Technical University of Denmark

# Stabilisation of Biological Phosphorus Removal from Municipal Wastewater

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# Ph.D. Thesis of

Ulrich Krühne

with the title

# Stabilisation of Biological Phosphorus Removal from Municipal Wastewater

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# Summary

The biological phosphorus removal (BPR) from wastewater has developed considerably during the last decades and is applied in many present wastewater treatment plants (WWTP) all over the world. The process performance and the control of the BPR are under the influences of daily and seasonal variations of the influent wastewater concentrations and are not yet always guaranteed. Even though the scientific knowledge and practical experience has reached a high level of understanding of the involved key-processes it is still necessary to apply chemical precipitation of phosphorus during the time periods, where the complete BPR can not be achieved. The understanding of the main phenomena involved into such failure of BPR and the development of operational or control strategies to overcome these deficiencies are the main areas of investigation of this thesis.

Investigations of the failure of BPR have been performed on an alternating pilot plant, receiving municipal wastewater. The pilot plant is equipped with an automatic measurement system based on the flow injection analysis (FIA) principle. Continuos analysis of the ammonium ($NH_4$-N), nitrate (as NOx-N) and phosphorus ($PO_4$-P) was performed in all important places of the plant.

Based on literature studies and investigations of the available pilot plant measurement data experimental designs were developed to produce operational conditions where the BPR failed. The process was investigated during periods of low influent concentrations and increased hydraulic load, with subsequent re-establishment of normal conditions. A process disturbance of this type results in an increase in the phosphate concentration level in the effluent, shortly after the wastewater returns to normal strength.

During the first part of the thesis it was examined if an extended version of the activated sludge model No. 2 (ASM2) including denitrification by phosphate accumulating organisms (PAO) can be calibrated and validated on the existing system. A set of parameter was determined through a simple evolutionary parameter estimation strategy. This parameter set was used during the whole investigation. The prediction of the dynamic model was used for development of new operational and control strategies.

Based on the model simulations an external carbon source addition (ECSA) was designed in order to overcome the BPR process failure. With the help of such addition, the internal carbon storage compounds could be maintained at a high level, indicated by poly-hydroxy-alcanoate (PHA) measurements and the accumulation of phosphorus in the effluent could be avoided. Experimental investigations imply that the ECSA together with a reduction of aeration time during periods of low organic influent concentration could improve and stabilise the BPR.

The identification of a minimum PHA level, necessary to ensure complete BPR, was however not possible. The failure of BPR was sometimes observed even when comparatively high internal PHA concentrations were present. The experiments where therefore further investigated with help of the model. The study indicates that a PHA limitation is not the only factor affecting the recovery of the BPR process during such

periods. The actual amount of PAO present in the system during and after such disturbance can play a role in the deterioration of BPR.

In the last part of the thesis the obtained understanding through the operational investigations was used for the design of a model predictive control (MPC) strategy for the BPR system under low influent concentrations. The MPC strategy is based on the addition of an ECSA keeping the internally stored carbon products at a high level. A simple model-based observer estimating the unmeasured influent soluble organic or internal PHA concentrations is used. This observer improves the robustness operation of the addition significantly. The MPC control performance is compared to a simple feed-forward control design, which also is based on the estimated organic influent concentrations. It is shown that the simple feed-forward as well as the more advanced MPC strategies can improve the BPR without major interference with the other biological processes. With increasing complexity of the strategy the amount of external added carbon could be significantly reduced while the effluent $PO_4$-P concentration could be kept below the required concentration of 1mgP/L

# Resumé (in Danish)

Biologisk fosfatfjernelse fra spildevand er blevet udviklet betydeligt gennem de sidste årtier og rensningsanlægi hele verden benytter denne proces. Idet drift og regulering af processen i høj grad afhænger af de daglige og sæsonbetonede udsving i spildevandets sammensætning, er tilfredstillende resultater ikke garanteret. Selvom videnskabelig indsigt og praktisk erfaring har medført en øget forståelse af de primære processer, er kemisk udfældning af fosfat stadig nødvendig inden den biologiske fjernelse påbegyndes. Hovedområderne i denne afhandling omfatter forståelsen af fænomenerne, der er skyld i den til tider begrænsede effektivitet af biologisk fosfatfjernelse med henblik på udvikling af drifts- og reguleringsstrategier, som kan øge effektiviteten.

Den eksperimentielle undersøgelse af biologisk fosfatfjernelse er udført på et alternerende pilotanlæg, der behandler kommunalt spildevand. Pilotanlægget er udstyret med et automatisk målesystem baseret på strømnings-injektions-analyse (flow injection analysis FIA) princippet. Kontinuerlige sammensætningsanalyser af ammonium ($NH_4$-N), nitrat (som NOx-N) og fosfat ($PO_4$-P) har dermed været muligt på alle vigtige steder af anlægget.

På basis af eksisterende litteratur og analyse af tidligere data fra pilotanlægget, er driftsbetingelserne hvor den biologiske fosfatfjernelse mislykkes, blevet bestemt. Formålet var at kunne reproducere disse data ved nye eksperimenter, der kunne anvendes til videre undersøgelser. Anlæggets opførsel er blevet undersøgt inden perioder, hvor spildevandet er blevet fortyndet som følge af forøget hydraulisk belastning med efterfølgende reetablering af nominelle koncentrationer og hydraulisk belastning. En sådan procesforstyrrelse resulterer i en forhøjet fosfatkoncentration–i udløbet umiddelbart efter reetablering af normale driftsforhold.

I den første del af projektet blev der fokuseret på at undersøge en udvidet version af aktiveret slam model nr. 2 (activated sludge model No. 2 ASM2) med inkludering af denitrifikation af fosfatakkumulerende organismer. Det blev undersøgt hvorvidt det er muligt at kalibrere modellen således at den svarer til pilotanlægget. Det var muligt ved hjælp af en simpel evolutionær metode at bestemme et parametersæt, der gav det ønskede resultat. Parametersættet blev ikke ændret under undersøgelsesforløbet. Den udviklede dynamiske model blev benyttet til udvikling af drifts- og reguleringsstrategier.

På baggrund af simuleringer af modellen er tilføjelse af eksterne kulstofforbindelser (external carbon source addition ECSA) blevet udviklet for hjælpe fosfatfjernelsen. Ved tilføjelse af ekstra kulstofforbindelser kunne interne, akkumulerede kulstofreserver blive bevaret på et højt niveau, indikeret af poly-hydroxy-alcanoate (PHA) målinger og undgåelse af fosfatakkumulering i udløbet fra anlægget. Eksperimentielle undersøgelser viser at ECSA, sammen med reduktion af beluftningen i perioder med lav koncentration af organisk materiale, kan forbedre og stabilisere den biologiske fosfatfjernelse.

En identifikation af det minimal PHA niveau, der stadig muliggør succesfuld biologisk optagelse af fosfat har ikke været muligt. Svigtende fosfatoptagelse kunne observeres selvom høje interne kulstofreserver eksisterede. Eksperimenterne blev derfor videre undersøgt med hjælp af modellen. Simuleringer antyder at lave PHA koncentrationer ikke er den eneste faktor, som påvirker reetableringen af biologisk fosfatfjernelse efter forstyrrede perioder. Antallet af fosfatakkumulerende organismer i systemet kan også have stor betydning.

I den sidste del af afhandlingen benyttes forståelsen af drifts-undersøgelser til at udvikle en modelunderstøttet reguleringsstrategi (model predictive control MPC) til biologisk fosfatfjernelse under påvirkning af lave indløbskoncentrationer. Strategien er baseret på tilføjelse af kulstofforbindelser for at holde mængden af interne kulstof-forbindelser på et højt niveau. En simpel modelbaseret komponent estimerer de ikke målte, opløste organiske forbindelser og interne PHA koncentrationer. Denne komponent forbedrer den robuste virkning af kulstoftilføjelse væsentligt. Effekten af den modelbaserede strategi sammenlignes med en simpel feed-forward reguleringsstrategi, der også er baseret på estimering af ikke målte organiske indløbskoncentrationer. Det viser sig, at såvel simpel feed-forward og mere avancerede reguleringsstrategier kan forbedre biologisk fosfatfjernelse uden større effekt på de andre biologiske processer. Mængden af tilføjede kulstofforbindelser kan reduceres betydeligt uden at øge udløbskoncentrationen af fosfat på bekostning af øget kompleksitet af reguleringsstrategien.

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# Introduction

This chapter conveys information about the motivation and objectives of the presented work. The introduction chapter is completed by an outline of the thesis chapters.

## Motivation

Biological wastewater treatment processes play a significant role in our society. The main objective of wastewater treatment is the preservation of aquatic environmental resources and the protection of our society from hygienic harmful substances and micro-organisms through reduction of pollutant concentrations. The perception of wastewater treatment facilities is however frequently dominated by negative impression, since the plants may be causing odour problems, eutrophication of receiving water bodies or the augmentation of local water fees.

The technical application of treatment processes must be reliable, simple, inexpensive and effortless to operate. Thus an economic optimisation can prescribe the necessary control equipment, maintenance and staff to satisfy pollutant concentrations in the effluent of a treatment imposed by the authorities. Modern wastewater treatment includes today besides removal of organic matter also nitrogen and phosphorus removal. The motivation for the additional phosphorus and nitrogen removal can be found in the problems associated with eutrophication of receiving waters. A consequence of the non-treatment would be to favour growth of micro-organisms and vegetation in the water bodies at the expense of higher organisms e.g. fish. The simple and powerful concept is to eliminate the nutrients, which are necessary for the growth of micro-organisms causing eutrophication. Due to economical and ecological reasons, most wastewater treatment facilities employ the activated sludge process (ASP) wherein the wastewater is contacted with a broad mixture of aerobic bacteria, the activated sludge. The activated sludge serves as a catalyst for the conversion of the wastewater-pollutants to harmless gaseous products or biomass, which can be removed by sedimentation.

Historically the process has developed from simple conversion of organic matter (carbon compounds) over biological nitrogen removal (BNR) to biological phosphorus removal (BPR). Even though the BPR phenomenon was reported the first time in 1959 it needed decades to be applied in the ASP. Nevertheless thanks to the experience of operators and the increasing knowledge about the involved biological processes gained by researchers, the biological phosphorus removal has been established during the last years at many treatment sites all over the world.

The performance of the BPR process is influenced by the varying influent conditions and the desired effluent phosphorus concentration is frequently exceeded. At many wastewater treatment plants (WWTP) a typical disturbance of the process can be observed after weekends. The influent pollutant concentration of the wastewater is decreased during the weekend due to a reduced industrial production. At the subsequent day of normal influent wastewater strength the BPR is no longer sufficient to remove the influent phosphorus load. Consequently the phosphorus concentration in the effluent increases. The BPR recovers usually after some hours or days. Such typical behaviour occurs also when the influent wastewater concentration is reduced due to rain events or seasonal influences such as vacation times. Most of the WWTP with BPR have therefore a second strategy for the phosphorus removal. The option of chemical precipitation is applied during the time periods, where the BPR is not achieved.

Although knowledge about BPR has increased considerably during the last decade the understanding of the BPR failure has been not sufficient to overcome the problem.

A further motivation for investigation of operational and control aspects of the BPR is that the level of control in such systems is still considerably low. This is directly connected to the lack of measurement equipment in the ASP, caused by high prices for the analysis technology or the absence of measurement techniques in general. In opposition to the control strategies applied to the BNR processes, the biological removal of phosphorus is not considered in many control strategies. It is therefore a challenge to obtain reliable performance of the BPR based on the availability of new analysis systems and to develop the necessary control or operational strategies. In future, when measurement sensors will be available on a reasonable economical background such strategies can be applied in full scale applications.

## Objectives

The main goal of this work is to improve the operational and control strategies in the activated sludge process with a focus on the biological phosphorus removal (BPR). The activated sludge process was investigated in order to

- improve the understanding of BPR behaviour under normal and disturbed situations. The disturbances include flow and concentration changes of the influent wastewater such as during rain events or weekly variations
- to explain the failure of BPR during disturbed situations ()
- identify control handles which allow better control performance during disturbed operation
- validate the identified operational and control strategies

The normal behaviour of the BPR process as well as during wastewater composition disturbances was investigated, with the purpose of determining a correlation between internal storage compounds and the phosphorus removal capabilities. The plant data from the recent years has been extensively analysed and pilot plant scale experiments have been performed with the intention to identify the limiting factors of the biological phosphorus dynamics.

In the subsequent part, the modelling of the process was performed with the use of an extended version of the Activated Sludge Model No. 2 (ASM2). The application of this model to explain and predict the process behaviour was related to the conclusions, drawn from the previous part. The investigation demonstrates how available models can sufficiently represent the transient behaviour of a pilot plant during wastewater flow and composition variation.

The last part of the thesis concentrates on pinpointing of feasible control handles and formulation of operational or control strategies. The development of control algorithms and the testing of control strategies for improved P-removal during normal and disturbed operations were explored.

## Outline of the Thesis

The main contribution from the thesis is presented in the four last chapters, which can be read independently. The first part of the thesis conveys the necessary background to the reader who is not familiar with the biological processes, the control of ASP and the experimental set-up. The intention of the first two chapters is to pass the key information needed for the understanding of the later four main chapters. The reader familiar with wastewater treatment can start the reading with chapter 4, were the investigated phenomenon is presented. A brief description of each chapter follows during the next paragraphs.

### Chapter 1: Basic Biological Processes

The processes involved in wastewater treatment are described with focus on the biological phosphorus removal. A literature review and a short summary of the modelling of the BPR is given. Other processes and reactions such as carbon removal, nitrification and denitrification are briefly discussed.

### Chapter 2: Control of the Activated Sludge Process

The control problems connected to the ASP are presented. First, general aspects such as main control objectives and problems in the ASP plant dynamics, measurements and candidate variables for manipulation of the process are discussed. The presentation of control loops conveys an overview about local controllers. The discussion about models describes the aspects of parameter identification for structured and unstructured models and advanced control strategies. Three examples of the present state of the art of control in the ASP are given in a literature review. The first example is the control of the dissolved oxygen concentration followed by the operation and control of the nitrogen removal processes. Finally an overview is given on the operation and control of the BPR process.

### Chapter 3: Material and Methods

The investigated alternating pilot plant is presented and discussed along with the automatic measurement system, the flow injection analysis (FIA) system. The design of model experiments used during the investigations is presented.

### Chapter 4: The Investigated Phenomena

The measurement data from the pilot plant, which performs BPR were extensively studied for the case of insufficient elimination of phosphorus from wastewater. These investigations demonstrated that the process cannot maintain the phosphorus concentrations below the limiting values under specific varying influent conditions. The performance fails either after low influent concentrations with subsequent re-establishment of the average concentration levels or after an increase of the influent wastewater strength. A model experiment was therefore designed to study this behaviour.

## Chapter 5: Parameter Estimation for the ASM2 Model Incorporating Denitrification by Phosphate Accumulating Organism

The behaviour of the pilot scale biological phosphorous removal process (BPR) of the alternating BIODENIPHO$^{TM}$ type is investigated during a period of normal inlet wastewater feed composition variations. A calibrated version of an extended activated sludge model No. 2 (ASM2), which includes denitrification by phosphate accumulating organism (PAO) can be used over large time periods to predict the behaviour of the main components in the system. A sensitivity analysis has been performed in order to focus on the estimation of the important parameters. The actual parameter estimation was performed by an evolutionary estimation procedure. The relevant calibration and validation experiments are presented. The necessary influent characterisation is described and a correlation of the influent organic compounds with the phosphorus release in the anaerobic tank is proposed.

## Chapter 6: Investigation of an Operational Strategy for the BPR Under Low Influent Concentrations

The behaviour of the pilot scale biological phosphorus removal process (BPR) of the alternating type was investigated during periods of low influent concentrations and increased hydraulic load. The accumulation of phosphorus in the system was prevented by the addition of an external carbon source either to the influent or to the effluent from the anaerobic reactor in form of sodium acetate. With this addition, the internal carbon storage compounds could be maintained at a high level, demonstrated by poly-hydroxy-alcanoates (PHA) measurements. Several levels of acetate addition were investigated experimentally in order to determine a minimal amount of internally stored carbon, which could ensure the stabilisation of BPR during dynamic influent conditions. Determination of an optimal level was however not possible. The failure of the BPR process was observed even when high concentrations of PHA could be detected. Furthermore reduction of aeration time during periods of low influent concentrations was investigated. It was demonstrated that BPR was stabilised by combining a reduction of aeration time with carbon source addition, thereby maintaining the internal stored carbon at a higher level. This combined control action resulted in a desired high BPR activity when the normal strength of the influent wastewater was re-established.

## Chapter 7: Model Assisted Investigation of an Operational Strategy for the BPR at Low Influent Concentrations

An operational strategy to support the biological phosphorus removal (BPR) process during situations of low influent concentrations and increased hydraulic load such as rain events was investigated. The addition of an external carbon source to the influent or the effluent of the anaerobic reactor avoided the increase of phosphorus in the effluent. In this way the internal carbon storage compounds in the form of poly-hydroxy-alcanoates are maintained at a high level during the disturbance and a possible PHA limitation is avoided when the normal influent composition is re-established. The identification of a minimum concentration of PHA necessary to ensure BPR was not possible and a dependency of the PHA concentration on the location of the addition was observed. The failure of the BPR process was sometimes observed even when comparatively high concentrations of PHA could be detected. During this investigation an extended version of the activated sludge model No.2 (ASM2), which includes denitrification by phosphate accumulating organisms (PAO), is used for the detailed analysis of the experiments. The model predicted the phosphorous build-up after the process disturbance as well as the performance during the stabilized experiments. Assisted by the model, the investigations indicate that a PHA limitation is not the only factor affecting the recovery of the BPR process during periods of low influent concentrations.

