without effluent quality, being the final overall costs slightly lower than the decentralized control structures.

4.8 Final product of the retrofitting methodology for EBPR applied to the Manresa WWTP

The developed methodology for retrofitting existent plants to perform the EBPR applied to the Manresa WWTP, which its secondary wastewater treatment operates as an A/O configuration, led to an A^2/O configuration using two of the six available anoxic reactors as anaerobic reactors. Such configuration produces an effluent stream with a total P concentration about 69% lower than the total P effluent concentration of the current configuration which represents a total reduction of 82.28% throughout the WWTP. The operating costs without considering the cost of the effluent quality (current Catalonia model) would decrease around 3.9% (A^2/O-3-MPC) compared to the current plant configuration. In case of prizing the effluent quality, the benefits of the retrofit solution would be around also 3.9% (A^2/O-3-MPC, less operating costs) if compared to the A/O Manresa WWTP of nowadays.

The control structure A^2/O-1 is the most conventional control structure of an A^2/O plant configuration where the ammonium, nitrate and phosphate at the effluent are controlled, respectively by the dissolved oxygen setpoint in the aerobic basins, the internal and the external flowrate recycles. Nevertheless, such control structure, in terms of robustness, loses performance to the control structure A^2/O-3 since the total P at the effluent in case of strong external P load disturbances is lower than the control structure A^2/O-3, although the latter control structure presented worse results in terms of total N after strong disturbances of NH_4^+ at the influent. The lower costs of control structure A^2/O-3 are observed again when such control structure is running with the optimized setpoints compared to the control structure A^2/O-1. Finally, the model predictive controller using the same variables of the control structure A^2/O-3 (A^2/O-3-MPC) presented the best performance of total operating costs and effluent quality costs amongst all the tested control structures. Such result was expected since the full model is used by the centralized controller avoiding extreme correlation effects of the manipulated variables. Such control structure is the most recommend control structure of all the tested control structures.

The proposed solution for upgrading the WWTP of Manresa would cost about € 165.000,00 which is, probably, much less than the fines for not producing an effluent with the required quality defined by the government. Such investment cost would be paid in about 4.5 years with the reduction of the operating costs provided by the retrofitting solution.

Chapter 5: Conclusions

The developed work pointed out a strong necessity of retrofitting WWTP in Catalonia and probably in other countries in order to implement EBPR and, the most fundamental, to systematically remove the amounts of phosphorus determined by the legal limits. Following this necessity, this work presented a retrofitting methodology for upgrading an existent WWTP to remove simultaneously COD, N and P, with the minimum number of changes as possible. The proposed methodology strongly states for using the maximum number of available plant data of the existent WWTP in order to calibrate a process model where also kinetic and stoichiometric parameters of the biomasses involved in the wastewater treatment will be determined. The model calibration step is a novel methodology which uses the lowest possible number of calibrating parameters to achieve the best model response fitting the real plant data. The calibration procedure is based on the usage of a relationship between the D and modE criteria of the FIM calculation.

As the current plant is an A/O WWTP, no parameters related to the biological P-removal appear in the 10 most impacting seeds. On the other hand, in all the tested subsets appears K_{PRE} or K_{RED}, parameters linked to the P-chemical precipitation. Y_H and b_H are present in all the subsets, with high values of parameter confidence interval, which indicate less reliable calibrating values. Parameter $\eta_{NO3,D}$ is the parameter that provides more information about the plant behaviour (lowest CCF and VCF when this parameter is inside the calibration set), despite its lower value (0.0296) and more than 50% of confidence interval (default ASM2d value is 0.80). Such value indicates that a poor denitrification process is occurring in the plant, caused by, probably two factors: a lack of easily biodegradable carbon source and some amount of DO transported from the aerobic zone to the anoxic one.

Applying the same calibration procedure but using the influent composition factors as parameters (multipliers of the original influent composition, which characterization was performed in laboratory experiments), keeping the model ASM2d with its original parameters, it was possible to conclude that:

- Different optimized factors that multiply the influent vectors for each variable of the influent were found. For example, a value of 1.414 of f_{SNH4} of the S_I seed means that the ammonium vector of original plant data increased 41.4% in order to minimize the cost function.
- From the 10 tested seeds, only 4 different calibrating subsets were created, which means that the influent variables participate in the same processes with almost the same importance. It is not possible to affirm that one part of the variables is more important that other one of this group.
- Comparing the results of f_{XTSS} and f_{XS} seeds it is possible to observe that the result of f_{XTSS} seed explains better the outputs than the result of f_{XS} seed, although the inclusion of S_F in the former subset increases correlation among parameters. In addition, the calibration methodology did not allow the simultaneous presence of X_S and X_{TSS} in any calibration subset, probably due to the high correlation between these variables.
- Nitrate data are correlated to the S_F data, since in both created subsets where f_{SNO3} appears (seeds f_{SNO3} and f_{SI}), high parameter confidence interval values are reported. The existence of such a correlation is evident in the subset created by the f_{SNO3} seed, since this subset is made up only by f_{SNO3} and f_{SF}.

Such procedure applied to the influent concentration is a way to evaluate the uncertainty of the influent characterization. The same procedure also was applied to the operational variables (manipulated variables in the control structures), where it could be concluded that:

- In any control structure, the purge flowrate was employed to maintain the biomasses in the basins and because there is a strong correlation between the biomass recycle flowrate and the own purge flowrate, fact that could bring some extra conflicts to the control system and probably would increase the operating costs.

- The dissolved oxygen in the aerobic basins is the most powerful operating variable since it was decided not to include the purge flowrate to the control structures.

The calibrated model is the base for introducing P removal process, preserving the biomasses characteristics of the existent plant. A set of possible plant configurations is created based on the specific characteristics, limitations of the existent plant (and the place it is installed) and design premises. All the plant configuration candidates of the retrofit have their robustness tested as they are submitted to abrupt changes in P and N loads. The most cost-effective and naturally stable solution has a new control structure systematically designed for increasing the control performance.

The proposed methodology was tested in a full scale WWTP plant (Manresa WWTP, Catalonia). At the same time the proposed retrofitting methodology tests different possible alternatives for EBPR (A^2/O-S, A^2/O-D, BARDENPHO and UCT) in an existent plant with a fair and systematic set of rules for comparisons, control structures are developed and recommended to minimize operating costs and to reject load disturbances. The main result indicates that for the current A/O plant, the best alternative for improving the EBPR processes considering criteria of prizing the effluent quality, of lowering the operational costs and investment costs should be an A^2/O configuration with two anaerobic reactors which are two of the six anoxic reactors already existent in the current plant (A^2/O-D). The proposed alternative could be almost 15% more stable than the existent plant in the case of presence of external P disturbances in the influent. Such configuration produces an effluent stream with a total P concentration about 69% lower than the total P effluent concentration of the current configuration which represents a total reduction of 82.28% throughout the WWTP (which represents a mass of 4.5 tons per year not released to the Cardener River).