## Chapter 8: Model Predictive Control for a Biological Phosphorus Removal System under Low Influent Concentrations

The biological phosphorus removal (BPR) process was previously studied during situations of low influent concentrations and increased hydraulic load. It was demonstrated that the accumulation of phosphorus can be avoided or significantly reduced when an external carbon source was added prior to the anaerobic reactor. Since the design of such addition is dependent on many influencing variables which are difficult to access by analytical measurements the design of a model-based observer can significantly improve the operational robustness. This chapter investigates the design of both a receding horizon observer that estimates the unmeasured influent soluble organic concentrations and of different control strategies. Non-linear predictive control has been developed, based on a calibrated and validated version of an extended version of the ASM2 incorporating denitrification by the PAO. The non-linear model predictive control law is investigated in simulation studies to stabilise the BPR process during load disturbances. The model predictive control performance is compared to a simple feed-forward control law. It is demonstrated that both control strategies can improve the BPR without major interference with the nitrogen removal processes. With increasing complexity of the control strategy the amount of external added carbon could be significantly reduced while the effluent $PO_4$-P concentration could be kept below the concentration of 1 mgP/L. The best performance was obtained with a model predictive control strategy, which maintained the internal PHA concentration and used a flexible aeration time in the aerated tanks.

# Biology and Control of the Activated Sludge Process

# 1. Basic Biological Processes

The introduction of nutrient containing wastewater into the receiving water bodies would support growth of micro-organism and thus lead to low oxygen concentrations. Extermination of higher organisms, which need oxygen combined with growth of algae and other micro-organism would lead to an eutrophication of the water body. One possible remedy to eutrophication is the removal of carbon, phosphorus and nitrogen compounds from wastewater.

Many wastewater treatment facilities employ the activated sludge process (ASP) wherein the wastewater is contacted with a broad mixture of micro-organisms, the activated sludge. The activated sludge serves as a catalyst for the conversion of the wastewater-pollutants to harmless gaseous products or biomass, which can be removed by sedimentation.

The most important groups of organisms and micro-organism can be divided into bacteria, fungi, algae, protozoa and metazoa. The occurrence and distribution depend strongly on the entering wastewater and the conditions at the plant. An overview of the different organism can be found in Henze et al (1997). The selection for the different organisms in wastewater treatment plants is mainly a function of the substrate, the electron acceptor (oxygen or nitrate), the settling and flocculation characteristics, the temperature, the growth rate and the freely suspended life forms.

The chemical conversions in a biological wastewater treatment system are mainly carried out by the micro-organism. The first objective of micro-organisms is to survive under substrate limiting conditions. With respect to life functions the following rough separation can be made

- biological growth
- hydrolysis
- decay and lysis

The micro-organism live on available substrate gives rise to population growth and their death is observed as lysis and decay. The hydrolysis process has the function to cut up larger organic molecules into smaller degradable ones and improves therewith the substrate supply. It allows the micro-organisms to survive under substrate limiting conditions, which is the normal situation of municipal wastewater. A typical lifecycle for micro-organisms consists of the hydrolysis of slowly degradable matter (for example in particulate form) into easily degradable matter, which may be soluble. This is further hydrolysed into very easy degradable matter, i.e. substrate (acetic acid, methanol, propionic acid, glucose, ammonium, nitrite etc.) that are used for the growth of the biomass.

The processes of nitrification, denitrification and biological phosphorus removal are presented below in more detail, since nutrients, i.e. phosphorus and nitrogen play a dominant role in the life and growth of micro-organisms. For both nutrients, the necessity for the elimination from the wastewater is directly comprehensible.

## 1.1.Aerobic Heterotrophic Conversion of Organic Matter

The supplied organic matter of a biological wastewater treatment plant is either oxidised to carbon dioxide or in combination with nutrients, assimilated by the micro-organisms during growth processes. The passage of unchanged organic components through a wastewater treatment system is solely possible for non-biodegradable or inert compounds. The aerobic conversion of organic matter is primarily performed by a group of organisms named heterotrophic organism. The group of heterotrophic organisms is very large and contains for example *Comamonas-Pseudomonas, Alcaligenes, Pseudomonas (*fluorescent*), Paracoccus, Aeromonas, Flavobacterium micrococcus*....(Hiraishi et al 1989). Factors influencing the aerobic, heterotrophic conversion of organic matter are temperature, oxygen, pH, toxic substances, nitrogen and phosphorus (see also Schlegel and Zaborosch, 1992 and Voet, 1995).

## 1.2.Nitrogen Removal

The removal of nitrogen compounds is performed in two steps. When the water reaches the plant most of the nitrogenous compounds in the raw wastewater are already converted to ammonium. The first step of conversion is the nitrification process during which ammonium is converted by autotrophic organisms into nitrate. An intermediate of this conversion is nitrite. In the second step of nitrogen removal, nitrate is used as electron acceptor for the conversion of organic matter by heterotrophic organisms and is transformed into molecular nitrogen. This process is called denitrification.

### 1.2.1.Nitrification

A small group of organisms, the autotrophic organisms, performs the nitrification process. These organisms use carbon dioxide for cell synthesis and gain energy from the oxidation of ammonium with oxygen (Schlegel, 1992). The nitrification process is performed in two steps. During the first reaction ammonium is oxidised to nitrite by a group of organism called *Nitrosomonas*. In the second step the nitrite is further oxidised to nitrate by a group of organism which is known as *Nitrobacter* (Henze et al. (1997) or Teichfischer et al (1995)).However Wagner et al (1996 and 1998) have investigated several sewage treatment plants with in situ analysis methods and their experimental results indicated disagreement with the above common understanding in the way that the as present expected micro-organism could not be identified in the system. However, the common knowledge is presented here.

Oxidation of ammonium:

$$NH_4^+ + \frac{3}{2}O_2 \rightarrow NO_2^- + H_2 0 + 2H^+ \qquad \text{eq. 1.1}$$

Oxidation of nitrite:

$$NO_2^- + \frac{1}{2}O_2 \rightarrow NO_3^- \qquad \text{eq. 1.2}$$

The group of nitrifying bacteria is rather homogenous and characterised by a low growth rate. The cause for the slow growth rate is the small energetic yield coupled to the oxidation of ammonium and nitrite. The nitrification process is therefore often problematic from an operational point of view such that they are washed out if the sludge retention time is too small.

The carbon source for autotrophic bacteria is the dissolved carbon dioxide that has to be reduced before it can be assimilated into the cell structure of the micro-organism. The reduction of the carbon source is linked to the oxidation of the nitrogen source i.e. ammonium or nitrite. The details of this reduction will be omitted here and only the resulting chemical equation for such nitrification including growth by *Nitrosomonas* and *Nitrobacter* is presented:

$$NH_4^+ + 1.86\,O_2 + 1.98\,HCO_3^- \rightarrow 0.02\,C_5H_7NO_2 + 0.98\,NO_3^- + 1.88\,H_2CO_3 + 1.04\,H_2O \qquad \text{eq. 1.3}$$

with $C_5H_7NO_2$ as biomass for both organisms

The oxidation of nitrite is assumed to be a single step reaction, while the oxidation of ammonium is executed in several intermediate steps. Factors limiting nitrification are alkalinity, temperature, oxygen, pH and the presence of inhibiting and toxic substances.

### 1.2.2. Denitrification

Heterotrophic micro-organisms can convert organic substrates in the presence of nitrate to biomass and carbon dioxide. This conversion is called denitrification and is performed by the same type of heterotrophic organisms that are normally using oxygen for their growth and respiration. Most of the denitrifying organisms are facultative able to use both oxygen and nitrate as energy source, but preferably use oxygen as oxidising agent.

The reaction consists of a number of intermediate steps e.g.:

$$NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2 \qquad \text{eq. 1.4}$$

Most of the intermediates are toxic or not desired in wastewater treatment plants. Nitrite is for example inhibiting the growth and activity of micro-organism and is therefore used in the food industry as preservative. Nitric oxide was used as poison gas during the First World War and dinitrogen oxide is used for anaesthesia and is a greenhouse gas. The stoichiometric equation of the overall denitrification process without consideration of the intermediate products is:

$$\frac{1}{70}C_{18}H_{19}O_9N + \frac{1}{5}NO_3^- + \frac{1}{5}H^+ \rightarrow \frac{1}{10}N_2 + \frac{17}{70}CO_2 + \frac{1}{70}HCO_3^- + \frac{1}{70}NH_4^+ + \frac{1}{5}H_2O \qquad \text{eq. 1.5}$$

For the growth of the heterotrophic organism due to anoxic conditions the incorporation of nitrogen by the use of ammonium or nitrate is possible. The equations are:

$$\begin{array}{l} 0.61\,C_{18}H_{19}O_9N + 4.54\,NO_3^- + 4.15\,H^+ + 0.39\,NH_4^+ \rightarrow \\ C_5H_7NO_2 + 2.27\,N_2 + 5.98\,CO_2 + 5.15\,H_2O \\ \hline \end{array} \qquad \text{eq. 1.6}$$

$$0.65\,C_{18}H_{19}O_9N + 4.89\,NO_3^- + 4.89\,H^+ \rightarrow C_5H_7NO_2 + 2.27\,N_2 + 6.70\,CO_2 + 5.12\,H_2O \qquad \text{eq. 1.7}$$

If ammonium is the nitrogen source during growth (eq. 1.6) a maximum yield of 0.47 kg biomass/kg organic matter can be estimated. For nitrate (eq. 1.7) a maximum yield of 0.44 kg biomass/kg organic matter is obtained. As long as ammonium is present in wastewater it will serve as nitrogen source for the growth of micro-organisms.

Both denitrification and nitrification processes depend on environmental influences like temperature, oxygen, or the pH variations. In contrast to the nitrification process alkalinity is produced during denitrification. A broad variety of organic substances can be used as organic substrates for the denitrification.

Besides the described nitrification/denitrification principles there exist alternative nitrogen removal possibilities, which are under investigation. One of them is for example the Anammox process, where the ammonium is oxidised under anaerobic conditions (Jetten et al 1998) or the aerobic deammonification (Hippen et al 1998). Van Loosdrecht and Jetten (1996) supply an exemplary overview about the reactions involved in the nitrogen removal processes.

## 1.3.The Biological Phosphorus Removal (BPR)

### 1.3.1. Basic Principle

A long time period has elapsed, between the first reports of biological phosphorus removal (Srinath et al. 1959, Alarcon et al. 1961, Barnard et al. 1974, Fuhs and Chen 1975) and the detailed investigation of the biological phosphorus removal during the last decade. The reason for this long time delay can be found in the non-existent ecological conscience of a generation of politicians and the successful use of chemical precipitation for the elimination of phosphorus from wastewater. With increasing knowledge about the impact of pollution through nutrients like phosphorus, the effort to remove such substances has increased (EU Directive 91/271/EEC).

An effective way for the elimination of phosphorus from wastewater would be the phosphorus uptake in reactors with isolated species of micro-organisms, operated at their optimal performance. But the identification of single organisms like the *Acinetobacter spp.,* responsible for the BPR process (Wentzel et al. 1989) could not be confirmed in practice (Wagner et al. 1993). The task of BPR is assumed to be performed by a rather broad group of micro-organisms (Henze et al. 1995), the phosphate accumulating organisms (PAO). The anaerobic substrate accumulation and storage are assumed to be unique for the PAO. This internal carbon pool ensures a competitive advantage over other heterotrophic organisms. Other heterotrophic organisms were also reported to be capable of storing substrate under anaerobic conditions, especially when glucose rich waste-waters are treated. In those organisms glycogen is stored and no accumulation of phosphorus is reported to occur (Cech and Hartmann 1990).

The general features of biological phosphorus removal are presented in figure 1.1. During anaerobic conditions readily biodegradable substrate in form of acetate is converted to AcetylCoA with the Adenosintriphosphate (ATP) as an energy carrier. Polymerisation of the AcetylCoA to poly-hydroxy-alcanoates (PHA) can be accomplished while consuming reduction equivalents in form of NADH. The consumption of acetate and the conversion to PHA is coupled to the hydrolysis of poly-phosphate, which is released via the cell membrane into the bulk phase and partly used for the generation of ATP. During anaerobic conditions cations are released as well e.g. $Mg^{2+}$, $Ca^{2+}$ and $K^+$, in order to maintain the charge balance (see Comeau et al. 1987, Gerber et al. 1987 and Rickard et al. 1992).

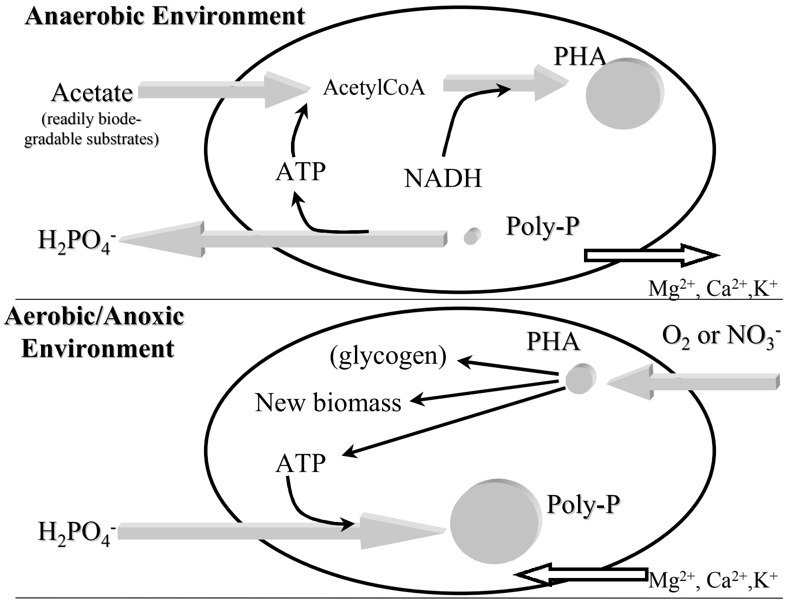


Figure 1.1. The biochemical model of the biological phosphorus removal

During aerobic/anoxic conditions the released phosphorus and an additional amount of phosphorus is again sequestered and stored in the poly-phosphate pool while consuming of ATP. In the presence of an electron acceptor like oxygen or nitrate, new biomass is formed, ATP produced and substrate may be stored in the form of glycogen. Cations are taken up since the charge balance of the cell must be equilibrated. In recent investigations it was shown that this aerobic uptake of ortho-phosphate is also performed with nitrite as electron acceptor (Meinhold et al. 1998).

The concept of the anaerobic storage of acetate (Wentzel et al. 1988) was corrected to readily biodegradable substrates or short chain fatty acids with the investigations of Comeau (1989) on the impact of different substrates on the biological phosphorus removal. Comeau observed that the anaerobic storage also took place for other substrates than acetate. This observation was confirmed in a later study by Satoh et al. (1996). The anaerobic characteristics seem to be different from system to system. Cech and Hartmann 1990 observed a non-favourable behaviour of the BPR process when glucose was used as organic substrate. Carucci et al. (1995) reported opposite results. The positive impact of fermentation products as substrate is however undisputed (Daigger et al. 1995, Lötter and Pitman 1992 and Randall et al. 1994) and acetate is assumed to play a significant role in the anaerobic environment.

The central question during the last decade was how the organisms could supply the necessary reduction equivalents in form of NADH in order to equalise the redox balances. Wentzel (1986) and Comeau (1986) proposed the tricarboxylic acid cycle pathway (TCA) to be responsible for the NADH regeneration. In the TCA cycle one mole of AcetylCoA is converted to 4 moles of NADH with simultaneous production of ATP and carbondioxid evolution. In contrast to this suggestion Mino et al. (1987) and Arun et al. (1988) assumed that the Embden Meyerhof Parnas pathway (EMP) was the main mechanism for the NADH supply. This hypothesis was increasing the complexity of the process such that glycogen is involved in this pathway. 1 mole of glycogen is converted to 2 moles of AcetylCoA, 4 moles NADH, 2 moles $CO_2$ and 3 moles ATP. The dynamics of the glycogen was observed in further studies e.g. Matsuo et al (1992), Satoh et al (1992 and 1994), Cech and Hartmanm (1993), Liu et al. (1994) and Mino et al. (1995). Wentzel et al. (1991) accepted the contribution of glycogen in the BPR process and discussed the Mino model with a degradation of glycogen via the Entner-Doudoroff pathway (ED). In contrast to the EMP pathway only 2 moles of ATP are formed.

*In vivo* $^{13}$C-NMR and $^{31}$P-NMR experiments (Pareira et al. 1996) have indicated that the NADH production was obtained through the glycogen degradation. Pareira et al. (1996) found evidences for the contribution of the EMP pathway and the TCA pathway at the same time. Maurer et al. (1997) showed in $^{13}$C labelled substrate batch experiments and a NMR investigation that metabolised substrate and internal stored glycogen are both involved in the synthesis of PHA. In the subsequent aerobic period the glycogen is formed from PHA. As NADH producing mechanism, the ED pathway is suggested.

The subsequent phosphorus uptake period was thought to require oxygen as electron acceptor (Lötter et al. 1986). The P-uptake however, was reported also under anoxic conditions (Gerber et al. 1987, Kuba et al. 1993, Bortone et al. 1994 and Kerrn-Jespersen et al. 1994) and even nitrite was found to be a possible electron acceptor (Meinhold et al. 1998).

The anoxic uptake of phosphorus was in these investigations found to be much slower than the aerobic uptake. This slower uptake phenomenon can be induced by simultaneous phosphorus release, observed by Gerber et al. (1987). The simultaneous P-uptake and release can be favoured by zonation in biofilms or flocs of micro-organisms (Kayser et al. 1985). Another possible explanation is the existence of two groups of PAO. One group, which can take up phosphorus under aerobic conditions exclusively (PAO) and one, which can use nitrate as electron acceptor as well, the denitrifying PAO (DNPAO). Meinhold et al. (1999) proposed a bio assay to determine the relative amount of DNPAO in the system, based on the aerobic and anoxic initial P-uptake rates in two parallel batch experiments.

### 1.3.2. Process Modelling of the BPR process

From the previous paragraph it becomes clear that the biological phosphorus removal process is not yet fully understood. The development of mathematical models is strongly dependent on the available knowledge about the involved processes. The first attempts for the mathematical description of the BPR processes are made by Wentzel et al (1988, 1989 a, b and 1992). These first attempts were based on the concept of the TCA pathway being responsible for the supply of reduction equivalents (Comeau/Wentzel 1986).