The RGA and the minimized condition number were applied to four sets of variables of the A^2/O-D alternative, which were classified as “decentralized control structures”. The most diagonal-dominant RGA was obtained to the control structure A^2/O-3. Only two of the four set of variables are not strongly coupled, as they have a lower minimized condition number (close to the unity). They are the structures A^2/O-3 and A^2/O-4. Both control structures do not have the phosphate concentration at the effluent as a control variable which is strongly correlated, according to the identified model, to the nitrate concentration, both in the effluent and the anoxic zone. This competition between the phosphate in the effluent and nitrate could be arisen from the fact that external recycling flowrate is bringing nitrate to the anaerobic zone and affecting the phosphate removal process in some extent.

The presented minimized condition number also infers that the performance of the control structures A^2/O-3 and A^2/O-4 are less sensitive to the speed of the designed controllers when all the control loops are closed, since their minimized condition number is close to one along all the observed range of frequencies. On the other hand, if the control structure A^2/O-2 were used instead of the A^2/O-3 and A^2/O-4, much care would be taken not to tune the process controllers for fast movements. With fast movements, the degree of correlation under the different variables of the control structure would be maximized and the operating costs would certainly increase.

Better than the control structures A^2/O-1, A^2/O-2, A^2/O-3 and A^2/O-4 is the control structure A^2/O-3 with optimized setpoints, balancing the uncertainties of the model identification procedure, sensors and processes noises and limitations in the tuning rules of decentralized controllers.

The centralized control structures presented the best results even though they are more complex to be implemented. The best control structure for the A^2/O plant configuration was the A^2/O-3-MPC since the ability of the MPC controller to avoid undesired correlation amongst the manipulated variables decreases conflicting control actions which could increase the operating costs and not allow improving the effluent quality.

This is not the end.
It is not even the beginning of the end.
But it is the end of the beginning.
Winston Churchill

Chapter 6: Future Works

The proposed retrofitting methodology allows to better understanding the current plant since it states for a model calibration using historical plant data and at the same time indicates the most cost-effective solution for implementing the EBPR processes in the existent WWTP. Besides, a more stable control structure is designed for the new plant, which guaranteed an increase of control performance compared to the current WWTP.

One of the advantages of the proposed retrofitting methodology is that the generated plant model is obtained with the lower number of calibrating parameters, avoiding high parameters variability. Other important point of the proposed methodology is the fact that all the simulations use the current plant influent files, using real data and making the proposed solution feasible.

Despite the benefits of using the proposed methodology, some important issues should be evaluated in future works:

- To check if the RDE criterion, which was used to choose the parameter subset for model calibration, is totally independent of the size of the system, i.e., if it is the most fair criterion to compare subsets of different sizes

- Plant reactor hydraulics models should be improved to take into account the spatial gradients of the pollutants in the basins, making the simulations more reliable.

- Air distribution models in the aerobic zones could be included in the retrofitting analysis.

- Other control structures and type of controllers could be tested instead of the standard PID controllers, so-well accepted by the industrial personnel.

- The evaluation of the historical population growth to better resize the existent plant for future flowrate and increments of pollutant loads.

- To include microbiological risks of foam and biomasses malfunction as a function of the operating conditions (let the microbiological risk be one more variable of the cost function).

Appendix

A.1. ASM2d Model

The ASM2d is an acronym for Activated Sludge Model nº2 with denitrifying PAO. It appeared in literature in 1999 and reasonable describes COD, N and P processes removal (Henze *et al.*, 1999). The model is compound by 19 state variables and 21 processes. The list of variables is presented in Table A1. The values of the ASM2d parameters and the stoichiometric coefficients used were taken/calculated from Henze *et al.* (1999) and Gernaey and Jørgensen (2004) and are presented in Table A2 and A3, respectively.

Table A.1: ASM2d state variables.

Symbol	Description	Symbol	Description
S_{O2}	Dissolved oxygen concentration, [g O_2 m^{-3}]	X_S	Slowly biodegradable substrates, [g COD m^{-3}]
S_F	Readily biodegradable soluble organic substrate, [g COD m^{-3}]	X_H	Heterotrophic organisms, [g COD m^{-3}]
S_A	Fermentation products VFA, [g COD m^{-3}]	X_{PAO}	Phosphorus accumulating organisms, [g COD m^{-3}]
S_I	Inert soluble organic material,[g COD m^{-3}]	X_{PP}	Polyphosphate, [g P m^{-3}]
S_{NH4}	Ammonium plus ammonia nitrogen, [g N m^{-3}]	X_{PHA}	Cell internal storage product of PAO, [g COD m^{-3}]
S_{N2}	Gaseous nitrogen, [g N m^{-3}]	X_{AUT}	Nitrifying organisms, [g COD m^{-3}]
S_{NO3}	Nitrate plus nitrite nitrogen, [g N m^{-3}]	X_{TSS}	Total suspended solids, TSS, [g TSS m^{-3}]
S_{PO4}	Inorganic soluble phosphorus, [g P m^{-3}]	X_{MeOH}	Metal-hydroxides, involved with chemical removal of phosphorus, [g TSS m^{-3}]
S_{ALK}	Alkalinity of the wastewater, [mol HCO_3^- m^{-3}]	X_{MeP}	Metal phosphate, [g TSS m^{-3}]
X_I	Inert particulate organic material, [g COD m^{-3}]		

Process kinetics [$ML^{-3}T^{-1}$].

Hydrolysis processes

Aerobic hydrolysis (process 1)

$$proc_1 = K_h \frac{S_{O2}}{K_{O2}+S_{O2}} \frac{X_S/X_H}{K_X+X_S/X_H} X_H$$

Anoxic hydrolysis (process 2)

$$proc_2 = K_h \eta_{NO3} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{S_{NO3}}{K_{NO3}+S_{NO3}} \frac{X_S/X_H}{K_X+X_S/X_H} X_H$$

Anaerobic hydrolysis (process 3)

$$proc_3 = K_h \eta_{fe} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{S_{NO3}}{K_{NO3}+S_{NO3}} \frac{X_S/X_H}{K_X+X_S/X_H} X_H$$

Heterotrophic organisms: X_H

Growth on fermentable substrates, S_F (process 4)

$$proc_4 = \mu_H \frac{S_{O2}}{K_{O2}+S_{O2}} \frac{S_F}{K_F+S_F} \frac{S_F}{S_F+S_A} \frac{S_{NH4}}{K_{NH4}+S_{NH4}} \frac{S_{PO4}}{K_P+S_{PO4}} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} X_H$$

Growth on fermentable substrates, S_A (process 5)

$$proc_5 = \mu_H \frac{S_{O2}}{K_{O2}+S_{O2}} \frac{S_A}{K_A+S_A} \frac{S_A}{S_F+S_A} \frac{S_{NH4}}{K_{NH4}+S_{NH4}} \frac{S_{PO4}}{K_P+S_{PO4}} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} X_H$$

Denitrification with fermentable substrates, S_F (process 6)

$$proc_6 = \mu_H \eta_{NO3} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{S_{NO3}}{K_{NO3}+S_{NO3}} \frac{S_F}{K_F+S_F} \frac{S_F}{S_F+S_A} \frac{S_{NH4}}{K_{NH4}+S_{NH4}} \frac{S_{PO4}}{K_P+S_{PO4}} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} X_H$$

Denitrification with fermentable substrates, S_A (process 7)

$$proc_7 = \mu_H \eta_{NO3} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{S_{NO3}}{K_{NO3}+S_{NO3}} \frac{S_A}{K_A+S_A} \frac{S_A}{S_F+S_A} \frac{S_{NH4}}{K_{NH4}+S_{NH4}} \frac{S_{PO4}}{K_P+S_{PO4}} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} X_H$$

Fermentation (process 8)

$$proc_8 = q_{fe} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{K_{NO3}}{K_{NO3}+S_{NO3}} \frac{S_F}{K_F+S_F} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} X_H$$

Lysis (Decay) (Process 9)

Original equation:

$$proc_9 = b_H X_H$$

Modified by Gernaey and Jørgensen (2004) and used in this work:

$$proc_9 = b_H \left[\frac{S_{O2}}{K_{O2}+S_{O2}} + \eta_{H,NO3,end} \frac{K_{O2}}{K_{O2}+S_{O2}} \frac{S_{NO3}}{K_{NO3}+S_{NO3}} \right] X_H$$

Phosphorus accumulating organisms (PAO): X_{PAO}

Storage of X_{PHA} (Process 10)

$$proc_{10} = q_{PHA} \frac{S_A}{K_A+S_A} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \frac{X_{PP}/X_{PAO}}{K_{PP}+X_{PP}/X_{PAO}} X_{PAO}$$

Aerobic storage of X_{PP} (Process 11)

$$proc_{11} = q_{PP} \frac{S_{O2}}{K_{O2}+S_{O2}} \frac{S_{PO4}}{K_{PS}+S_{PO4}} \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}} \frac{K_{MAX}-X_{PP}/X_{PAO}}{K_{IPP}+K_{PHA}-X_{PP}/X_{PAO}} X_{PAO}$$

Anoxic storage of X_{PP} (Process 12)

$$proc_{12} = q_{PP}\,\eta_{NO3}\,\frac{K_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{PO4}}{K_{PS}+S_{PO4}}\,\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\,\frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}}\,\frac{K_{MAX}-X_{PP}/X_{PAO}}{K_{IPP}+K_{PHA}-X_{PP}/X_{PAO}}\,X_{PAO}$$

Aerobic growth on X_{PHA} (Process 13)

$$proc_{13} = \mu_{PAO}\,\frac{S_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{NH4}}{K_{NH4}+S_{NH4}}\,\frac{S_{PO4}}{K_{PS}+S_{PO4}}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\,\frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}}\,X_{PAO}$$

Anoxic growth on X_{PHA} (Process 14)

$$proc_{14} = \mu_{PAO}\,\eta_{NO3}\,\frac{K_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{NH4}}{K_{NH4}+S_{NH4}}\,\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\,\frac{S_{PO4}}{K_{PS}+S_{PO4}}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\,\frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}}\,X_{PAO}$$

Lysis of X_{PAO} (Process 15)

Original equation:

$$proc_{15} = b_{PAO}\,X_{PAO}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}$$

Modified by Gernaey and Jørgensen (2004) and used in this work:

$$proc_{15} = b_{PAO}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\left[\frac{S_{O2}}{K_{O2}+S_{O2}}+\eta_{P,NO3,end}\,\frac{K_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\right]X_{PAO}$$

Lysis of X_{PP} (Process 16)

Original equation:

$$proc_{16} = b_{PP}\,X_{PP}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}$$

Modified by Gernaey and Jørgensen (2004) and used in this work:

$$proc_{16} = b_{PP}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\left[\frac{S_{O2}}{K_{O2}+S_{O2}}+\eta_{PP,NO3,end}\,\frac{K_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\right]X_{PP}$$

Lysis of X_{PHA} (Process 17)

Original equation:

$$proc_{17} = b_{PHA}\,X_{PHA}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}$$

Modified by Gernaey and Jørgensen (2004) and used in this work:

$$proc_{17} = b_{PHA}\,\frac{S_{ALK}}{K_{ALK}+S_{ALK}}\left[\frac{S_{O2}}{K_{O2}+S_{O2}}+\eta_{PHA,NO3,end}\,\frac{K_{O2}}{K_{O2}+S_{O2}}\,\frac{S_{NO3}}{K_{NO3}+S_{NO3}}\right]X_{PHA}$$

Nitrifying organisms (autotrophic organisms): X_{AUT}

Aerobic growth of X_{AUT} (Process 18)

$$proc_{18} = \mu_{AUT} \frac{S_{O2}}{K_{O2,AUT} + S_{O2}} \frac{S_{NH4}}{K_{NH4,AUT} + S_{NH4}} \frac{S_{PO4}}{K_P + S_{PO4}} \frac{S_{ALK}}{K_{ALK,AUT} + S_{ALK}} X_{AUT}$$

Lysis of X_{AUT} (Process 19)

Original equation:

$$proc_{19} = b_{AUT}\, X_{AUT}$$

Modified by Gernaey and Jørgensen (2004) and used in this work:

$$proc_{19} = b_A \left[\frac{S_{O2}}{K_{O2,AUT} + S_{O2}} + \eta_{A,NO3,end} \frac{K_{O2,AUT}}{K_{O2,AUT} + S_{O2}} \frac{S_{NO3}}{K_{A,NO3} + S_{NO3}} \right] X_A$$

Chemical phosphorus removal

Precipitation with $Fe(OH)_3$ (Process 20)

$$proc_{20} = k_{PRE}\, S_{PO4} X_{MeOH}$$

Redissolution (Process 21)

$$proc_{21} = k_{RED} X_{MeP} \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$$

Table A.2: Parameter values of the ASM2d model. The temperature of reference is 15ºC.