The IAWQ Task Group's Activated Sludge Model No. 2 (ASM2) was introduced by Gujer et al (1995). It improved an existing model for nitrification, denitrification and carbon removal, the Activated Sludge Model No. 1 (ASM1, Henze et al 1987) considerably by the introduction of the phosphate accumulating organism (PAO). The addition of a reaction term, including the denitrifying characteristics of the PAO, was necessary and proposed by Mino et al (1995) and Schmidt et al (1994) in order to consider the observations made by several research groups. The extended version of the IAWQ task group (ASM2d) uses such additional reactions assuming that the PAO can incorporate phosphorus under anoxic and aerobic environmental conditions (Henze, 1998). The production and consumption of glycogen is however not considered. Dold and Briggs (1995) included chemical precipitation of phosphorus to the ASM2. In their case study they found the simultaneous precipitation in a nitrifying plant to be more sludge producing than in a comparable plant with biological phosphorus removal only.

Smolders et al (1995a, b, c, and d) presented a structured metabolic model to describe the dynamic behaviour of storage compounds in the anaerobic and aerobic zones of the biological phosphorus removal process. The model incorporates the concentration of poly-phosphate, poly-ß-hydroxy-butyrate and glycogen as internal storage compounds and reflects therewith in a more specific way the reality of the BPR process. Filipe and Daigger (1998) refined the model by the assumption of a different transport mechanism of acetate into the cell. The consideration of the anoxic uptake of phosphorus by PAO found its expression in a metabolic model presented by Kuba et al (1996) and Murnleitner et al (1997). This model is based on the structure suggested by Smolders et al (1995a, b, c, d). The model has shown, that both aerobic and denitrifying phosphorus removal systems, can be described with the same model, and therewith the same stoichiometric relationships.

The anoxic phosphorus uptake was included into a mechanistic model proposed by Barker and Dold (1997), where the nitrogen removal is based on the ASM1 model and the biological phosphorus removal on the modified Wentzel (1986) model.

## 1.4. Anaerobic Processes

Anaerobic processes are defined as environmental conditions where neither oxygen nor electron donors as nitrate are present. Such conditions are from an energetic point of view very uncomfortable for the micro-organisms. The evolutionary developed strategies for survival are, in comparison to the previous presented groups of micro-organisms, more advanced. Many of the anaerobic bacteria exist only in the absence of oxygen, like e.g. methane-forming bacteria. A significant number of anaerobic bacteria live in symbiosis. One of the advantages of anaerobic processes is the relatively low amount of formed biomass.

The basic mechanism of a simplified three step anaerobic degradation of organic matter follows a simple pattern. Particulate and large dissolved molecules are extra-cellularly hydrolysed into small dissolved molecules. In an acid producing step, acetic acid and hydrogen are formed with subsequent methane and carbon dioxide evolution. The organisms are divided into acid producing or methane producing bacteria. Anaerobic processes are recently applied in Denmark for sludge digestion. This process reduces the amount of produced sludge, hence the financial expenses.

Anaerobic processes are, as the aerobic or anoxic processes, influenced by the supply of nutrients and other conditions such as alkalinity, pH, toxic substances and temperature. The highest biomass specific substrate removal rate is reached for thermophillic processes in a temperature range between 50 C and 70 C. Nevertheless mesophillic processes are widely used with temperatures between 30 C and 40 C.

For the included anaerobic reactor of a biological phosphorus removal system only anaerobic hydrolysis of slowly biodegradable matter and fermentation from soluble organic matter to acetic acid is considered.

# 2. Control of the Activated Sludge Process

Modern wastewater treatment includes today besides organic also nitrogen and phosphorus removal. The motivation for the additional phosphorus and nitrogen removal can be found in the problems associated with eutrophication of receiving waters. The simple and powerful concept is to eliminate the nutrients necessary for growth of micro-organisms which cause eutrophication. Due to economical and ecological reasons, most wastewater treatment facilities employ the activated sludge process (ASP) wherein the wastewater is contacted with a broad mixture of micro-organisms, the activated sludge. The activated sludge serves as a catalyst for the conversion of the wastewater-pollutants to harmless gaseous products or biomass, which can be removed by sedimentation.

As it can be anticipated from the complexity of the biochemical reactions, which have been described in chapter 1, the operation and control of activated sludge processes constitute a nontrivial problem.

- **The primary research effort is therefore the identification of operational procedures and control strategies that will establish high effluent quality under varying load.**

Knowledge from the fields of microbiology, wastewater process design, operation and control engineering must all contribute in order to fulfil the specified research objective.

In the following chapter, an overview is given about control of wastewater treatment plants. It is especially focussed on the activated sludge process and will lead via the basic phenomena involved in the ASP process via dissolved oxygen control (DO) to control of biological nitrogen and biological phosphorus removal. In particular biological phosphorus removal will be addressed Literature reviews and general introductions in control of the ASP can be found in Andrews (1992 and 1995), Beck (1986), Briggs and Grattan (1992), Eckenfelder and Grau (1992), Garett jr. (1998), Harremoës et al (1993), Lant and Steffens (1998), Lindberg (1995), Marsili-Libelli (1995), Ohto (1998), Olsson (1992, 1998a and b), Stephenson (1992a), Stimson (1993) and Vassos (1993).

## 2.1.Main Control Problems in ASP

The performance of the majority of wastewater treatment plants is maintained by the well-experienced staff rather than by scientific based control techniques. The operators of wastewater treatment systems are conscious of the vital changes, connected to the ASP mostly by the monitoring of the alternating hydraulic rates, concentrations and compositions. The concerns of the operators are to

- Maintain the operation of the plant and to escape from major failures,
- Keep the limits for C, N and P, while the operating costs are low,
- Compensate for variability,
- Maintain good settleability.

The process is exposed to disturbances, which are often changing significantly in amplitude. Control actions have frequently a non-linear quality and alternate in structure depending on the operating condition. The control actions are often reduced to the simple rule

**"Rescue the plant"**.

In many cases the well-experienced team can not even accomplish this seeming simple control objective.

## 2.2.General Aspects

The intention of this section is to mediate the necessary background for the control of the activated sludge process. Plant dynamics and measurements are discussed as well as the possible process actuators which are candidates for the manipulation of the process. Simple control loops are explained and the basic ideas of a PID controller of feedforward control are presented.

### 2.2.1.Plant Dynamics

A typical treatment plant has a wide span of dynamics presented in figure 2.1:

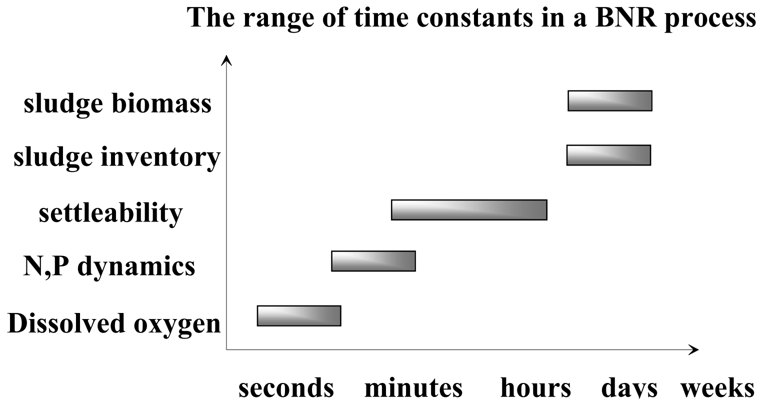


Figure 2.1. Typical time constant ranges for the involved processes in ASP

The variety of different and often time varying constants of the coupled processes makes the control of an ASP complicated. The control problem is of multivariable nature and the manipulation of a variable has frequently an impact on several other process variables.

The growth of the different biomass fractions in the system e.g. demands days to weeks and can therefore only be influenced on a long-term perspective. Seasonal influences have even longer time constants and are not to manipulate at all. The impact of cold weather on the biomass especially the autotrophic organism is strong. All processes with significantly long time constants like growth processes can be affected over weeks, due to the lower temperature. Settleability of the sludge can be influenced by different causes, like growth of filamentous organisms or hydraulic disturbances. Depending on the reasons the impact on the settleability will occur after several minutes, hours or weeks. The nutrient removal processes have time constants in the range of minutes. The respiration and transfer of oxygen are the fastest processes and therefore the dissolved oxygen concentration can change from second to second. Hydraulic disturbances play a dominant role in the ASP process and propagate in 20 to 40 minutes through a plant.

### 2.2.2.Measurements

In order to control the ASP a broad amount of measurements should be collected but this would lead to considerable operation costs. The monitoring of all significant process variables is not feasible. This faces the operation management to take decisions in order to reduce the analytical effort. Examples of important types of measurements are shown in figure 2.2:

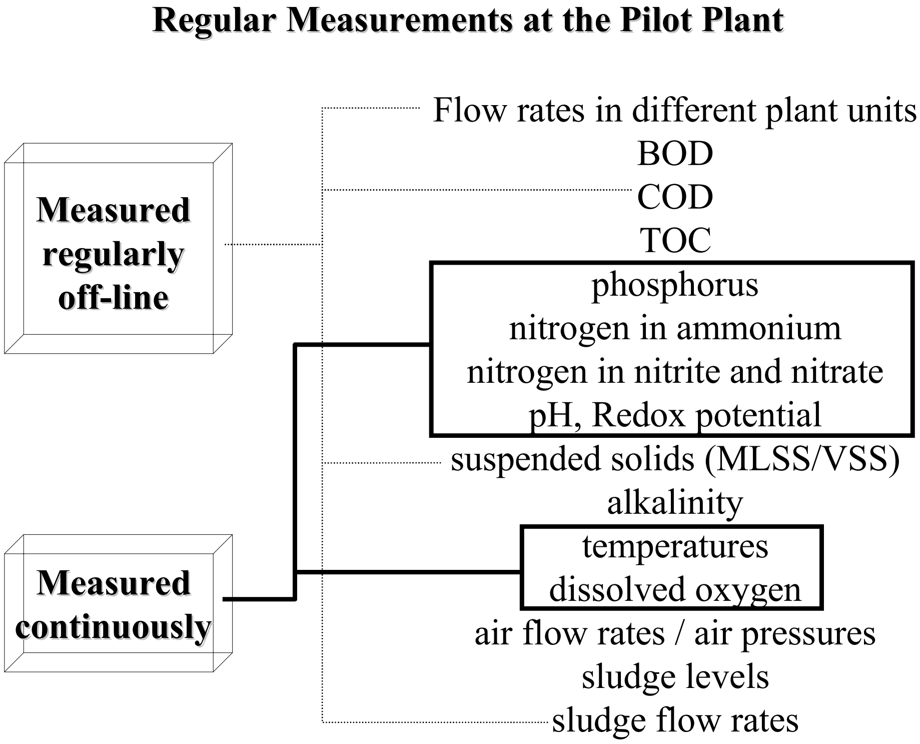


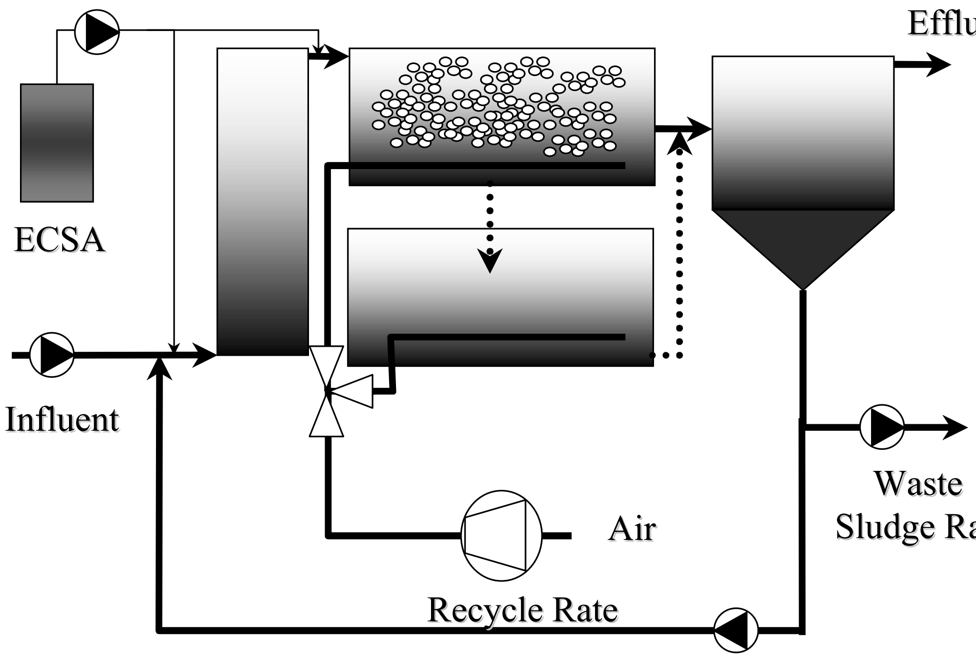
Figure 2.2. Regular measurements at the pilot plant.

Genaey et al (1996) as well as Vanrolleghem and Verstrate (1993) provided an overview about the state of the art in sensor technologies. Isaacs et al (1992, 1994 and 1998a) and Pedersen et al (1990) provided a more specific insight into the monitoring of wastewater treatment systems. Common indirect measurements are the Oxidation-Reduction-Potential (ORP) (Barnes et al 1985, Charpentier et al 1998, Menardiere et al 1991, Wareham et al 1993 and Wouters-Wasiak et al 1994), pH measurements (Wett et al 1998 and Pröll and Nazmul 1994) or the oxygen utilisation rate (OUR) (Surmacs-Gorska et al 1995). As an example for latest developments about measurement techniques Wagner et al (1994) illustrated the development of a rRNA-targeted probe specific for the genus *Acinetobacter* and its application for *in situ* monitoring in activated sludge. Nielsen and Onnerth (1996) proposed strategies for the handling of large amounts of on-line information.

### 2.2.3. Variables for Manipulation

The variables, which can be manipulated in an ASP, are limited. A typical ASP set-up including biological phosphorus removal is illustrated in figure 2.3:

**Variables for Manipulation**



- air flow rate and its spatial distribution
- return sludge flow rate
- waste sludge flow rate
- external carbon source addition (ECSA) or chemical dosage
- cycle length, tubing and internal flows

Figure 2.3. ASP set-up with variables that can be manipulated

An ASP is multivariable. A change of one influent variable effects several output variables, which frequently can not be separated from each other. In this way the change of one manipulated variable will simultaneously affect also other variables which have to be controlled too. Since concentrations and flows change often independently from each other, the control problem becomes of multivariable input multivariable output (MIMO) type. An overview about possible interactions of the control actuators is given in figure 2.4.

**Interactions of the Control Actuators**

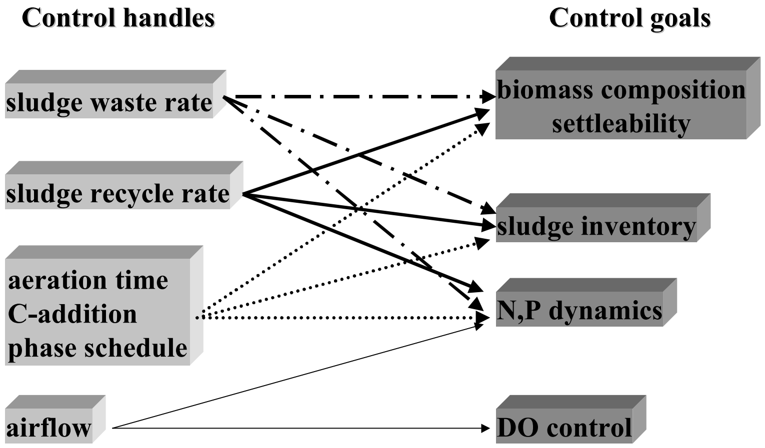


Figure 2.4. Possible coupling between the control handles and control variables

## 2.3. Control Loops

The classical way in which plants are controlled is the implementation of local control loops operated independent from each other. These local controllers have frequently the main purpose to react to small deviations around a steady state operation than to significant process disturbances. In many situations the well-experienced operators are overruling even such local control loops. Often the impact of the operators becomes even more important when the level of automation and control equipment of the process increases whereas the opposite should be the goal. This status is the result of insufficient process knowledge and often the absence of reliable on-line analysis systems.

The future dominant role of computer systems in local control loops and advanced process control is unquestionable. The computer assistance will develop simultaneously the control of fast feedback processes and help in design of operational control strategies for processes with slow dynamics. The impact of interactions in these processes can often be observed only gradually and with much analytical effort. With respect to complex interactions computer calculations can be provide powerful tool to predict the behaviour of the process over a longer time horizon. As an intermediate step to the incorporation of on-line models for assisting operators, the use of expert systems or knowledge based strategies can become important. In such systems, described by Barnett (1992), Collins and Ellins (1992) and Ladiges and Kayser (1993), the operation of the plant is guided by information, which has been gathered during previous experience.