Parameter	Value	Parameter	Value	Parameter	Value
Hydrolysis		**PAO**		**Autotrophs**	
K_h	2.46	q_{PHA}	2.46	μ_{AUT}	0.61
K_{O2}	0.2	K_{PP}	0.01	b_A	0.09
K_X	0.1	q_{PP}	1.23	$\eta_{A,NO3,end}$	0.33
η_{NO3}	0.6	K_{PS}	0.20	$K_{A,NO3}$	0.50
K_{NO3}	0.5	K_{PHA}	0.01	$K_{O2,AUT}$	0.50
η_{Fe}	0.4	K_{MAX}	0.34	$K_{NH4,AUT}$	1.00
Heterotrophs		K_{IPP}	0.02	$K_{ALK,AUT}$	0.50
μ_H	4.23	μ_{PAO}	0.82	**Phosphorus chemical removal**	
K_F	4.00	b_{PAO}	0.14	k_{PRE}	1.00
K_{NH4}	0.05	$\eta_{P,NO3,end}$	0.33	k_{RED}	0.60
K_P	0.01	b_{PP}	0.14		
K_{ALK}	0.10	$\eta_{PP,NO3,end}$	0.33		
K_A	4.00	b_{PHA}	0.14		
q_{fe}	2.11	$\eta_{PHA,NO3,end}$	0.33		
b_H	0.28				
$\eta_{H,NO3,end}$	0.5				

Table A.3: Stoichiometric parameter values of the ASM2d model.

Process (j) → Variable ↓	1	2	3	4	5	6	7	8	9	10
S_{O2}				-0.6	-0.6					
S_{F}	1.0	1.0	1.0	-1.6		-1.6		-1.0		
S_{A}					-1.6		-1.6	1.0		-1.0
S_{I}										
S_{NH4}	0.01	0.01	0.01	-0.022	-0.07	-0.022	-0.07	0.03	0.031	
S_{N2}						0.21	0.21			
S_{NO3}						-0.21	-0.21			
S_{PO4}				-0.004	-0.02	-0.004	-0.02	0.01	0.01	0.4
S_{ALK}	0.001	0.001	0.001	-0.001	0.021	0.014	0.036	-0.014	0.002	0.009
X_{I}									0.1	
X_{S}	-1.0	-1.0	-1.0						0.9	
X_{H}				1.0	1.0	1.0	1.0		-1.0	
X_{PAO}										
X_{PP}										-0.4
X_{PHA}										1.0
X_{A}										
X_{TSS}	-0.75	-0.75	-0.75	0.9	0.9	0.9	0.9		-0.15	-0.69
X_{MeOH}										
X_{MeP}										

Process (j) → Variable ↓	11	12	13	14	15	16	17	18	19	20	21
S_{O2}	-0.2		-0.6					-18			
S_{F}											
S_{A}							1.0				
S_{I}											
S_{NH4}			-0.07	-0.07	0.031			-4.24	0.031		
S_{N2}		0.07		0.21							
S_{NO3}		-0.07		-0.21				4.17			
S_{PO4}	-1	-1	-0.02	-0.02	0.01	1		-0.02	0.01	-1	1
S_{ALK}	0.016	0.021	-0.004	0.011	0.002	-0.016	-0.016	-0.6	0.002	0.048	-0.048
X_{I}					0.1				0.1		
X_{S}					0.9				0.9		
X_{H}											
X_{PAO}			1.0	1.0	-1.0						
X_{PP}	1.0	1.0				-1.0					
X_{PHA}	-0.2	-0.2	-1.6	-1.6			-1.0				
X_{A}								1.0	-1.0		
X_{TSS}	3.11	3.11	-0.06	-0.06	-0.15	-3.23	-0.6	0.9	-0.15	1.42	-1.42
X_{MeOH}										-3.45	3.45
X_{MeP}										4.87	-4.87

A.2. Influent Characterization

As commented in the main text, *Orhon et al.* (1994) developed a method to determine the values of S_I, X_I, X_S and S_F (ASM2d states) in the effluent, using the well-know measurement of the COD. Such method allows makes an interface between the COD and ASM2d state variables.

The experimental determination of S_I and X_I is performed in two parallel CST Reactors, one of them fed with raw WWTP influent and the other one fed with filtered WWTP influent. Both reactors operate as long as all the biological reactions have been ceased and daily analysis of total COD and the soluble COD are performed. At a sufficient time, both values of COD of the two systems will be approximately constant. At the end of the experiment, the relationship between the initial and final values of total COD and soluble COD of both systems will help to estimate S_I and X_I.

X_S is present at the beginning of the experiment for reactor 1 (with raw influent, without filtering) and it is not for reactor 2 (with filtered WW). At the end of the experiment, in both systems X_S and S_F are no longer exists, different of and S_P and X_P that are produced by the microorganisms along the experiment time. S_P and X_P are, respectively, soluble and particulate residual biodegradable matter, product of microorganism activity. X_I is present at the end of the experiment only in reactor 1 (no filtered WW). With these observations, it is possible to write a system of equations as follows:

Reactor 1 (Fed with raw wastewater)	Reactor 2 (Fed with filtered wastewater)
$C_{T0} = S_{F0} + X_{S0}$ Eq. A.1	$C_{T0} = S_{T0}$ Eq. A.4
$C_{T1} = X_{I1} + S_{I1} + X_{P1} + S_{P1}$ Eq. A.2	$C_{T2} = X_{I2} + S_{I2} + X_{P2} + S_{P2}$ Eq. A.5
$S_{T1} = S_{I1} + S_{P1}$ Eq. A.3	$S_{T2} = S_{I2} + S_{P2}$ Eq. A.6

In equations A.2 and A.3 the lowercase "1" means the values at the end of the experiment in reactor 1. The same notation is used for reactor 2, in equations A.5 and A.6. The lowercase "0" in equations A.1 and A.4 means "initial value" for variables in reactor 1 and 2, respectively. Variable C_T means the total substrate concentration in reactors. S_T means total soluble substrate. X variables are the particulate variables while S variables indicate soluble variables. For a better understanding of the whole experiment, Figure A.1 shows an illustration of the historical data of total COD and total soluble COD.

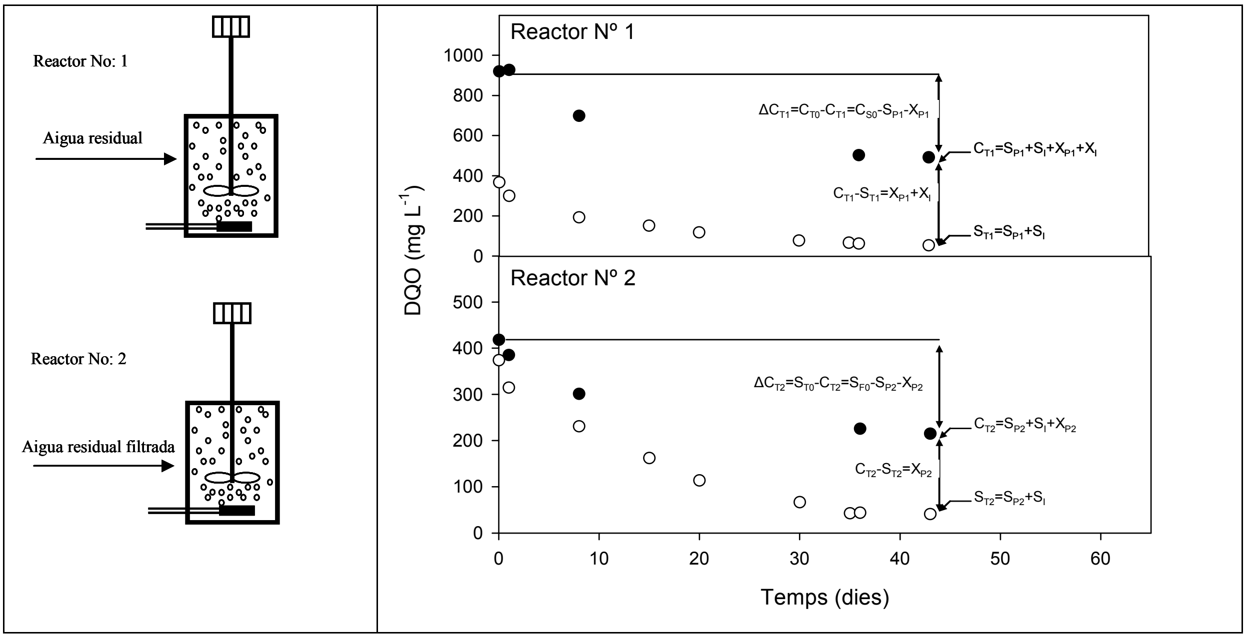


Figure A.1: Illustration of the lab scale reactors, total COD and total soluble COD data for determining S_I and X_I fractions in the secondary stage influent in a WWTP (• Total COD, ○ Total soluble COD).

Using the equations A.1 to A.6, X_I is determined with equation A.7.

$$X_I = (C_{T1} - S_{T1}) - \left\{ [C_{T2} - S_{T2}] \cdot \frac{[C_{T0} - C_{T1}]}{[S_{T0} - C_{T2}]} \right\} \qquad \text{Eq. A.7}$$

Similar procedure should be performed to determine S_I.

$$S_I = S_{T1} - \left\{ \frac{S_{T1} - S_{T2}}{1 - \left[\dfrac{S_{T0} - C_{T2}}{C_{T0} - C_{T1}} \right]} \right\} \qquad \text{Eq. A.8}$$

S_F value can be obtained by taking the value of total soluble COD of reactor 2 at the beginning of the experiment for determining XI and SI and resting the value of SI (obtained by Eq. A.8).

$$S_F = COD_{Soluble\,(filtered\ WW)} - S_I \qquad \text{Eq. A.9}$$

Finally, X_S is determined by using measures of total COD in reactor 1.

$$X_S = DQO_{total} - (S_A + S_F + S_I + X_I) \qquad \text{Eq. A.10}$$

In Eq. A.10, S_A should be considered null (no conditions of fermenting X_S to produce S_A in the urban sewage system) and the rest of variables were already been determined.

A.3. The Simulation Environment

The water line of the simulated A^2/O plant configuration was implemented in Matlab/Simulink® and the main screen is presented in Figure A.2.

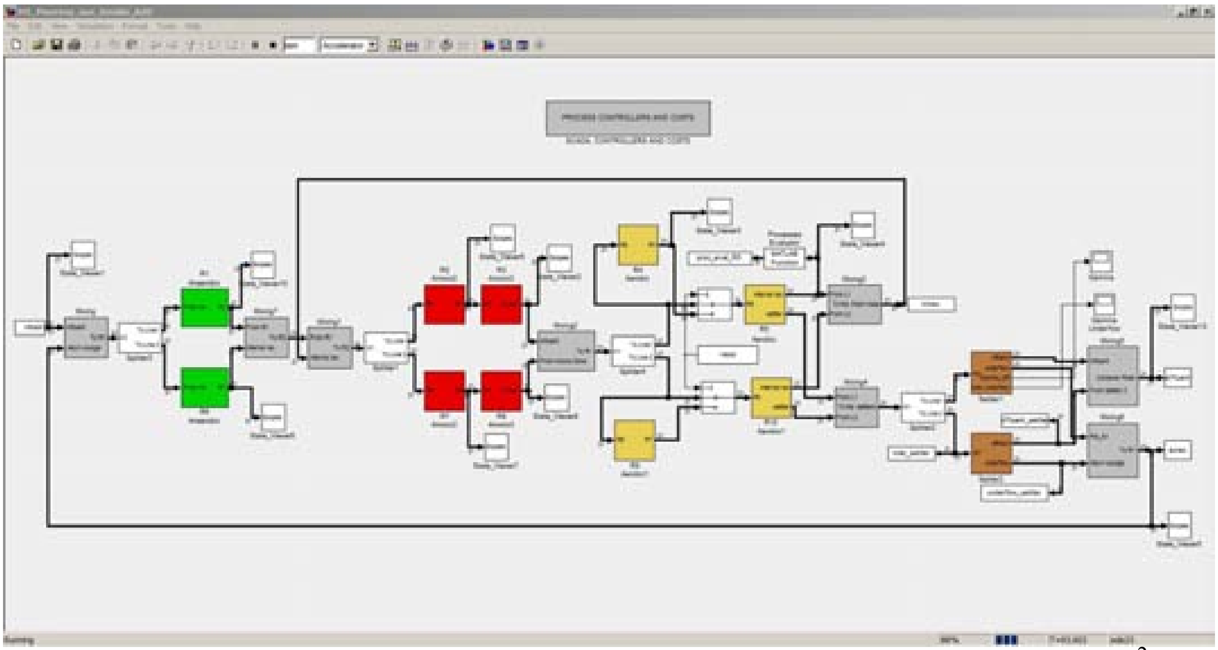


Figure A.2: Main screen of the simulated biological part of the proposed A^2/O-D configuration for implementing the EPBR in the Manresa WWTP, used in this work.