### 2.3.1. Simple Controller

A great number of local controllers are present at different units in a wastewater treatment plant. Their objective is to maintain controlled variables in specific regions. This is frequently achieved by simple strategies without the use of models. A separation between open loop and closed loop controllers can be made. In open loop, the control actions are often based on a timer. Examples for such loops are the control of sludge transporting pumps or of the aerators of the reactors. A qualitative representation of such control actions are shown in figure 2.5:

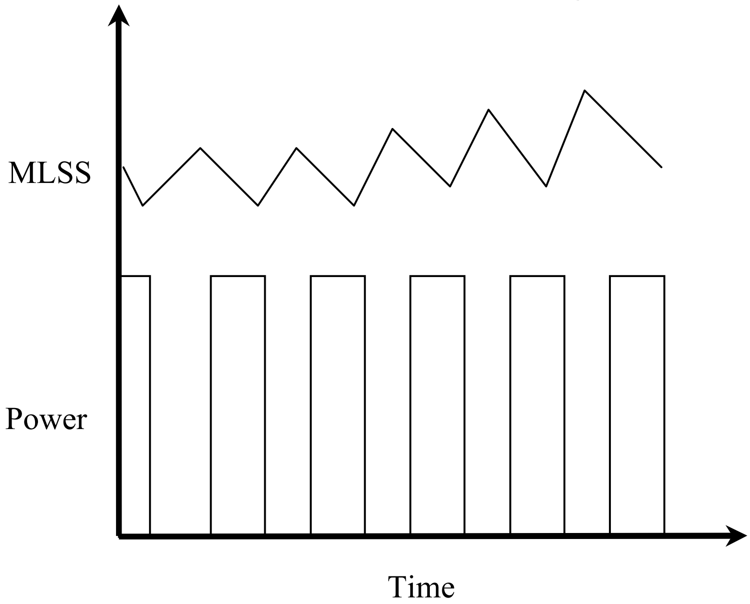


Figure 2.5. On-Off control of dissolved oxygen concentration

In closed loop control actions, the PID controller is used in the overwhelming part of treatment plants The basic principle is demonstrated in the next subchapter.

### 2.3.2. Feedback Controller

In a feedback controller (figure 2.6.) the input to the regulator is the output error, which is the difference between the reference signal (setpoint) and the measurement of the output y. The controller output is a linear combination of functions of the output error, the integral of the output error and the derivative of the output error. In this way it is possible to counteract the disturbances in a flexible way. A major problem is the identification of the time constants and the gain factor for such controller. Examples for tuning procedures can be found in Babatunde et al (1994) or Stephanopolous (1984).

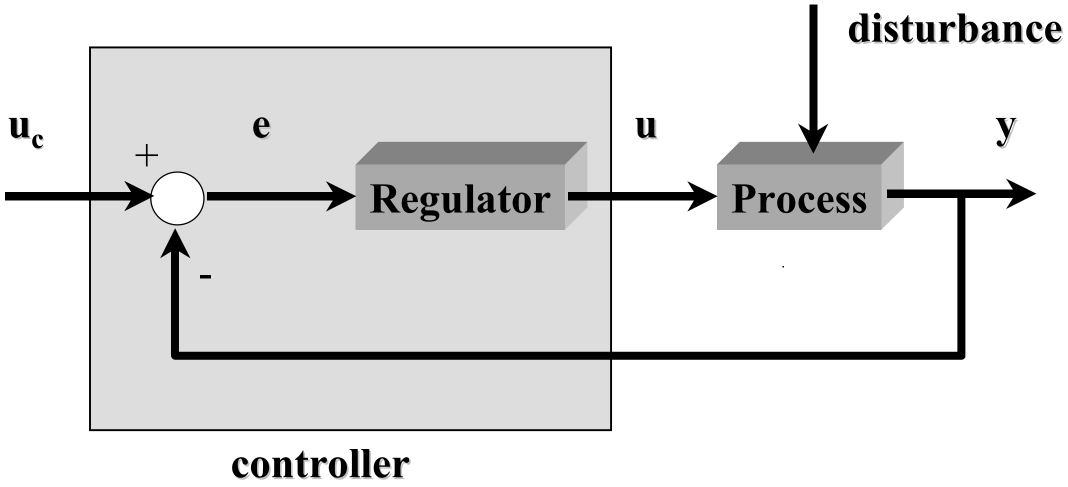


Figure 2.6. Feedback control structure

The PID controller is the most common controller used in chemical process control and hence it is also frequently used in control of wastewater treatment processes. The addition of chemicals, the control of flows or even the dissolved oxygen concentration is often controlled by this simple concept. The application of such uncomplicated control strategy is strictly limited. As soon as the normal characteristics of the ASP dominates (non-linear or time variant behaviour), the PID control is difficult or infeasible. Time delays, time varying or unknown parameter, interactions between the biological processes or non-linear parameters will complicate the tuning of the PID controllers. Often the tuning is difficult or impossible due to their multivariable and nonlinear characteristics. Very often the design of a setpoint is not easy to obtain. Models or at least an understanding of the process is needed for the advanced control of the ASP.

### 2.3.3. Feedforward Control

An example for a simple local controller using knowledge or a model is the feedforward control structure. It overcomes the obvious limit of feedback during which the corrective actions can first be taken when the influence is seen at the output of the system. In many process control applications it is possible to measure the disturbances coming into the system. Measurements of these disturbances can be used to perform control actions before the impact is noticed at the output of the process. This control structure is named feedforward control and the response of such feedforward control will be considerably faster than a simple feedback structure. The basic principle is demonstrated in the following figure 2.7:

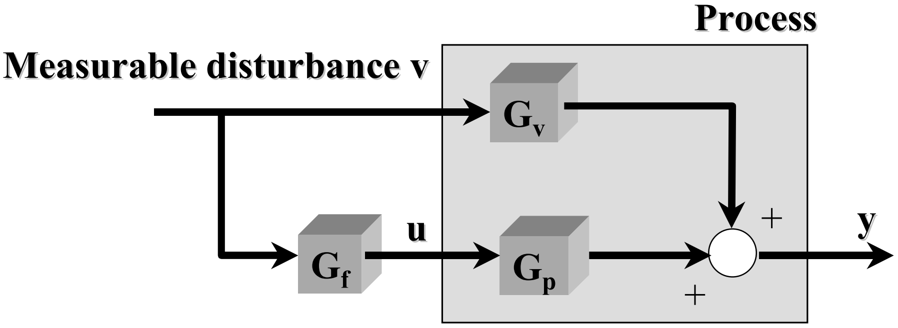


Figure 2.6. Feedforward control structure

The objective in the feedforward control structures is to determine the transfer function $G_f$ of the controller such that the influence of the measurable disturbance v can be adjusted or reduced. A combination of feedforward control and feedback is in general possible.

Examples for local feedback loops or feedforward control are:

- Production of a well defined air flow rate to the aerators
- Dissolved oxygen control
- Dosage control of chemicals (denitrification or phosphorus removal) is often based to some extend on feedback, such as flow rate

Any control that will outperform the local control actions must be based on quality-related or model-related behaviour. The controller has to get its information from several sensors or from estimated variables. The choice of the setpoint is often nontrivial and closely related to the choice of operating conditions.

## 2.4.Models

For the successful feedback control of the activated sludge process, a general understanding of the investigated system is necessary. A reliable model of the dynamic system and the analysis of the response to process disturbances are basic prerequisites. The trade off between relatively simple on-line models and complex structured models can be seen as a major problem in the automation of a biological wastewater treatment plant. In biological systems, the assumption that any experiment can be repeated is not true. The process behaviour is often not predictable due to the lack of understanding or significant change of the environmental conditions. The detection of the change in operating conditions is often done with the help of recursive identification techniques (Ljung and Söderström, 1983 and Ljung 1987), which is a powerful tool in this respect. In such recursive methods the input and output information of a process is observed over a time horizon and a often linear model is used for the prediction of the future output values. An example for such models will be given in the next subchapter.

### 2.4.1. Models for Control

The applied models for control are usually simple or reduced forms of more complex or structured models. One of the prerequisite characteristics of such model is that it can be validated by measurements from an existing monitoring system of the controlled plant. The models can be of pure statistical nature or based on conservation balances in which case the model parameters have a physical interpretation. Nevertheless engineering scientists usually prefer structured models, while in practice input-output models are most often used. Such models may be derived from actual input-output measurements using suitable estimation algorithms.

As a typical example of input-output models a time series model is presented [Beck (1986)]. Generally the models are time-invariant and linear and are adapted to specific operating conditions, which limits their range of application.

$$y(t_k) = -a_1 y(t_{k-1}) - a_2 y(t_{k-2})\ldots - a_n y(t_{k-n}) + b_0 u(t_k) + b_1 u(t_{k-1}) + \ldots b_n u(t_{k-n})$$
$$+ c_0 e(t_k) + c_1 e(t_{k-1}) + \ldots c_n e(t_{k-n})$$

y = process output
u = process input
e = process and measurement noise

$a_{i\ldots n}$, $b_{0\ldots n}$,$c_{0\ldots n}$ = constants

$$\theta = [a_1, \ldots, a_n, b_1, \ldots, b_n, c_1, \ldots c_n]^T$$

the regression vector is

$$\varphi = [y(t_{k-1}), \ldots y(t_{k-n}), u(t_k), \ldots, u(t_{k-n}), e(t_k), \ldots, e(t_{k-n})]$$

$$y = \varphi \cdot \theta \qquad \text{eq.2.1}$$

The updating of the parameter vector is like

$$\hat{\theta}(tk+1) = \hat{\theta}(t_k) + K \cdot [y(t_k) - \hat{y}(t_k)]$$

$K$ is a gain factor

$y(t_k)$is the current measurement

$\hat{y}(t_k)$is the predicted measurement

This example describe in eq. 2.1 is an ARMAX model (auto-regressive, moving average model with an external input) and the parameter $a_i$, $b_i$ and $c_i$ are determined from measurements of y and u. Variables that are not measurable can be reconstructed by combining a first principal mathematical model with primary measurements. The parameter $a_i$, $b_i$ and $c_i$ may vary slowly with time. Using recursive estimation, the parameters can be tracked on-line and corrected for each new measurement obtained, provided that the process is persistently excited. The parameters are stored in a parameter vector θ.

### 2.4.2. Parameter Identification for Structured and Unstructured Models

Independent of the type of model used, the parameter values have to be estimated in order to apply the model during dynamic process investigations, different from the linearized steady state. The calculation time needed for the mathematical solutions of structured models has considerably decreased with increasing developments and advances in the computer industries. Therefore it is possible today to add knowledge to the time series approach. The model is significantly improved in this way and it is possible to obtain a higher accuracy of the system. Johansen (1996) presents general considerations about the identification of non-linear systems using empirical data and prior knowledge.

Typical examples of structured deterministic models are the models described in chapter 1 on biological processes involved in the BPR process. The structure of such models is complex and the number of parameters, which have to be estimated, can be high. One of the procedures for the parameter estimation of such structured or unstructured models is an evolutionary or genetic approach. In both procedures, the dynamic (often non-linear) model of the system is simulated and compared with experimental data. The adjustable parameters are modified until the best model fit to the measurements is obtained. A typical structure for such procedure is presented in figure 2.8:

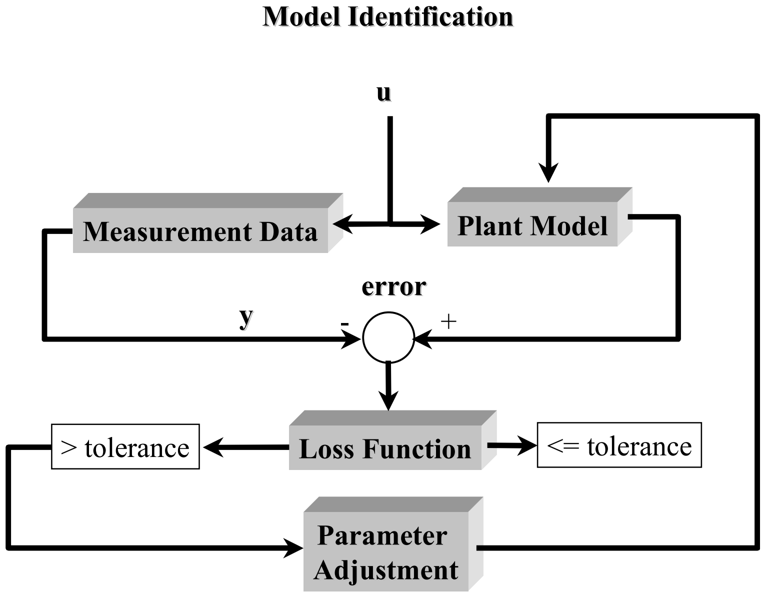


Figure 2.8. Parameter estimation for structured or unstructured models

A parameter estimation procedure is briefly presented with the example of a reaction rate of the Monod type having the following form:

$$r = \mu \cdot \frac{C_S}{C_S + K_S} \cdot X_{BM} \qquad \text{eq.2.2}$$

With r the reaction rate, μ the growth rate, $C_S$ the substrate concentration and $X_{BM}$ the biomass concentration.

It is assumed that the concentration of biomass is known and that the substrate concentration can be measured. This implies that the reaction rate can be calculated useing eq. 2.2. The growth rate is assumed to have a value of 3 $d^{-1}$ and the saturation concentration $K_S$ is assumed to be 20 $mgC_S/L$. The objective function is defined as

$$J = \sum_{1}^{i} \sum_{1}^{n} W_i \left( y_i - \hat{y}(\theta)_i \right)^2 \quad ; \quad y_i(0) \qquad \text{eq. 2.3}$$

y is the measurement of component i, $\hat{y}_i$ the model prediction of component i, $\theta$ the parameter vector, $y_i(0)$ the initial values, n the number of measurements which are used for the estimation procedure and $W_i$ a weighting factor for the different components. The simulation result of the parameter estimation is shown in figure 2.8.

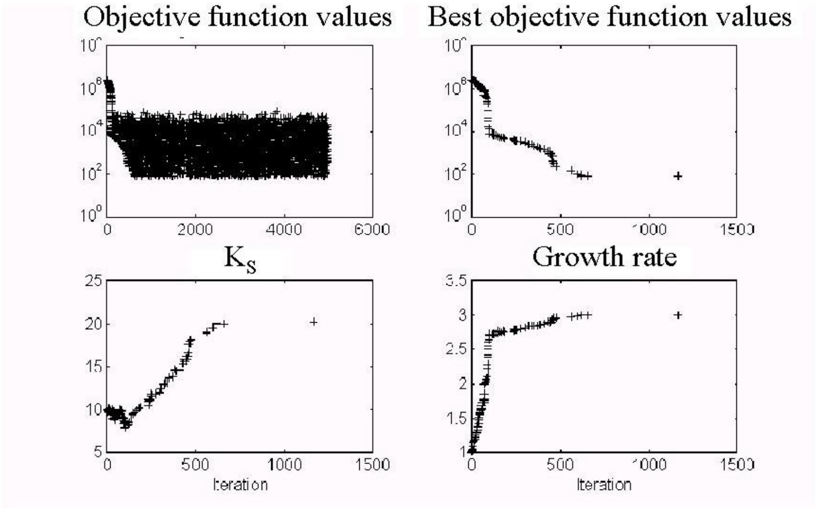


Figure 2.8. Simulation results of parameter estimation

It can be recognised how the objective function values (e.g. the sum of least squares between measurements and predictions in the upper left subfigure) are in the beginning very fast improved (from $10^8$ to $\sim 10^2$ ). Afterwards the variations of the parameters result only in very slow improvements of the objective function. In order to improve the overview only the first 1500 iterations are shown and for the objective values the best values are presented in the upper right part of figure 2.7. The development of the estimates are presented in the lower subfigures. In the left subfigure the transient of the saturation concentration is presented, while in the right subfigure the growth rate over the iterations is shown. In the lower subfigures it can be observed how the as unknown assumed parameters are moving into the direction of the "real" values. The growth rate is after approximately 600 iterations estimated to a value of 3 d-1 as well as the saturation concentration is at this point of time estimated to a value of appr. 20 mg/L. In all four subfigures a characteristic change of the slopes can be observed. This is coupled with the fast estimation of the growth rate, which approaches the region of the correct magnitude first. Thus the influence of the saturation concentration begins to influence the loss function approximately to the same extent as the variation of the growth rate.

A structural problem of such parameter identification is that the procedure could end in a local minimum. This would represent the case that the changes of parameter from iteration to iteration do not improve the objective values, while a potential still exists, for improvement. This could be the case, when simultaneously the amount of biomass and the growth rate is searched via an estimation procedure. Goldberg (1989) describes a genetic algorithm in order to overcome such local minima, while Johansen (1996) suggests the use of prior knowledge. However the work of Carstensen et al (1995) indicates that the statistical estimation of Monod-kinetic parameter from on-line measurements is possible. Marsili-Libelli (1989a, 1992a) describes the estimation of parameters or characteristic dynamics of wastewater treatment systems. Further examples for the adaptive estimation for non-linear bacterial growth systems are given by Dochain and Bastian (1984, 1990a and b), Hiraoka and Tsumura (1989), Jeppson and Olsson (1993), Jeppson (1995), Julien et al (1998) and Marsili-Libelli (1989). Jeppson and Olsson (1993) describe reduced order models for the on-line parameter identification of the activated sludge process. Vanrolleghem et al (1995) investigates the practical identifiability of a bio-kinetic model of the ASP.

## 2.4.3. Advanced Control Strategies in the ASP

A reliable dynamic model can be used for the implementation of advanced control strategies. A typical example is the application of optimal control in the wastewater treatment processes. An objective functional is solved and a control policy is chosen which optimises the functional. Model predictive control may be viewed as one implementation of an optimal control strategy where an explicit prediction of future plant behaviour is calculated with subsequent computation of the corrective control action, required to match the predicted output as closely as possible to a desired targeted trajectory.

The advantages model-based control strategies, which are frequently called model predictive control (MPC) systems, are obvious. They can be used for multivariable systems and handle interactions between different processes with ease. Time delays and other difficult process dynamics can be handled. Any kind of model can be used in a MPC control structure. Measurable disturbances are via the feedforward principle rejected, while the non-measurable disturbances can be eliminated via feedback of the error. Since the nature of MPC is an optimisation problem any kind of constraint and reference trajectory can be handled and the control effort can be optimised.

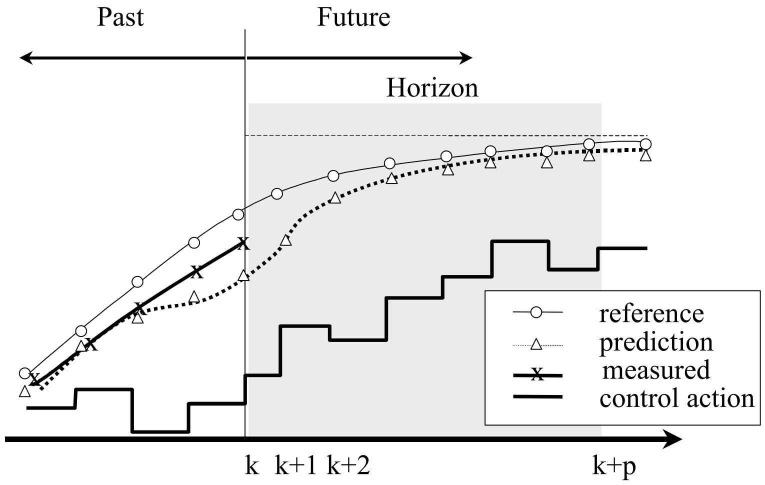


Figure 2.9. Model Predictive Control Strategy

Although model based control strategies are extensively used in chemical industries their application in wastewater treatment ASP is relatively scarce (e.g. Menzi and Steiner 1995). A reason for this circumstance may be the low level of on-line instrumentation and the lack of economical interest for better-controlled systems. While in chemical industry an improvement of the control is connected to a higher profit the improvement of a higher control level in ASP is primarily connected to higher economical effort.

Babatunde et al (1994), Deshpande (1989) or Morari and Lee (1998) provide overviews on model predictive control, while Chen and Shaw (1982), Mayne and Michalska 1990, and Michalska and Mayne (1993) explain the idea of receding horizon optimal control (RHOC). Applications of optimal control strategies are investigated by Kabouris and Georgakakos (1990), Kabouris et al (1992), Lukasse et al (1998b and c, 1999), Marsili-Libelli (1984) and Zhao et al (1994a). First investigations, where the idea of recursively identification was performed, are studies from Dupont and Sinkjær (1993) and Thornberg and Thomsen (1994).

Aspegren et al (1992), Chang et al (1998), Coen et al (1997 and 1998), Hiraoka and Tsumura (1989), Isaacs and Thornberg (1998) and Nielsen et al (1993) carried out further investigations with applications of model based control strategies or model based predictions. General aspects of the use of on-line models in the process control of ASP are discussed by Jumar et al (1998) and Lindberg (1998) studied specific aspects of multivariable modelling and control.

This chapter attempts an overview of process control in the ASP. Therefore a few other approaches are mentioned. Fuzzy control is investigated by Marsilli-Libelli (1992 a and b) and Tong et al (1980). Another topic of advanced control methodology in the ASP applies neural nets which were studied by Cote et al (1995), Kuo and Melsheimer (1998) and Minderman and McAvoy (1993) while Rauch and Harremoës (1999) propose a genetic algorithm for the real time control of urban wastewater systems. Information about stochastic control can be found in Kabouris and Georgakakos (1991) and Novotny and Capodaglio(1992). Sanchez and Cortes (1996) describe an integrated approach for the distributed architecture of a wastewater treatment supervision. Rosen and Olsson (1998) inspect the topic of disturbance detection. Knowledge based systems were investigated by Barnett (1992), Serra et al (1997) or Vanrolleghem et al (1991).

## 2.5. Dissolved Oxygen Control – an Example for Different Approaches

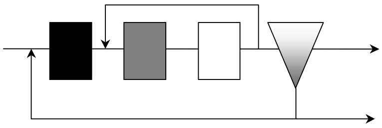
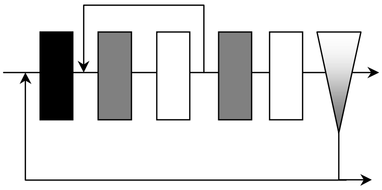
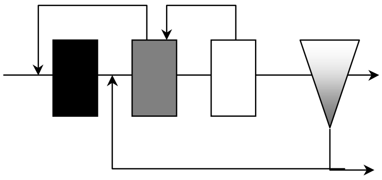
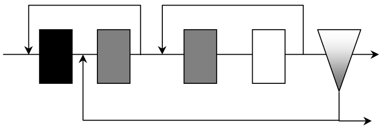
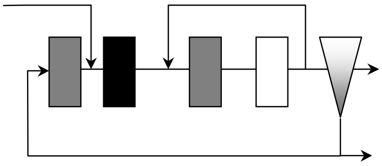
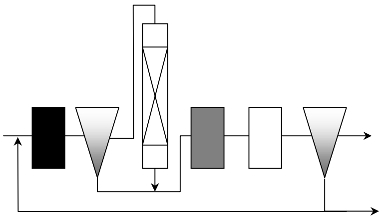
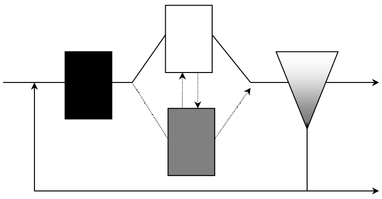
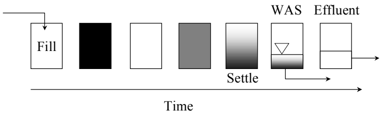
The dissolved oxygen concentration is due to the comparatively inexpensive measurement sensors the most controlled variable in the ASP. The problem to maintain a certain setpoint of the DO concentration e.g. 2 mg/L can be considered to be solved (Isaacs and Kümmel 1993; Lee et al 1998, Lindberg and Carlsson 1996b; Marsili-Libelli et al 1985; Olsson and Andrews 1981; Olsson et al. 1985b). The variety of solutions to the problem is extensive. It reaches from timer control, manual control, simple feedback control or cascade control (combination of DO setpoint and air flow control) to more advanced solutions like predictable parameter variations-gain-scheduling-control and self-tuning control. Meanwhile the research effort was focussed on the additional information that can be gained from DO measurements. The estimation and control of the biological activity is already described (e.g. by Olsson and Andrews 1978a and b). Hence the determination of the respiration rate in the activated sludge process has rapidly developed and is used for the control of the ASP as well as for the characterisation of influent (Brouwer et al 1998; Carlsson 1993; Edwards and Sherrard 1982; Holmberg and Olsson 1985; Holmberg 1987; Holmberg et al 1989; Klapwijk et al 1992 and 1998; Larose et al 1997, Lukasse et al 1997 and 1998a; Marsili-Libelli 1982 and 1990; Spanjers and Olsson 1992; Spanjers et al 1996 and 1998 and Vanrolleghem and Spanjers1998).

One of the associated troubles with the analysis of the respiration rate is the lack of reliability of the DO sensors. The proper functioning of the sensors have to be verified before the DO dynamics can be used for further analysis. Lindberg and Carlsson (1996b), Suescun et al (1998) and Spanjers and Olsson (1992) investigate the reverse filtering of measurements with the intention to detect faulty measurements.

## 2.6. The Operation and Control of Nitrogen Removal Processes

The nitrogen removal process is a rather complex interaction between autotrophic and heterotrophic organisms demanding different environmental conditions in order to establish nitrogen removal. In an aerobic reactor the nitrification takes place and afterwards in an anoxic reactor the nitrate is in presence of organic substrates converted to molecular nitrogen. The bottleneck in the process is the requirement of organic substrate for denitrification while on the other hand the nitrification has to be performed first, with simultaneous conversion of organic matter due to the presence of oxygen. The most commonly used concepts are the continuous flow process with recycle of the nitrified volume to the anoxic tank and the alternating concept, where the reactors are operated with alternating aeration and flow distribution. A possible immobilisation of the autotrophic organism in a biofilm reactor is also possible as the operation in sequencing batch mode. Descriptions of the processes can be found in Arvin (1985), Bortone et al (1994 and 1996), Morgenroth (1998), Thornberg et al (1993) and WRC (1984). The most common used processes in praxis are listed in table 2.1, including an anaerobic reactor for BPR:

Table 2.1. Frequently used processes for BNR

| | |
|---|---|
| Bardenpho |  |
| modified Bardenpho |  |
| UCT |  |
| modified UCT |  |
| Johannesburg |  |
| Dephanox™ |  |
| | **Alternating concepts** |
| Biodenipho™ |  |
| Sequencing Batch Reactors |  |

■ Anaerobic ▨ Anoxic □ Aerobic ▽ Settler ⊠ Biofilm Reactor

Control handle candidates for the BNR removal are the manipulation of the air-flow rate into the aerobic reactors, the sludge waste rate (WAS) or the aerated volume of the plant, which means the distribution of the air in a continuous system or the aeration time in the alternating system. The WAS was found to be unsuitable for the control of the N-removal process, since the connected interactions with the sedimentation tanks and the delayed impact of control action stands in opposition to the obtained improvements (Vaccari and Christodoulatos, 1989).

The focus in control of the nitrification process is in the overwhelming applications the control of the dissolved oxygen concentration at a setpoint value (see chapter 2.5). A completely different approach is the control of a flexible nitrification volume in order to compensate influent variations (Brouwer et al 1998).

The control of the denitrification takes place either via the re-circulation of the anoxic effluent from the aerobic reactor to the anoxic reactor or via the anoxic periods in the alternating concept. In the continuous approach two control handles are possible, the size of the flexible anoxic zones for example by the use of less aerators or the degree of re-circulation. For the alternating processes the cycle length can be variable, as well as the flow rate through the system. In summary two control handles are possible in both approaches. Typical examples for the control of different cycle length or flows between the alternating tanks are Isaacs (1996), Lukasse et al (1999), Thomsen et al (1998) or Zhao et al (1994 and 1995).

For both concepts a third possible control handle is the external addition of a carbon source (ECSA) to the anoxic zones or periods, which accelerates the denitrification process. Examples for such addition can be found in Barros and Carlsson (1998); Demynck et al (1994); Gerber et al. (1986); Hallin et al (1996), Isaacs et al (1993a and b, and 1994); Isaacs and Henze (1995) and Lindberg, Mavinic and Carley (1991) and Carlsson (1996). The main disadvantage of the very effective ECSA is the economical burden, if no inexpensive carbon source is available. The second drawback is the extra production of sludge. The ECSA should therefore only be applied when no other control or operational actions can improve the situation in the process. The importance of volatile fatty acids for the control of BNR processes was however investigated by Armiger et al (1993) when he controlled the waste load to biomass ratio (VFA/M) independent of hydraulic flow fluctuations.

Another feasible way to remove nitrogen is the simultaneous nitrification and denitrification in one reactor, where the dissolved oxygen concentration is kept at a low level (Kayser and Ermel 1985) like for example 0.5 $mgO_2/L$. A zonation in the activated sludge flocs takes place and ensures the nitrification in the outer zone, which is oxygen penetrated. The inner part of the floc is exposed to anaerobic conditions while the intermediate zone has anoxic environments, enabling denitrification.

Bundgaard and Pedersen (1991) performed investigations of operational factors affecting the BNR processes.

An evaluation of the quality of the different processes is not the intention of this thesis. Each process has advantages and disadvantages and the broad use of different design approaches illustrate that no optimal design of the nitrogen removal process has materialised yet.

## 2.7. The Operation and Control of Biological Phosphorus Removal

The level of complexity for the BPR is increased in comparison to the nitrogen removal process. A third group of micro-organism, the PAO, is enriched in the system via the introduction of an anaerobic reactor upstream of the aerobic or anoxic reactors and enables biological phosphorus removal. The PAO compete with the heterotrophic organisms for substrate and have developed a more complex strategy for growth and respiration than most of the other heterotrophic organisms. Cyclic changes between anaerobic/aerobic (or anoxic) conditions are a prerequisite condition for the survival of PAO as well as the accumulation of internal storage products like poly-phosphate, poly-hydroxy-alcanoates or glycogen.

In comparison with the other involved biological processes the BPR is relatively poorly understood. A large number of investigations can therefore be found were phenomenological aspects are explored. These phenomenological studies cover single organism cultures (Stante et al 1997 and Wentzel et al 1986), BPR under anoxic conditions (Bortone et al 1994 and 1996; Meinhold et al 1998 and 1999, Kerrn-Jespersen and Henze 1993; Kerrn-Jespersen et al 1994, Kuba et al 1993, 1994, 1996a and b and Wachtmeister et al 1997), the impact of different substrates (Carucci et al 1997, Comeau 1989 and Tasli et al 1997), pH influence (Bond et al 1999 and Smolders et al 1994) or possible magnesium and potassium limitations (Rickard and McClintock 1992).

The studies which are focussed on the operational factors affecting the BPR process are numerous (Ayesa et al 1998, Carlsson et al 1996; Jönsson et al 1996; Lee et al 1996; Lee et al 1997; Meinhold et al 1999; Morgenroth 1998; Rodrigo et al 1996; Satoh et al 1994; Schlegel et al 1992; Shehab et al 1996 and Wachtmeister et al 1997). Operational strategies using an external carbon source addition have been found to be favourable for the BPR process. The addition of external carbon improves the performance of BPR and a large fraction of influent readily degradable carbon is desirable (Lotter and Pittman 1992; Meinhold et al 1998; Quasim et al 1996; Randall et al 1994 and 1997; Teichfischer 1995 and Temmink et al 1996).

The implementation of control strategies for the biological removal of phosphorus is particularly small, which may be connected with the lack of reliable measurement equipment for the on-line monitoring of phosphorus or the financial efforts for the installation. A further limitation for advanced control strategies is the lack of understanding of the BPR process. The number of articles on control of BPR is very low. One central point of the investigations is the use of the Oxidation Reduction Potential (ORP) signal as control handle for the BPR. Charpentier et al (1989) investigated points of inflection of the ORP measurement data, which are possible to use for the control of wastewater treatment plants. With their help the aerobic, anoxic or anaerobic environment conditions can be detected. He demonstrated that the ORP control strategy could be transferred from pilot plant experiments to full-scale plants. Menardiere et al (1991) confirmed that the ORP-signal can be used for control purposes for the optimisation of C, N and P removal. The ORP signal was used for the aeration of the aerobic/anoxic reactor and it was used for the monitoring of the anaerobic conditions at the plant. It was illustrated that the simultaneous N and P removal is possible in a two-series reactor system, and the operating conditions in such a system can be controlled by setting ORP limits for operation. The operation was however dependent on the span of ORP limits. The experimental full-scale investigation revealed that the dilution of the influent wastewater composition has a negative impact on the phosphorus removal capacity. Sasaki et al (1993) investigated a 2-tank intermittent aeration of time sharing method and used a control system which is based on the ORP measurements. With help of the inflection or bending points the aerobic, anoxic and anaerobic periods of one cycle were designed. The investigations were performed on a pilot scale system with synthetic wastewater.

Larose et al (1997 and 1998) proposed a method to control the duration of an anaerobic period in a sequencing batch reactor with help of respirometric measurements. In his method samples were withdrawn from the anaerobic reactor phase aerated and thereafter the OUR was determined. A sudden change in the OUR dynamics was an indication of the complete consumption of acetate.

Based on these measurements the anaerobic phase length could be flexibly designed. The experimental investigations demonstrated that respirometry could successfully be used not only for the characterisation and control of aerobic processes but also for the flexible design of the anaerobic periods of a SBR.

The previous investigated control approaches for BPR processes are based on periodic sequences which possess special dynamic characteristics, used for the development of control strategies. Lee et al. (1999) examined a re-circulation plant by simulation. A genetic distributed parameter model-based control (GDPMC) strategy is the methodological focus of the investigation. The simulation study intends to control the entire BNR activated sludge plant by a multi-unit decentralised GDPMC strategy. The performance of the strategy has in comparison to well-tuned PI controllers in terms of the integral time absolute error (ITAE) improved the BPR. The control structure is based on an external carbon source addition and manipulation of the sludge recycle rate to maintain a maximum PHA uptake by the PAO in the anaerobic reactor. This goal is achieved by the simultaneous control of the acetate and $PO_4$-P concentration, in one of the compartments of the anaerobic reactor. For simulation purposes the ASM2 model is used and is validated with experimental data of a pilot plant. The determined parameters are similar to the default parameters of the ASM2. In some simulation cases the biological phosphorus removal is not sufficiently high to satisfy the required effluent limits. In this connection the conclusion that both the $PO_4$-P concentration and the acetate concentration have to be controlled to ensure low effluent $PO_4$-P concentrations is however not fully understandable. It seems that control of both $PO_4$-P and acetate concentrations is necessary but not sufficient to ensure low effluent $PO_4$-P concentration.

Considering the complexity and the importance of the BPR process, it is of strong interest to increase the effort in that area of control. An important prerequisite for the development of advanced control strategies in BPR processes is the availability of valid models. The work of Chang et al. (1998) investigates the prediction of effluent suspended solids from a dynamic enhanced BPR system.

Based upon the literature review there is a need for investigation of which disturbances are detrimental for BPR. If the understanding of those disturbances is possible control designs can be developed for handling the disturbances.

# 3. Material and Methods

## 3.1.The Pilot Plant

The biological phosphorus removal process occurs in a complicated network of biological reactions, performed by micro-organisms. The micro-organisms in the activated sludge culture compete for the limited substrate resources. To establish BPR, the culture has to be exposed to cyclic changes of environment in form of anaerobic and aerobic (or anoxic) conditions. For the nitrification process an appropriate long aeration period must be included whereas the aeration processes do not interfere with the denitrification process, where however an organic substrate is needed.

The investigated system is an alternating BIODENIPHO™ pilot plant that includes cyclic changes of flow and aeration in order to satisfy the above requirements. The plant and its control structure are presented in figure 3.1. The characteristic technical details are presented in table 3.1.