Apart from the process blocks, representing the anoxic and aerobic basins and the settlers, Figure A.2 shows the process controllers and the operating cost calculation module. The hydraulic and kinetic process models are implemented in C-MEX files and are called by the block diagram of Figure A.2. All the constant parameters are defined by running a script file before to run the block diagram. For complete information about the implementation of the simulated WWTP process, please send a mail to: vinicius.cunhamachado@gmail.com

A.4. Tools for Model Validation and Model Calibration

A.4.1. Sensitivity analysis

Sensitivity analysis allows making a ranking of the most important parameters that affect the outputs. Relative sensitivity of an output *i* (y_i) respect a parameter *j* (θ_j) is defined as (Reichert and Vanrolleghem, 2001),

$$S_{ij} = \frac{\theta_j}{y_i}\frac{dy_i}{d\theta_j} \qquad \text{Eq. A.11}$$

Norton (2008) proposed the utilization of algebraic sensitivity analysis because the numerical value of sensitivity applies only for a specific change from a specific value of θ_j, while the former provides algebraic relations. Numerical values of sensitivity are generally much less informative than an algebraic relation, but algebraic sensitivity analysis is not feasible if the equations of the model are complicated as in ASM2d. Therefore, the derivatives of equation A.11 were determined numerically by the finite differences method. The central difference approach with 10^{-4} (0.01%) as perturbation factor was used for the sensitivity calculations of each tested parameter around the default ASM2d value. This perturbation factor was selected because it produced equal derivative values with forward and backward finite differences (de Pauw, 2005).

The overall sensitivity of a parameter was calculated by adding absolute values of individual sensitivities. In our case, 5 output variables were declared (phosphate, ammonium, nitrate, total suspended solids and Kjeldahl nitrogen concentrations at the effluent). Hence, the overall sensitivity value of a parameter *j* (OS_j) was calculated with equation A.12.

$$OS_j = \left|S_{j,PO_4}\right| + \left|S_{j,NH_4}\right| + \left|S_{j,NO_3}\right| + \left|S_{j,XTSS}\right| + \left|S_{j,TKN}\right| \qquad \text{Eq. A.12}$$

A.4.2. The Fisher Information Matrix and Parameter Confidence Interval

The FIM summarizes the importance of each model parameter over the outputs, since it measures the variation of output variables caused by a variation of model parameters (Dochain and Vanrolleghem, 2001, Guisasola *et al.*, 2006). Algebraically, the FIM is represented by equation A.13.

$$FIM = \sum_{k=1}^{N} Y_\theta(k) \cdot Q_k^{-1} \cdot Y_\theta^T(k) \qquad \text{Eq. A.13}$$

For a FIM calculated for r output variables and p parameters, it is a p x p matrix, where k represents each sampling data point, Q_K is the r x r covariance matrix of the measurement noise, θ is the vector of p parameters, N is the total number of samples and Y_θ is the p x r output sensitivity function matrix, expressed by equation A.14.

$$Y_\theta^T(t) = \left[\frac{\partial y(t,\theta_0)}{\partial \theta^T}\right]_{\theta_0} \qquad \text{Eq. A.14}$$

where θ_0 is the complete model parameter vector used for calculating the derivatives and θ^T is the transposed parameter vector, which its elements are being studied. In the present study, the derivative shown in equation A.14 was numerically obtained by finite differences using a perturbation factor of 10^{-4} as in the sensitivity calculations. Mathematically was proved that the FIM provides a lower bound of the parameter error covariance matrix (Söderström and Stoica, 1989) as shown by equation A.15.

$$\operatorname{cov}(\theta_0) \geq FIM^{-1} \qquad \text{Eq. A.15}$$

This FIM property was used for calculating the confidence interval $\Delta\theta_j$ with equation 6 for a given parameter θ_j (Seber and Wild, 1989).

$$\Delta\theta_j = t_{\alpha,N-p}\sqrt{\mathrm{cov}(\theta_j)} \qquad \text{Eq. A.16}$$

where *t* is the statistical t-student with α = 95% of confidence and *N-p* degrees of freedom (number of experimental data points minus *p* parameters), and $\mathrm{cov}(\theta_j)$ was assumed as $FIM^{-1}{}_{jj}$.

As can be observed, the calculation of the parameter error covariance matrix using the FIM involves its inversion. To be invertible, the FIM should have a determinant different from zero and should not be ill-conditioned. To match these requirements any pair of matrix columns should not be very similar. As each column of the matrix represents a parameter, the determinant and the condition number of the FIM provides a reasonable measurement of the correlation of a set of parameters. Hence, parameters less correlated will easily provide a diagonal-dominant matrix. The FIM determinant (D criterion) and the ratio between the highest and the lowest FIM eigenvalue (modE criterion) can be used as criteria for parameter subset selection. A modE criterion value close to the unity indicates that all the involved parameters independently affect the outputs while the shape of the confidence region is similar to a circle (2 parameters) or a sphere (3 parameters) and not ellipses and ellipsoids as occur with correlated parameters. A high D criterion value means lower values of the diagonal elements of the covariance matrix and hence, lower confidence intervals of the parameters. As the D criterion is dependent on the magnitude of the involved parameters, this criterion was normalized (normD) according to Equation A.17.

$$normD = D \cdot \left\|\theta_P\right\|^2 \qquad \text{Eq. A.17}$$

where $\|\theta_P\|$ is the Euclidean norm of the parameter vector. Such normalization works as a scaling factor and allows comparisons among subsets with the same size but with different parameters.

From the system engineering point of view, it is important to include in the parameter subset those parameters that maximize the D criterion and minimize the modE criterion. Hence, the ratio between the normD and the modE criteria (RDE criterion) is proposed in the present work as an interesting index to define subsets of parameters for calibration. The RDE criterion (Equation A.18) establishes the capacity of a parameter subset to explain experimental data coupled to low uncertainty in the estimated parameters.

$$RDE = \frac{normD}{modE} \qquad \text{Eq. A.18}$$

A.4.3. Cost function construction and model validation

The calibration procedure was based on the minimization of a cost function already exposed in chapter 3. The optimization algorithm employed was the MATLAB® "*fminsearch*" based on the Nelder and Mead Simplex method (Lagarias *et al.*, 1998). *Fminsearch* is an unconstrained direct method and does not use numerical or analytical gradients of the cost function. The tolerances used were 10^{-4} and 10^{-5} for the parameters and for the cost function, respectively. Although in practice model parameters require constraints, the optimization method used was unconstrained because constraints may disrupt convergence properties and produce a less realistic covariance matrix (Checchi and Marsili-Libelli, 2005). However, a posterior analysis of results can easily detect unrealistic parameter estimations.

The analysis of the quality of the model calibration started from checking the system response with the default values of ASM2d parameters in initial simulations. These simulations were useful as a reference to compare how much the optimized parameter values improved the model predictions. Such comparison was performed through the Janus coefficient (Sin *et al.*, 2008), the CCF and the VCF values. The Janus coefficient is defined as the ratio between the sum of the squared difference between experimental validation data and model predictions and the sum of the squared difference between the calibration data and model predictions, according to equation A.19,

$$J^2 = \frac{\frac{1}{N_{VAL}} \sum_{1}^{N_{VAL}} \left(y_{EXP.} - y_{MOD.}\right)^2}{\frac{1}{N_{CAL}} \sum_{1}^{N_{CAL}} \left(y_{EXP.} - y_{MOD.}\right)^2} \qquad \text{Eq. A.19}$$

where N_{CAL} and N_{VAL} are the number of experimental data points used for calibration and validation, respectively, and $y_{EXP.}$ and $y_{MOD.}$ are the experimental data points and the model prediction vector, respectively. When J^2 is closer to the unity, the calibrated model provides a similar performance in calibration and validation data.

A.5. The black-box linear model

Based on the step tests data using the non-linear model developed with the systematic procedure of parameter calibration for the Manresa WWTP (A/O configuration) and the selected alternative for upgrading (A^2/O-D), linear models with several input and output variables were estimated. These models were employed to:

- calculate the RGA and the minimized condition number
- tuning the process controllers

The full linear models identified for the water line of the Manresa WWTP (A/O) and the selected configuration (A^2/O-D) are made of several FODT (First Order with Dead-Time) models, one for each input-output channel/pair. The representation of this function is showed below:

$$G(s) = \frac{y(s)}{u(s)} = \frac{K}{\tau s + 1} e^{-\theta s} \qquad \text{A.20}$$

Tables A.4, A.5 and A.6, show the parameters K (process gain), τ (time constant) and θ (dead time) for each input-output pair (channel) of the transfer function model amongst input and output variables of the A^2/O-D configuration (the selected configuration).

Table A.4: Gain of the linear model in each channel.

Gain, K	DO	Q_{RINT}	Q_{RAS}
NH_4^+ Eff.	-0.6976	-1.9588 10^{-6}	-6.1470 10^{-6}
NO_3^- Anox.	0.1643	14.240 10^{-6}	16.572 10^{-6}
NO_3^- Eff.	0.4802	-25.168 10^{-6}	-19.232 10^{-6}
PO_4^{3-} Anaer.	0.0169	1.6084 10^{-6}	-0.2181 10^{-6}
PO_4^{3-} Eff.	0.0250	1.2146 10^{-6}	1.7286 10^{-6}

Table A.5: Time constant of the linear model in each channel.

Time constant, τ[d]	**DO**	**Q_{RINT}**	**Q_{RAS}**
NH_4^+ Eff.	5.24	2.10	1.76
NO_3^- Anox.	4.95	0.42	0.84
NO_3^- Eff.	4.49	0.65	1.91
PO_4^{3-} Anaer.	5.83	2.34	75.4
PO_4^{3-} Eff.	3.67	2.98	3.94

Table A.6: Dead time of the linear model in each channel.

Dead time, θ[d]	**DO**	**Q_{RINT}**	**Q_{RAS}**
NH_4^+ Eff.	1.00	1.00	1.00
NO_3^- Anox.	1.00	1.00	1.00
NO_3^- Eff.	1.00	1.00	1.00
PO_4^{3-} Anaer.	1.00	1.00	1.00
PO_4^{3-} Eff.	1.00	1.00	1.00

The identified linear models have the structure/algorithm “Output-Error”, (OE) (Ljung, 1999). The OE model structure is represented in equation A.21.

$$y(t) = \frac{B(q)}{F(q)} u(t - n_K) + e(t) \quad \text{A.21}$$

where $y(t)$ is the output (controlled variable), $u(t\text{-}n_K)$ is the input (manipulated variable) at n_K sample intervals before the current time. The variable $e(t)$ is the prediction error. B and F are polynomials that represent the process model $G(q)$ (relationship between the input and the output) and their parameters should be identified. Polynomials B and F are expressed by equations A.22 and A.23.

$$B(q) = b_1 + b_2 q^{-1} + \ldots + b_{nb} q^{-nb+1} \quad \text{A.22}$$

$$F(q) = 1 + f_1 q^{-1} + \ldots + f_{nf} q^{-nf} \qquad \text{A.23}$$

where *nb* and *nf* are the orders of *B* and *F* respectively. Variable “*q*” is the shift operator. So, q^{-1} applied to *y*(*t*) produces *y*(*t*-1), which is the previous value of *y*. The coefficients of *B* and *F* are determined, therefore, solving an optimization problem, in which the squared prediction error is minimized over the whole set of input-output data of *N* entries. The optimization variables of this problem are the coefficients of *B* and *F*. The objective function is presented in equation A.24.

$$V_N = \sum_{t=1}^{N} \left(y(t) - \frac{B(q)}{F(q)} u(t - n_K) \right)^2 \qquad \text{Eq. A.24}$$

It is important to let clear that the identified model using OE algorithm is discrete and for tuning the process controllers, the OE model was converted to the continuous domain.

A.6. Methods for tuning of PI and PID controllers

Table A.7 shows the relationships between the transfer function model parameters and the tuning parameters of PI/PID controllers used in this work (Rivera *et al.*, 1986; Ogunnaike and Ray, 1994; Skogestad, 2003).

Table A.7: Tuning rules of PI/PID controllers used in this work.

Method	Process Model	K_P	τ_I	τ_D
IMC (internal model control)	$\frac{K}{\tau s+1}e^{-\theta s}$ $\tau_{CL}>0.8\theta$	$\frac{(2\tau+\theta)}{K\cdot(2\tau_{CL}+\theta)}$	$\tau+\frac{\theta}{2}$	$\frac{\tau\cdot\theta}{2\tau_{CL}+\theta}$
	$\frac{K}{\tau s+1}e^{-\theta s}$ $\tau_{CL}>1.7\theta$	$\frac{(2\tau+\theta)}{K\cdot 2\tau_{CL}}$	$\tau+\frac{\theta}{2}$	-
ITAE-s (good for setpoint changes)	$\frac{K}{\tau s+1}e^{-\theta s}$	$\frac{0.586}{K}\left(\frac{\tau}{\theta}\right)^{0.916}$	$\frac{\tau}{1.03-0.165\cdot\left(\frac{\theta}{\tau}\right)}$	
ITAE-d (good for load disturbances)	$\frac{K}{\tau s+1}e^{-\theta s}$	$\frac{0.965}{K}\left(\frac{\tau}{\theta}\right)^{0.855}$	$\frac{\tau}{0.674}\left(\frac{\theta}{\tau}\right)^{0.680}$	
Skogestad Correlations	$\frac{K}{\tau s+1}e^{-\theta s}$	$\frac{\tau}{K}\left[\frac{1}{\theta+\tau_{CL}}\right]$	$\min\left[\tau,4\cdot(\tau_{CL}+\theta)\right]$	