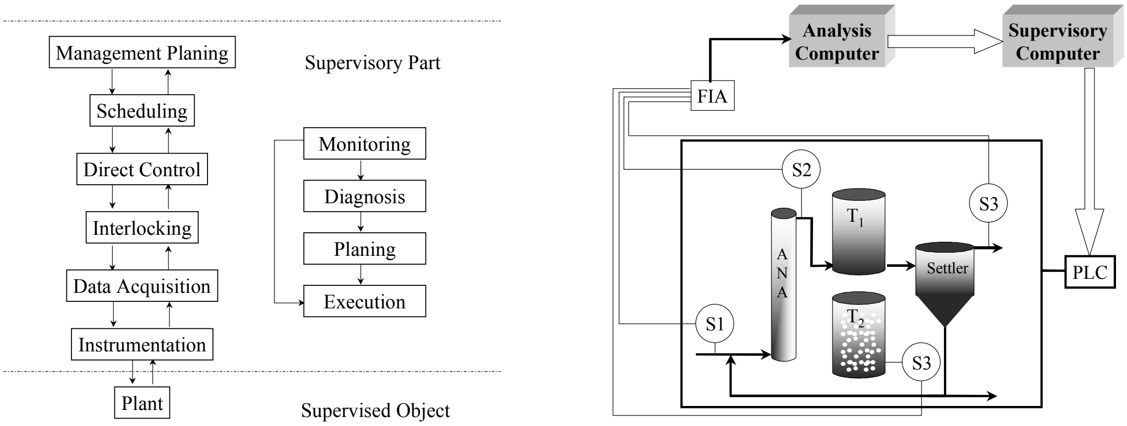


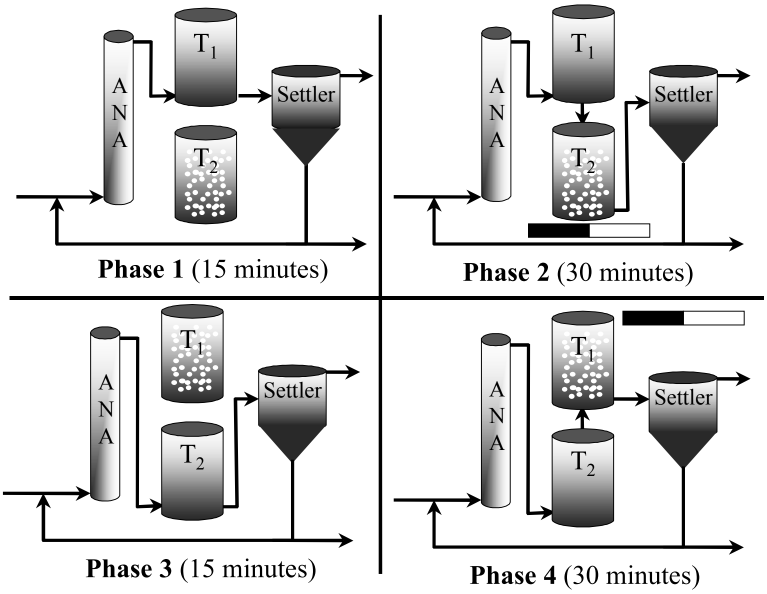
Figure 3.1. The Pilot Plant and the Control Structure

Table 3.1. Technical Specification for the Pilot Plant during Normal Operation Periods

| Volume | Anaerobic Reactor | Tank 1 | Tank 2 | Settler |
|---|---|---|---|---|
| in litre | 200 | 800 | 800 | 1000 |
| Flows | Influent | Return Sludge | Waste Rate | Effluent |
| in l/h | 90 | 90 | 2.5 | 87.5 |
| Average Inventory | MLSS Tank 2 | MLSS Return | MLVSS Tank 2 | MLVSS Return |
| in g/l | 3.5 | 7 | 2.8 | 5.6 |
| SRT | T | pH | DO | SVI |
| ~15 days | ~18  C | ~7.4 | 2 mg/l | ~110 ml/g |

Ammonium nitrogen ($NH_4$-N), nitrate plus nitrite nitrogen ($NO_x$-N) and ortho-phosphate ($PO_4$-P) are measured automatically by flow injection analysis (FIA) at the sample points S1-S4 shown in figure 3.1 which are the inlet wastewater, the exit of the anaerobic tank, in the aeration tank 2, and the effluent stream, respectively. An analysis computer receives the information of the FIA unit and transmits the measured values after mathematical processing to the supervisory computer equipped with a real-time multitasking software system FactoryLink. With help of this supervisory software program it is possible to introduce control actions which overrule a programmable logical controller (PLC) which has basic control authority

The BIODENIPHO™ system is flexible since it can be operated in many different schemes and cycle length. For the process investigated here one cycle consists of four phases and lasts 90 minutes. During all phases of a cycle the anaerobic reactor and the settler are operated as continuously fed reactors i.e. chemostats. The effluent of the anaerobic reactor is always passed to the anoxic tank of the phase as shown in figure 3.2. This operation particular ensures that the wastewater, which is still rich of soluble and particulate organic matter, supports the denitrification processes in the anoxic phase of the reactors, while the readily biodegradable organic matter is available for the phosphate accumulating organism in the anaerobic reactor.



**Phase 1** (15 minutes)

**Phase 2** (30 minutes)

**Phase 3** (15 minutes)

**Phase 4** (30 minutes)

Figure 3.2. Operation Schedule of the BIODENIPHO™ Pilot Plant (■□ indicates a partly aeration of the possible 30 minutes)

In phase 1, which lasts 15 minutes, the wastewater flows under anoxic conditions through the first tank into the settler, while the second tank is separated, and aerated. In tank 2 the denitrification takes place and in tank 1 nitrification as well as the remaining COD oxidation. In figure 3.3 the transient behaviour of ammonium, nitrate and phosphorus concentrations during a normal cycle are shown.

During the second phase which lasts 30 minutes the wastewater flow is switched via the second tank into the settler. During this phase the denitrification in the first tank comes to depletion. In the second tank the aeration is continued until either the ammonium concentration reaches the setpoint of 0.5 mg $NH_4$-N/L or the maximum aeration time is attained. In most of the experiments performed in this work the maximum aeration time is 30 minutes. Even though the aeration is stopped, the environment will still be aerobic since the oxygen utilisation rate (OUR) has reduced considerably, due to the decreased substrate concentrations. The shift to anoxic conditions can be observed in the phosphorus concentration in figure 3.3. The phosphorus uptake rate is slowed down but continued under anoxic conditions.

In the third and fourth phase, the same processes as for phase 1 and 2 takes place but in the other reactors and the accumulated phosphorus is removed via the wasted activated sludge from the bottom of the settler.

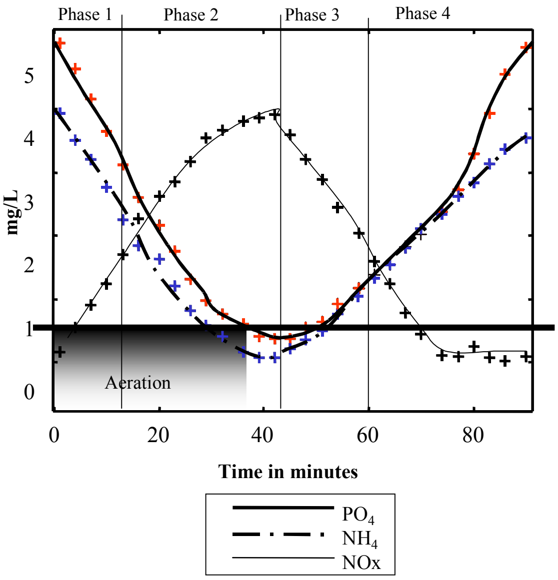


Figure 3.3. Transition concentrations in tank 2 during a normal cycle. Experimental measurements are connected with the indicated curves

During the fourth phase of the cycle, the phosphorus concentration increases significantly when the NOx-N concentration has dropped to a low level and anaerobic conditions are predominating. Under these abiotic conditions the phosphorus release due to the incorporation of readily biodegradable matter, not taken up in the anaerobic reactor, is prevailing. This knee in the $PO_4$-P concentration, corresponding to the complete consumption of NOx-N indicates that during anoxic conditions the anoxic uptake of phosphorus is a relevant process.

One of the advantages of the BIODENIPHO™ process when compared to re-circulation plants is the absence of large recycling volumes. The technical and the operating costs are therefore often smaller than in continuous re-circulation plants. A second advantage is the access to information on the biological activity via nitrification, denitrification and P-uptake or release rates. When on-line measurements are available this information can be used for the on-line estimation of process dynamics and kinetic parameters (e.g.Carstensen et al 1995).

## 3.2. The Flow Injection Analysis System

The Flow Injection Analysis (FIA) system is a technique, which allows the automatic execution of a complete analytical procedure including sample preparation, chemical reaction and detection. Reproducibility at fairly high sample rates is besides the automatic execution, one of the advantages of such a system. The method consists essentially of the injection of a precise volume of sample fluid into a moving carrier system, which may contain reagents with which the analysis compound reacts. The injected sample forms a zone, which propagates through the system and passes a detection unit, which records the excitation of the compound. In case that the compound can not be directly detected, the component must first be converted into a detectable component e.g. through a chemical reaction. The recorded signal is then interpreted with help of a calibration curve. General information about the principle of FIA are given by Ruzicki (1988).

The FIA set-up is schematically presented in figure 3.4a. It consists of a reagent pump, an injection valve, the reactor, which can be a coiled tube and the detector unit. For the majority of the time, the injection valve is bypassed. The injection takes place only for a short time interval. The introduction of a constant and well-defined volume of sample depends on the employed injection valve. Usually the volume of the cavity of the injection valve is well defined and determines the volume of injection. At the moment of injection, which is defined as start of a new sample analysis cycle, the defined sample volume becomes part of the carrier fluid transporting the sample to the detector unit.

The sample volume disperses into the carrier fluid while it is transported towards the detector unit. In this way the former plug-like volume of sample spreads and becomes more dispersed axially. On its way through the tube which is basically the reaction unit the reagents included in the carrier fluid are dispersing into the sample and the reaction occurs. The product of such reaction may be the formation of a colour, which ideally should be related linearly via the intensity to the concentration of the formed compound. A spectrophotometer, equipped with a flow through cell can be used for the detection of the produced compound. A typical shape of such a detected signal is shown in figure 3.4b.

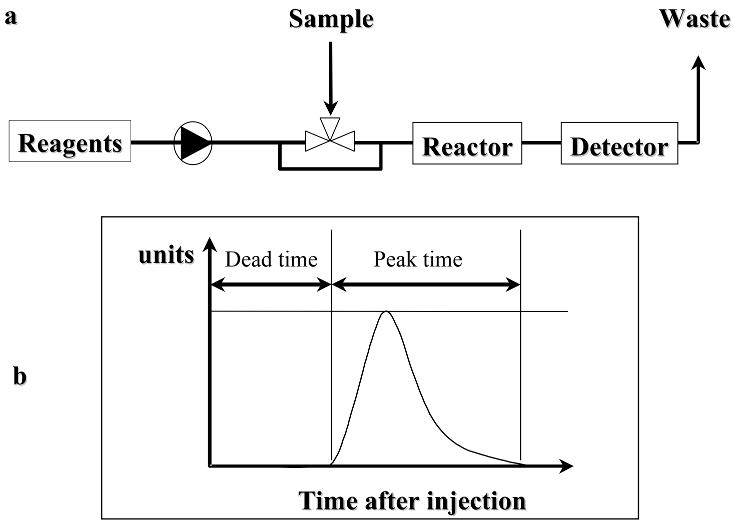


Figure 3.4. a) Schematic FIA components, b) FIA signal

The comparison of the peak height might be only one of the options for the determination of the sample concentration but it is commonly used since the application is very simple. Any drift of the peak height, which is caused for example by pump rate or reagent differences will also affect the peak height of the standard sample and can therefore be neglected, provided standard samples are analysed with a reasonable interval.

The reactions, necessary for the detection of phosphate, ammonium and nitrate are summarised in table 3.2. More detailed information can be found in Pedersen (1990).

The conversion of $PO_4$-P to a colorimetric compound necessary for the analysis is based on a two step reaction. In the first step the sample forms a complex with the molybdenum(VI) ion. In the second step the ion is reduced to the blue molybdenum(V) ion and the intensity of this colour is measured at 610 nm.

Table 3.2. Main chemical reactions involved in the FIA measurement system

| Component | Chemical Reactions | Detection Wavelength | |
|---|---|---|---|
| $PO_4$-P | $H_3PO_4 + 12H_2MoO_4 \rightarrow H_3P(Mo_{12}O_{40}) + 12H_2O$ | 610 nm | eq. 3.1 |
| | $2MO(VI) + Sn(II) \rightarrow 2Mo(V) + Sn(III)$ | | eq. 3.2 |
| $NH_4$-N | $NH_4^+ + OH^- \Leftrightarrow NH_3 + H_2O$ | 590 nm | eq. 3.3 |
| $NO_x$-N | $NO_3 \xrightarrow{\text{cadmium}} NO_2$ | 540 nm | eq. 3.4 |

The ammonia analyser is slightly more complicated than the phosphate analyser. These complications are due to inclusion of a gas diffusion module. The principle is based on the properties of ammonia. The pH value of the sample is increased by the injection of a basic reagent to values around 13 and the dissolved ammonia ion in the sample is converted to ammonium gas as described in equation (3.3). When the sample is passing a gas diffusion module the ammonia gas diffuses through a Celanese membrane from the donor to the acceptor side. At the latter side a reagent is found with a pH value around 6.8 and weak pH buffer characteristics. With help of a pH sensitive indicator the change of the pH value in the recipient is converted into a colorimetric signal which intensity is measured at 590 nm.

The nitrate analyser measures both nitrate and nitrite as nitrite. The method is based on the reduction of nitrate to nitrite when the sample is passing through a reaction element, which is covered with cadmium granules, coated with copper. The nitrite reacts with sulphanilamide, from the carrier fluid and forms a diazonium complex. The diazonium complex is reacting with another reagent to a diazo dye and the intensity is detected at 540 nm.

In figure 3.5 the overall set-up of the FIA measurement system is schematically illustrated. The system can be divided into the sample acquisition including a cross-flow membrane filtration unit (F1-F4), selection and transport part and the sample injection. The reaction and detection parts, which are here all lumped into the detection block. The monitored signals are passed to the controlling and analysing computer, which controls the injection valve and all the involved transport pumps in the system.

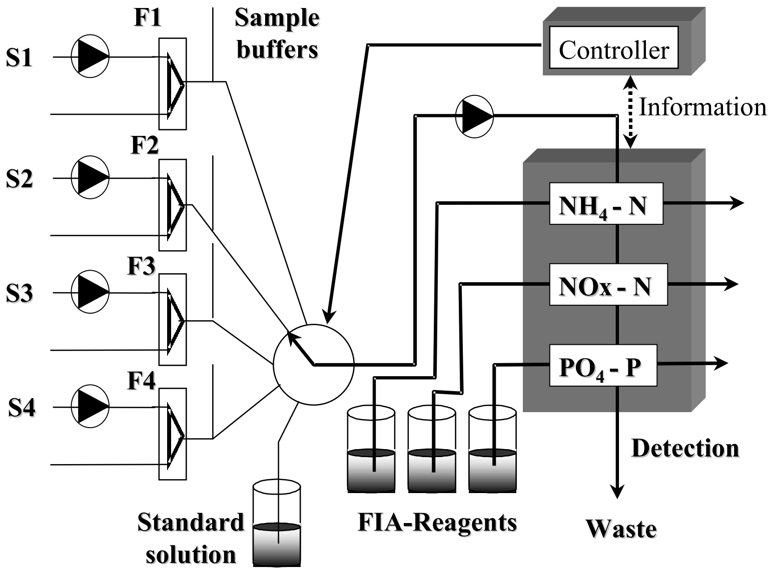


Figure 3.5. Plant-wide FIA measurement set-up

Table 3.3. Sample rates of the FIA measurement system

| | Influent | Anaerobic Reactor | Tank 2 | Effluent | Standard |
|---|---|---|---|---|---|
| Sample Rate | ~ all 12 min | ~ all 12 min | ~ all 3 min | ~ all 12 min | ~ all 12 min |

This basic description gives an overview of the ideas behind the set-up. Such a system needs an intensive effort to maintain a reliable performance. This effort is the reason why such measurement equipment can be found in scientific laboratories rather than in industrial applications. More detailed information can be found in Arvin (1985), Einfeldt (1992), Isaacs *et al.* (1992) and Pedersen *et al.* (1990 and 1988).

## 3.3. Model Considerations and Numerical Methods

For the simulation of the pilot plant a version of the ASM2 model was used, which was extended with denitrification by PAO. The model was implemented into Matlab/Simulink. The Simulink software is offering a simple and fast programming of complex systems due to the convenient user interface. The main effort of programming is in this way reduced using standard modules and their connection with each other. The individual programs are written in $C^{++}$ code and are so called S-functions, which are invoked from the Simulink structure. The final programs can be used either from the user-friendly Simulink interface or via the Matlab working environment and offers in this way a flexible use. The Simulink structure of the pilot plant is found in appendix number x as well as a $C^{++}$ program, which contains the code implementation of the extended ASM2 model.

The model was calibrated using a simple evolutionary strategy as described in more detail in chapter 5. The same set of model parameters is used for the simulations of all presented experiments. The set of parameters was found to be valid during a time period of more than two years. The parameters are with exception of the phosphorus release rate $q_{pha}$, similar to the default values of the original ASM2. The initial conditions for the biomass concentrations ($X_{AUT}$, $X_H$ and $X_{PAO}$) were to be estimated in order to predict the behaviour of the plant via the model. This estimation was in most of the presented cases performed by a simple manual adjustment of the initial values based on calculation of the reaction rates. The dynamics of the alternating process for the $PO_4$-P, $NH_4$-N and NOx-N concentration supports such a manual adjustment since the uptake rates can be directly determined based on the concentration profiles observed in the tanks.

The ASM2 model was selected, due to the broad acceptance of the previous model developed by the international task group on modelling of the International Association of Water Quality (IAWQ), the activated sludge model No. 1 (ASM1). This model was developed in order to describe nitrification, denitrification and carbon removal processes and is recognised by a broad range of international researchers. The challenge was to investigate if the ASM2 can be calibrated to sufficiently predict the pilot plant behaviour. This project do however not investigate neither observablility nor controllability for the ASM2.

The ASM2 had however to be extended in order to consider the anoxic phosphorus uptake phenomenon, observed in the studied pilot plant Krühne et al (1998) or Meinhold et al (1999). The original ASM2 model describes only the phosphorus uptake under aerobic environmental conditions and neglects the anoxic uptake of phosphorus by PAO. A typical effect resulting from such calculations are presented in figure 3.6.