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Kind of Participation:	Oral presentation
Congress:	The 10th IWA Conference on Instrumentation, Control and Automation (ICA 2009)
Publication Media:	CD
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Kind of Participation:	Poster
Congress:	11th Mediterranean Congress of Chemical Engineering
Publication Media:	CD
Place:	Barcelona, Spain
Date:	2008

Authors:	Rosa Redondo, **Vinicius Cunha Machado**, Maria del Mar Baeza, Javier Lafuente, David Gabriel
Title:	**On-line monitoring of gas-phase bioreactors for biogas treatment: hydrogen sulfide and sulfide analysis by automated flow systems**
Kind of Participation:	Poster
Congress:	XI ISAMEF: International Symposium on Analytical Methodology in the Environmental Field.
Publication Media:	CD
Place:	Pollensa, Mallorca, Spain
Date:	October, 2007

Authors:	**Machado, V. C.**; Trierweiler J. O. ; Secchi A. R.
Title:	**A new signal design tool for process model identification.**
Kind of Participation:	Oral presentation
Congress:	DYCOPS:7th IFAC Symposium on Dynamics and Control of Process Systems
Publication Media:	DYCOPS-2004 (7th IFAC Symposium on Dynamics and Control of Process Systems), 2004, Boston. CD DYCOPS 2004, 2004. v. 1. p. 177.
Place:	Boston, USA.
Date:	July, 2004

Authors:	**Machado, V. C.**; Trierweiler J. O.
Title:	**Which is the best criterion for identification of dynamic models?**
Kind of Participation:	Oral presentation
Congress:	DYCOPS: 7th IFAC Symposium on Dynamics and Control of Process Systems
Publication Media:	DYCOPS-2004 (7th IFAC Symposium on Dynamics and Control of Process Systems), 2004, Boston. CD DYCOPS 2004, 2004. v. 1. p. 1788.
Place:	Boston, USA.
Date:	July, 2004

Authors:	**Machado, V. C.**; Trierweiler J. O.; Secchi, A. R.
Title:	**Nova metodologia de projeto de perturbações multivariáveis aplicada à identificação de sistemas mal-condicionados (A novel design methodology for multivariate disturbances applied to the model identification of ill-conditioned systems)**
Kind of Participation:	Oral presentation
Congress:	CBA 2004 - XV Congresso Brasileiro de Automática –CBA (Brazilian Automation Congress)
Publication Media:	CD CBA 2004. Porto Alegre: UFRGS, 2004. v. 1. p. 1138-1148
Place:	Gramado, RS, Brazil
Date:	July, 2004

Authors:	**Machado, V. C.**; Secchi A. R.
Title:	**Vantagens e benefícios da implementação de um controlador preditivo em coluna de destilação (Advantages and benefits of implementing a model predictive controller in a distillation column)**
Kind of Participation:	Oral presentation
Congress:	4º Congresso Internacional de Automação, Sistemas e Instrumentação. (4th International Congress of Automation, Systems and Instrumentation)
Publication Media:	Congress Proceedings
Place:	São Paulo-SP, Brazil
Date:	November, 2004

Authors:	**Machado, V. C.**; Secchi A. R.
Title:	**Aplicação de uma nova sistemática de projeto de perturbações na identificação de modelos dinâmicos em uma unidade de destilação. (A novel method for designing disturbances for model identification of a distillation unit)**
Kind of Participation:	Oral presentation
Congress:	XV COBEQ – Congresso Brasileiro de Engenharia Química (COBEQ-Brazilian Chemical Engineering Congress)
Publication Media:	CD – COBEQ2004. ABEQ, 2004, v.1.
Place:	Curitiba, Brazil
Date:	September, 2004

Authors:	**Machado, V. C.**; Ribeiro, L. R.; Rodrigues, C. M.; Trierweiler, J. O; Secchi A. R.
Title:	**Plantas experimentais de engenharia química monitoradas via Internet (Pilot-plants for chemical engineering education operated by the Internet)**
Kind of Participation:	Poster
Congress:	XV COBEQ – Congresso Brasileiro de Engenharia Química (COBEQ-Brazilian Chemical Engineering Congress)
Publication Media:	CD – COBEQ2004. ABEQ, 2004, v.1.
Place:	Curitiba, Brazil
Date:	September, 2004

Authors:	**Machado, V. C.**; Trierweiler J. O.; Secchi, A. R.; Teixeira, H.; Lusa, L. P.; Miranda, F. C. P. R.
Title:	**Planejamento de perturbações para a identificação de modelos dinâmicos de plantas industriais (Disturbances design for identification of industrial dynamic models)**
Kind of Participation:	Oral presentation
Congress:	3º Congresso Internacional de Automação, Sistemas e Instrumentação. (3rd International Congress of Automation, Systems and Instrumentation)
Publication Media:	Congress Proceedings
Place:	São Paulo-SP. Brazil
Date:	November, 2003

Contribution Papers

Authors: **Vinicius Cunha Machado**, Gladys Tapia, David Gabriel, Javier Lafuente, Juan Antonio Baeza.
Title: ***Systematic identifiability study based on the Fisher Information Matrix for reducing the number of parameters in calibration of an activated sludge model***
Journal: Environmental Modelling and Software
Volume: 24 Pages 1274-1284 Date: 2009
Place of publication: London, England

Authors: **Vinicius Cunha Machado**, David Gabriel, Javier Lafuente, Juan Antonio Baeza.
Title: ***Cost and Effluent quality controllers design based on the relative gain array for a nutrient removal WWTP.***
Journal: Water Research
Volume: 43 Pages 5129-5141 Date: 2009
Place of publication: London, England

Authors: Guillermo Baquerizo, Juan Pedro Maestre, **Vinicius Cunha Machado**, Xavier Gamisans, David Gabriel.
Title: ***Long-term ammonia removal in a coconut fiber-packed biofilter: Analysis of N fractionation and reactor performance under steady-state and transient conditions.***
Journal: Water Research
Volume: 43 Pages 2293-2301 Date: 2009
Place of publication: London, England

Authors: Rosa Redondo, **Vinicius Cunha Machado**, Maria del Mar Baeza, Javier Lafuente, David Gabriel.
Title: ***On-line monitoring of gas-phase bioreactors for biogas treatment: hydrogen sulfide and sulfide analysis by automated flow systems***
Journal: Analytical and Bioanalytical Chemistry
DOI: 10.1007/s00216-008-1891-5 Date: 2007
Place of publication: Berlin, Germany

Authors: **Machado, V. C.**; Schmidt, A. M.; Azambuja, D. S.
Title: ***Electrodissolution of Cu-Zn Alloys in Acetate Media***
Journal: *Journal of Brazilian Chemistry Society*
Volume: 11 Pages: 387-392 Date: 2000
Place of publication: Brazil