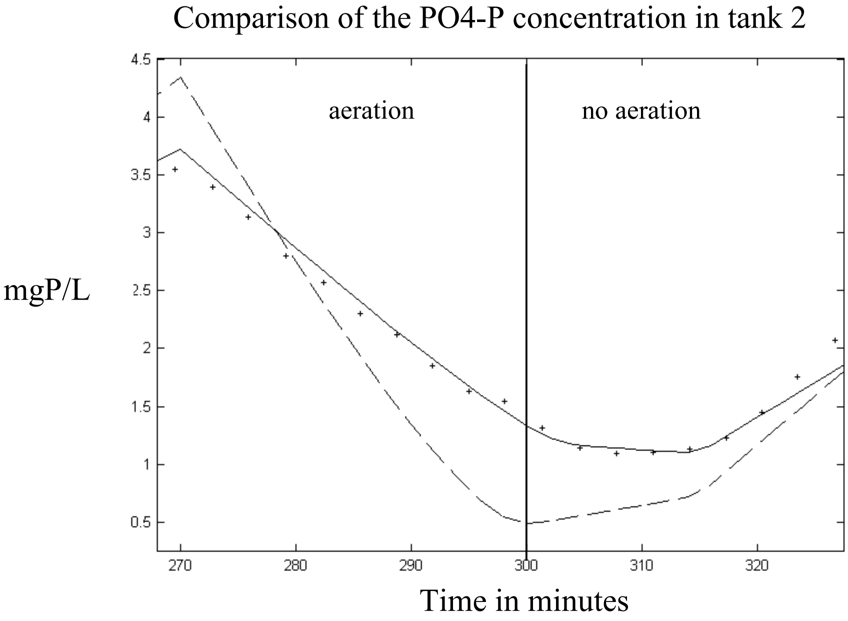


Figure 3.6. PO$_4$-P concentrations calculated by the original ASM2 (dashed line, with best fit of parameter) and extended ASM2 (solid line, again fitted to data) and measurements (+) in tank 2

In this figure the measured phosphorus concentration in tank 2 is presented along with the simulations by the original ASM2 model and the proposed extended version presented in chapter 5. It can be seen that for the calculations with the standard model the phosphorus is already released (around 300 minutes) when the aeration is stopped, while for the ASM2x model and the measurement values the phosphorus concentration is kept low until 318 min.

Figure 3.6 was developed to demonstrate the main difference between the extended version of the model and the standard version. It must be emphasised here that for the simulations a calibrated version of the original ASM2x version was used while the effort of calibration of the ASM2 model was comparably low. The slope for the standard version is therefore relatively steep and the amplitude of the concentration is larger than for the concentration calculated with the calibrated ASM2x. The main difference between the two model is however the behaviour of the process after the stop of aeration. In the standard model the PAO begins to release phosphorus while for the extended version the phosphorus is still taken up due to the presence of nitrate, which is used as an electron acceptor instead of oxygen. The nitrate is present in both cases and is not shown.

# 4. The Investigated Phenomena

## 4.1.Introduction

A practical application for the elimination of phosphorus from wastewater is the chemical precipitation, which is used successfully all over the world in many wastewater treatment plants (WWTP). The general intention to avoid the usage of chemical reagents (if possible) as well as the increased requirements by the authorities concerning effluent phosphorus concentration values is supporting the implementation of biological phosphorus removal in existing plants or in new constructions. It is therefore of interest to understand the process detailed enough in order to maintain the BPR during all disturbed and normal operational situations. Especially the failure of BPR, meaning that the phosphorus concentration in the effluent exceeds the limiting values, due to an insufficient uptake of phosphorus by the biological processes, is of interest.

Carucci et al. (1999) described the microbial competition for the organic substrates and its impact on enhanced biological phosphorus removal (EBPR) systems under conditions of changing carbon feed. Temmink et al. (1996) studied the recovery of BPR after periods of low organic loading and Teichfischer (1995) analyses the stabilisation of the BPR process in general.

These investigations report that the dilution of the organic load by rain events or periodic changes in composition frequently results in an increase of the phosphate concentration in the aerobic or anoxic reactors, when the influent organic concentration returns to the normal wastewater strength. Temmink et al (1996) suggests different recovery times for anoxic/aerobic P-uptake and anaerobic P-release to explain this phenomenon. During a period of low inlet wastewater composition the PHA stores in the bacteria are depleted due to the reduced amount of soluble organic components in the influent wastewater. After re-establishment of normal conditions the PHA storage must first be replenished before P-uptake can recover while the P-release recovers instantly. This hypothesis is supported by Brdjanovic et al. (1998) who performed experiments in which the impact of excessive aeration on the BPR process is studied. These investigations observed the deterioration of BPR with a simultaneous depletion of the PHA stores.

One possibility to overcome the problem could be the maintenance of internally stored carbon at high concentration level by the addition of an external carbon source, suggested by Temmink et al (1996) and Teichfischer et al (1995). A different strategy could be the reduction of aeration time, limiting the unnecessary consumption of internal PHA during the disturbed influent conditions as suggested by Brdjanovic et al (1998) as well as by Temmink et al (1996).

However the impact of a carbon source addition on the internal carbon storage compounds have recently been reported by Krühne et al (2000) and Urbain et al (2000). Such operational strategies are today only used under particular governmental constraints or technical limitations. They were nevertheless used to support the BPR under transient influent concentration variation and reduced chemical precipitation of phosphorus.

In the following subchapter the behaviour of the pilot plant under transient influent conditions will be shown and analysed. Based on such typical examples of disturbed periods the development of model disturbance experiments will be explained.

## 4.2. Investigation of Measurement Data

The examination of the BPR in full scale WWTPs is difficult since only few facilities have phosphorus measurements with sufficient sampling frequency installed. Measurement data from the described pilot plant was therefore extensively studied for the occurrence of insufficient elimination of phosphorus from wastewater. These investigations demonstrated that the BPR process can not maintain the effluent phosphorus concentrations during varying influent conditions. The performance fails either during low influent concentrations with subsequent re-establishment of the average concentration levels or during the increase of the influent wastewater strength. In both cases the increase of the influent wastewater strength seems to cause the failure of BPR An example demonstrating failure of BPR process is shown in figure 4.1.

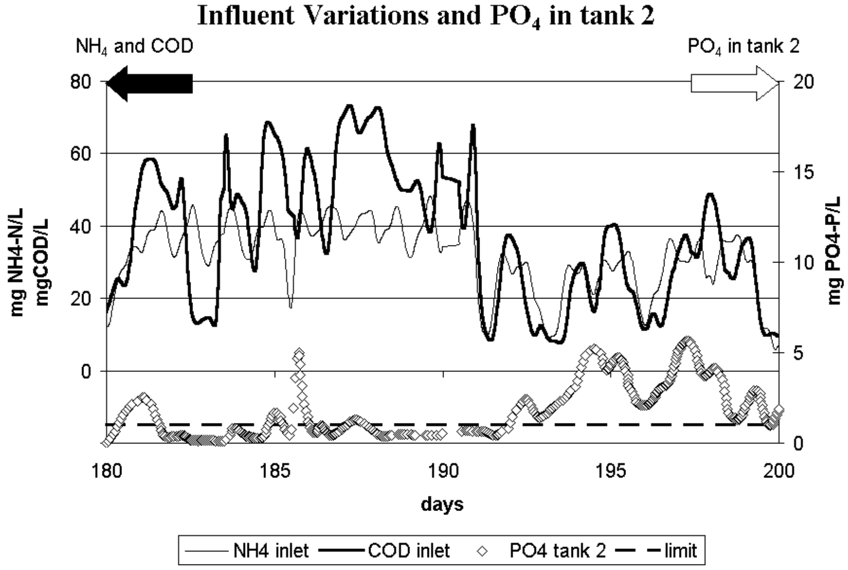


Figure 4.1. Influent readily biodegradable COD and $NH_4$ concentration and the response of the $PO_4$ concentration in tank 2 for the days 180 - 200 in 1998. COD is estimated based upon P-release in the anaerobic reactor

Figure 4.1 shows the measured ammonium influent concentration and the response of the phosphorus concentration in the activated tank of the plant. The influent COD concentration was estimated from the phosphorus measurements in the anaerobic reactor and the influent phosphorus concentration. This estimation is based on the phosphorus release in the anaerobic reactor due to the presence of readily biodegradable substrate. The difference between the phosphorus concentration from the anaerobic reactor and the influent phosphorus concentration must be proportional to the influent readily biodegradable substrate. In figure 4.1 it was assumed that the influent readily biodegradable COD is two times the measured difference of the phosphorus concentrations. The value of 2 could frequently be observed in experiments when the influent concentration of readily biodegradable COD was analytically determined. The exact value of the influent COD concentrations is in this qualitative analysis however not of relevance, since only an overview should be obtained to design experiments for the investigation. The trajectory of the respective components and their relation is of much more interest, in order to design future experiments.

The limiting effluent value of 1 mgP/L (required by Danish authorities) is for several periods exceeded already in tank 2 and hence in the effluent. The BPR is regarded as failing during such time intervals. It is remarkable, that the periods of failure are relatively short when the wastewater has a high influent strength (days 180 to 190). In the second part of the data set (days 190 to 200) the limiting value is exceeded during most of the days. During both high and low influent wastewater concentrations the qualitative trajectory of the phosphorus concentration in the activated tank follows the estimated influent ready biodegradable substrate concentrations. Since most of the BPR failures take place when the strength of the wastewater increases, such cases can be considered as important periods for further investigations.

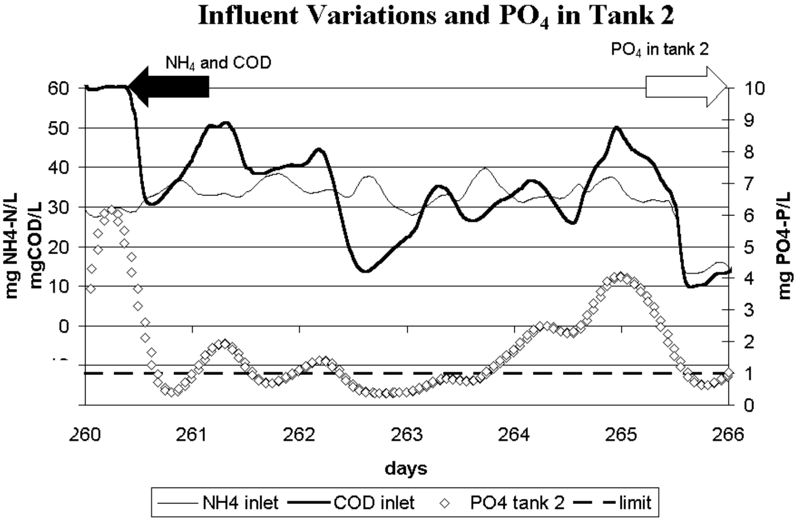
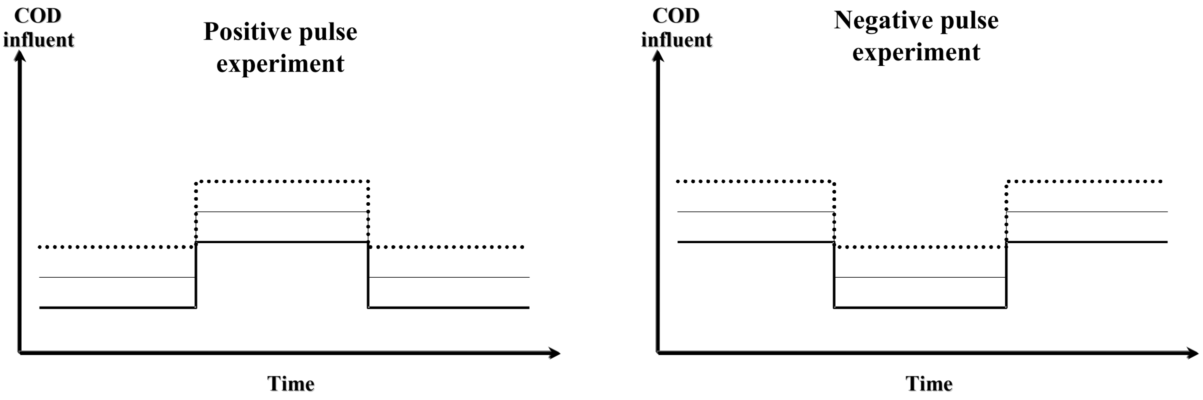


Figure 4.2. Influent readily biodegradable COD and $NH_4$ concentration and the response of the $PO_4$ concentration in tank 2 for the days 260 - 266 in 1998.

The measurements in figure 4.2 are presented over a period of six days to render the presentation more clear. At day 260.5 to 261 the estimated influent COD concentration increases by approximately 20 mgCOD/L (from ~25 to 45 mgCOD/L). Such increase also occur at day 262.5 (from ~10 to ~30 mgCOD/L) and 264.5 (from ~20 to ~40 mgCOD/L). The impact of such increases is for all three cases different. In the third case a strong accumulation of phosphorus in the activated sludge tanks is induced, while for low influent concentrations the impact is less severe. From day 263 to 264.5 the influent COD concentration is relatively constant even though an accumulation of phosphorus takes place in the aerated tanks. Thus it can be stated that the sudden augmentation of the organic load has an impact on the process performance of the BPR but the magnitude of the impact seems to depend upon the level of readily biodegradable COD.

For further investigation of BPR failure during an essential task is the design of a model experiment that can be used for detailed analysis of the problem. The idea of such an experiment is to develop a reproducible scenario. A suitable experiment could be the increase of wastewater concentration to a different level, as illustrated in figure 4.3a. To complete the observations an inverse experiment, the simulation of a rain event, could be performed as demonstrated in figure 4.3b.

One of the advantages of the pilot plant investigation is the operation with real wastewater, since the operational conditions are very close to the reality of a WWTP. The use of real wastewater constrains on the other hand such experiments due to the actual load disturbances caused by seasonal or weather influences. Especially the variations of the influent conditions are difficult to predict. These constraints render scheduling and design the operational conditions difficult. The use of partly synthetic wastewater instead could overcome such problems and could support the detailed investigation of the phenomenon. The augmentation of the organic load by addition of carbon sources like acetate, methanol or ethanol to stabilise the influent conditions could be possible but the response to such perturbations may be different from real wastewater composition changes and hence open to interpretation.



a b

Figure 4.3. Suitable model experiments for the investigation of the failure of BPR. a) Pulse experiment with increasing wastewater concentration. b) Pulse experiment with dilution of the influent wastewater

The pulse increase of the influent wastewater strength, shown in figure 4.3a, can be achieved by storage of large volumes of wastewater with a concentration above the usual wastewater strength. In the subsequent normal periods the stored wastewater could be used for the desired influent concentration augmentation. This procedure however would have two substantial disadvantages:

- The dependency on a real wastewater composition change, which in practice can mean to wait several days or weeks until the change takes place. During fall and wintertime the period can even be months.
- The biological processes, taking place in the storage tank, could lead to a partial conversion of important substances. The volume of the existing storage facilities will furthermore limit the duration of the experiment.

The experimental design was therefore selected as illustrated in figure 4.3b. The desired decreased strength of the influent wastewater is easily achieved by a dilution with tap water upstream of the pilot plant. The tap water is brought to the same temperature as the influent wastewater by using a storage tank. The dilution experiments will however be affected by the diurnal variation as well. The probability of normal influent wastewater characteristics is nevertheless higher than attempting increased influent wastewater compositions.

In Conclusion:

During this first part of the thesis an overview was given about the involved basic biological processes and the most common control concepts used in control of activated sludge processes. The investigated pilot plant and the technical background were briefly presented and a problem definition was established.

The purpose of the thesis is to overcome the described problematic dynamic plant responses to influent variations. In the following chapters the experimental and simulation results are presented including a dynamic model calibration and the examination of an operational and control strategy.

# Results

# 5. Parameter Estimation for the ASM2 Model Incorporating Denitrification by Phosphate Accumulating Organism

ABSTRACT

The behavior of a pilot scale biological phosphorous removal process (BPR) of the alternating BIODENIPHO$^{TM}$ type is investigated during a period of normal inlet wastewater feed composition. A calibrated extended version of the activated sludge model No. 2 (ASM2), which includes denitrification by phosphate accumulating organism (PAO) can be used over a large time period to predict the behavior of the main components in the system. A sensitivity analysis has been conducted in order to focus on the estimation of the important parameters. The actual parameter estimation was performed by an evolutionary estimation procedure, which is briefly presented as well as the relevant calibration and validation experiments. The necessary influent characterisation is described and a correlation of the influent organic compounds with the phosphorus release in the anaerobic tank is proposed.

KEYWORDS

ASM2, PHA, biological phosphorus removal, denitrification by PAO, parameter estimation and validation, wastewater treatment.

## 5.1.Introduction

Models, which describe activated sludge processes, are essential both for the improved understanding of these processes as well as an improved design, operation and control. For nutrient removal processes incorporating biological phosphorus removal (BPR) the IAWQ task force on activated sludge process modelling has developed the Activated Sludge Model No. 2 (ASM2). One aspect of BPR processes not included in the ASM2 model is the possibility for at least a fraction of the phosphorus accumulating organisms (PAO) to denitrify, as observed in several investigations. Current investigations imply the existence of denitrifying phosphorus accumulation organisms (DNPAO). These micro-organisms are capable of using $NO_3$ as well as $O_2$ as electron acceptor for their growth or internal storage of polyphosphate. These organisms were extensively studied and described by Kuba et al. (1993, 1994, 1996a, b and c) and Smolders et al. (1994a, b, 1995a, b, c and d). In the work of Meinhold *et al.* (1998) the fraction of the DNPAO in the system investigated in this study were found to be in the range of 40-60% of the PAO.

The user of a deterministic model faces always the question about which aspects to consider. On one hand all key phenomena must be included, while on the other hand the model should be as simple as possible for the intended purpose. Compromises must be made, since the complexity of the reality can only be approximated. In the case of the ASM2 the model component representing the cell internal carbon storage products of the PAO is an example for such a compromise. Even though it is recognised that the internal stored compound glycogen plays an important role during the BPR (Kuba *et al.*,1994), it is not included in the model as an independent component, but lumped with other polymers like poly-hydroxy-alkanoates (PHA) in one model compound. Therefore the analytical measured PHA concentrations can not be compared directly with the modelled concentration of $X_{PHA}$. The model is nevertheless due to the basic structure used by a broad community of researchers and engineers despite of such deficiencies.

The development of operational or control strategies without a suitable model is very difficult if not unfeasible without experimental investigations. Therefore this study is made in order to confirm if the extended ASM2, which considers denitrification by PAO, can be used for the analysis of a BIODENIOPHO™ pilot plant. Since the model contains a large amount of parameters it is of significant interest if an estimated set of parameters will be valid over a long period or if the prediction will change with the time. The model will therefore be calibrated on an average influent situation and then validated under different influent conditions. The necessary calibration procedure is briefly presented as well as a sensitivity analysis, which has the intention to reduce the amount of parameters which have to be calibrated. In this way it is examined if the model can be used despite of the structural deficiencies for the analysis of the existing plant under different influent compositions. Subsequent the model is tested on a set of data which has been recorded with a time difference of one year and which is approximately 20 times longer than the data on which the model was calibrated. After the confidence into the model and the estimated set of parameters is obtained, it will be used subsequently for the development of control and operational strategies with the purpose to maintain the BPR process during problematic influent conditions.

## 5.2.Material and Methods

### 5.2.1.The Pilot Plant

An alternating BIODENIPHO™ pilot plant process is employed in this study. The plant and the basic alternating operation is shown in figure 5.1 and is described in e.g. Isaacs *et al.* (1992), Einfeldt (1992), Arvin (1985) and Pedersen *et al.* (1990). This is an activated sludge process for biological C, N and P removal incorporating cyclic changes in flow and aeration.

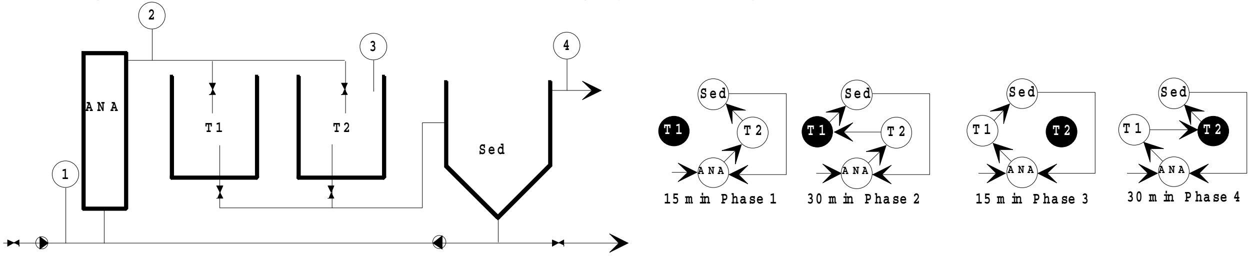


Figure 5.1. The pilot plant and the flow and aeration pattern during a standard 90 min cycle, black circles indicate an aerated tank, air supply to the aerated tanks is terminated when the ammonia concentration has dropped to a setpoint concentration (0.5 mgN/L).

Ammonium nitrogen ($NH_4$-N), nitrate plus nitrite nitrogen ($NO_x$-N) and ortho-phosphate ($PO_4$-P) are measured automatically by flow injection analysis (FIA) as described in Isaacs *et al.* (1992) at the sample points 1-4, which are the inlet wastewater, the exit of the anaerobic tank, in the aeration tank 2, and the effluent stream respectively (see figure 5.1). PHA were measured as described in Smolders *et al.* (1994) with minor modifications. MLSS was determined according to Standard Methods of the APHA (1985).

### 5.2.2.The Extended Model

The motivation for this investigation arises from the question if the incorporation of the denitrifying capabilities of PAO will result in a proper description of the pilot plant behaviour, which shows denitrification activity by PAO. If this is possible the model can be used for further investigation and development of control strategies to obtain a better performance of the process.

Two additional reaction rates for the denitrifying abilities of the PAO were implemented into the existing ASM2 model. The structure of the ASM2 model was retained in such that the number of states was unchanged, two new reaction rates and three new parameter were introduced. The new reactions incorporate the anoxic growth of PAO on PHA and the anoxic phosphate storage on PHA. The reaction rates are shown in table 5.1, while the new values related to the stoichiometric matrix are found in table 5.2. The modelling approaches were taken from Mino *et al* (1994) and Isaacs *et al.*(1994)

The necessary energy for the anoxic uptake of ortho-phosphate and the subsequent storage as cell internal poly-phosphate is received from the anoxic respiration of poly-hydroxy-alkanoates. The kinetic expression for this process is identical to the aerobic uptake of phosphate with the difference that an anoxic rate constant is introduced ($q_{PPNO3}$)as a new parameter. The anoxic growth of PAO is assumed at take place exclusively at expense of the internal carbon stores in form of poly-hydroxy-alkanoates (PHA). And as in the case for the anoxic storage of phosphorus a rate factor is introduced ($q_{PAONO3}$) which is not as large as for the aerobic growth of PAO. The internal carbon storage compound PHA is defined as in the ASM2. That means that it includes the internal storage products of the PAO, which are primarily PHA and glycogen. The PHA concentration is herewith a functional variable, which is needed for modelling purpose and cannot directly be compared with the analytically measured PHA.

Table 5.1: Kinetic Rate Expressions

| | |
|---|---|
| uptake rate | $q_{PPNO_3}\frac{S_{PO4}}{S_{PO_4}+K_{PO4}}\cdot\frac{K_{O2}}{S_{O2}+K_{O2}}\cdot\frac{S_{NO3}}{S_{NO3}+K_{NO3}}\cdot\frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}}\cdot\frac{K_{MAX}-X_{PP}/X_{PAO}}{K_{MAX}-X_{PP}/X_{PAO}+K_{IPP}}\cdot X_{PAO}$ |
| growth rate | $q_{PAONO_3}\frac{S_{PO_4}}{S_{PO4}+K_{PO4}}\cdot\frac{K_{O2}}{S_{O2}+K_{O2}}\cdot\frac{S_{NH_4}}{S_{NH_4}+K_{NH4}}\cdot\frac{S_{NO3}}{S_{NO_3}+K_{NO3}}\cdot\frac{S_{ALK}}{S_{ALK}+K_{ALK}}\cdot\frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}}\cdot X_{PAO}$ |

Table 5.2: Stoichimetric values for the new reactions

| Component | $S_{NO3}$ | $S_{PO4}$ | $S_{N2}$ | $X_{PAO}$ | $X_{PP}$ | $X_{PHA}$ |
|---|---|---|---|---|---|---|
| Uptake | $-\frac{Y_{PHAd}}{2.86}$ | -1 | $\frac{Y_{PHAd}}{2.86}$ | | 1 | $-Y_{PAOd}$ |
| Growth | $-\frac{(1-Y_H)}{Y_H\cdot 2.86}$ | $-i_{PBM}$ | $\frac{(1-Y_H)}{Y_H\cdot 2.86}$ | 1 | | $\frac{-1}{Y_{PAOd}}$ |

The presented structure of the model seems to be outdated since several experimental investigations indicate the existence of two groups of PAO (literature). On the other hand the incorporation of another organism into the model would lead to a considerable increase of its complexity since also internal storage compounds should be considered. The justification for the here presented attempt lies in the ease of the implementation. If the resulting model is successful it may be used under consideration of its structural limitations.

### 5.2.3. The Experiments

In a *calibration experiment*, the extended model was calibrated to pilot plant data collected over a 12 hour period. The data include ammonia, nitrate and phosphate concentrations measured automatically every 3 minutes at sample point 3 and every 12 minutes at sample points 1,2 and 4 (see figure 5.1). Manual samples were taken to determine concentrations of total COD, filtered

COD and acetate at sample point 1 and to determine the PHA level in the sludge at sample point 3. The evolutionary strategy was employed to estimate the initial conditions and the model parameters. One third of the available data was employed in the calibration, the remainder being used for model validation.

In a *validation experiment*, performed 3 months later, the ability of the calibrated model to describe a disturbance in the inlet water composition was tested. The normal inlet water was diluted by a rain event over several hours. Phosphate, ammonia and nitrate were measured automatically every 12 minutes at sample points 1, 2 and 4, and every 3 minutes at sample point 3 during a period of almost 24 hours. Manual samples were taken for PHA at sample point 2 (every 3 minutes for three selected aerated phases). Samples for measurement of total COD, soluble COD and acetate in the inlet water were taken with an autosampler each 60 minutes. The model parameter values determined during the calibration experiment were employed for simulation and the initial concentrations were determined using the evolutionary strategy on the first third of the available data points.

In a *long term experiment* a long set of continuous measurement data of the pilot plant was used in order to test the model over a time horizon of 10 days. Since the FIA-system analyses only ammonium, nitrate and phosphate concentrations, the influent organic compounds had to be estimated on approximates. Phosphate, ammonia and nitrate were measured automatically every 12 minutes at sample points 1, 2 and 4, and every 3 minutes at sample point 3 during a period of almost 10 days. The remaining unknown influent components were related to the phosphorus release in the anaerobic reactor.

### 5.2.4. The Parameter Estimation

*The Evolutionary Strategy:* The presented model contains 50 parameters and 17 state variables, neglecting the precipitation processes. The necessary effort for the estimation of appropriate values of those parameters is quite high even though the parameters connected to the nitrification and denitrification processes are well accepted and confirmed by experimental investigations throughout the recent years (literature). Therefore a methodological approach must be chosen in order to obtain a reliable set of parameter within a reasonable time frame. During this investigation an evolutionary strategy has yielded convincing results and will therefore be shortly described.

During the evolutionary strategy, see also Born and Bellman (1980), illustrated in figure 5.2, a starting set of parameters is chosen, e.g. the default parameters recommended by Henze *et al.*(1995). A simulation is performed and an appropriate objective function is calculated. Then the set of parameters is changed by random choice and the simulation and estimation of the objective function is performed again. After the comparison of the new objective function and the old objective function the new set of parameter is stored or discarded, depending on the development of the objective function. Subsequently, the loop is repeated until either the objective function has reached a desired value or the number of iterations exceeds a maximum number of iterations.

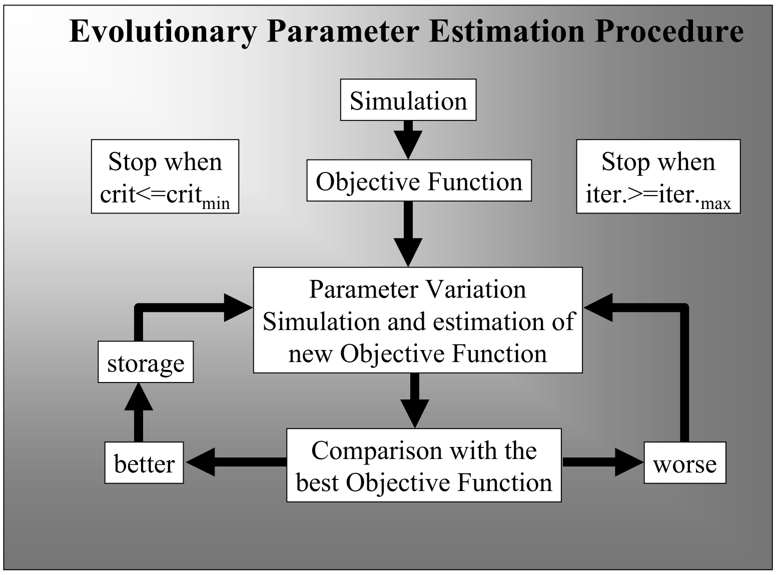


Figure 5.2. The evolutionary strategy principle

The objective function was:

$$J = \sum_{1}^{i} \sum_{1}^{n} W_i \left(y_i - \hat{y}(\theta)_i\right)^2 \quad ; \qquad y_i(0) \qquad \text{eq. 5.1}$$

y is the measurement of component i, $\hat{y}_i$ the model prediction of component i, $\theta$ the parameter vector, $y_i(0)$ the initial values, n the number of measurements which are used for the estimation procedure and $W_i$ a weighting factor for the different components.

As a starting point one third of the calibration data was used for the estimation of the parameter vector while the remaining part was used for validation purposes. The perturbation of the parameter vector was performed as follows:

$$\theta_{i+1,j} = r_j \theta_{i,j}$$
$$\text{where } 0 \le r_j \le 0.03 \text{ and randomly chosen} \qquad \text{eq. 5.2}$$

*The Sensitivity Analysis:* A possibility to accelerate the parameter estimation procedure is to reduce the amount of parameters, which are possible candidates for the calibration routine, via a sensitivity analysis. A sensitivity analysis is an appropriate procedure, in which the model and its parameter are investigated in order to find the significant parameters, which afterwards will be calibrated. The performed method is based on the idea to perform a simulation with a default set of parameters and the subsequent alteration of the single parameters. The deviation from the nominal parameter set is mathematically formulated as:

$$S_i = \left(\frac{J_\times}{J_n}\right)_i \qquad \text{eq. 5.3}$$

In this equation S is a sensitivity value, J is the above described objective function, x stands for the new objective function value, n for the nominal objective function value and i for the degree of deviation from the nominal parameter value. i has values between 1 and 5 in which 3 is the nominal value, 1 is a 50% deviation, 2 a 75% deviation, 4=150% deviation and 5 a 200% deviation from the nominal parameter value. High sensitivity values for a parameter indicate that this parameter with the given measurements is a suitable candidate for the calibration routine, while small values should lead to an elimination of this parameter from the estimation procedure, since the objective function is not sensitive to variations in this parameter.

In figure 5.3 the results of a sensitivity analysis for the BPR related parameters is presented. The analysis is performed from the best set of parameters, which has been found by the evolutionary strategy with the 13 parameters related to the BPR. It is obvious that only half of the investigated parameters have a significant influence upon the objective function. They are the yield coefficients ($Y_H$, $Y_{PAO}$ and$Y_{PO4}$), the aerobic uptake rate ($q_{pp}$) and growth rate ($\mu_{pao}$), and the anoxic uptake rate ($q_{ppno3}$). It is remarkable that for some parameters the direction of the deviation has a strong impact on the sensitivity while for others the impact is negligible. This nonlinear phenomenon stresses the importance of the appropriate starting values during such an analysis. If the analysis is started in the wrong region, no sensitivity may be detected if an inappropriate parameter disturbance is chosen.

Special attention has to be dedicated to the initial concentrations of the biomass components, since the model is using Monod term kinetics. The fractions of the biomass can unfortunately not be measured. Considering the equations in table 5.1 it is obvious that the same values for the kinetic expressions can be reached with either a high rate constant ($q_{ppNO3}$, $q_{PAO}$) and low concentrations of $X_{PAO}$ or low rate constants and high concentrations of $X_{PAO}$. In order to avoid such difficulties the estimation procedure is applied sequentially.

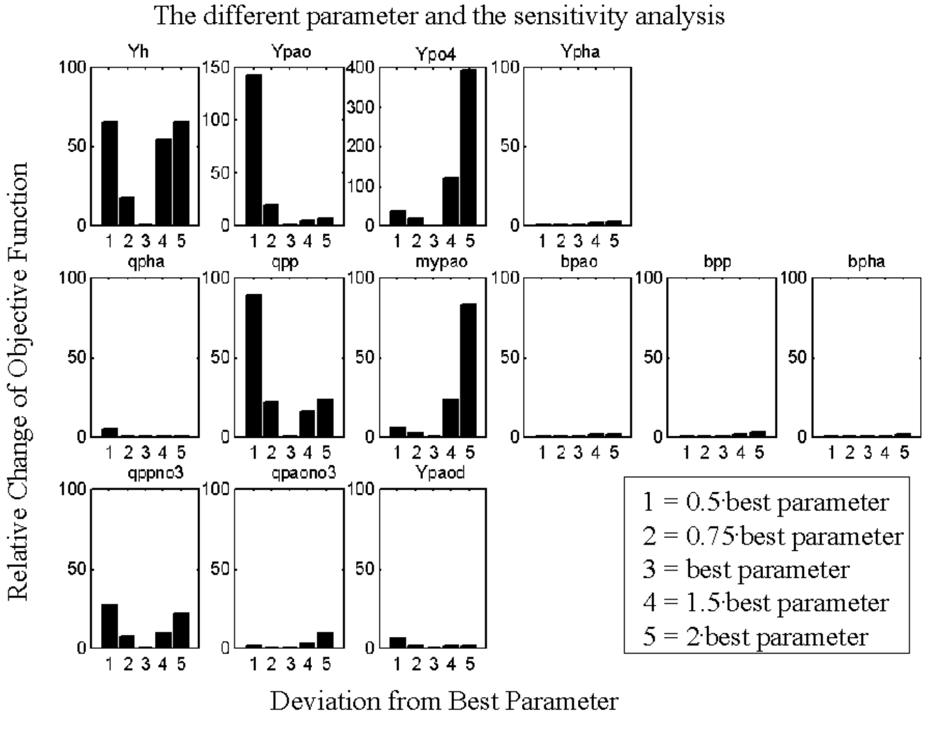


Figure 5.3. The sensitivity analysis results

First the initial conditions of the autotrophic organism are fixed, since the pilot plant is operated with an ammonium setpoint control strategy. The weight for the ammonium concentrations is increased while the other weights are set to low values and the estimation procedure is applied. After some dozen repetitions a satisfying fit is obtained. If this step is not performed first, the aeration periods will be determined wrong and therewith this incorrect aeration time will influence the further estimation procedure. As a second step in this sequential procedure the initial concentrations for the heterotrophic organism will be fitted by increasing the weights for the NOx concentrations. Again the procedure is performed and the initial concentrations are obtained after some dozen loops. In the last step of this procedure the parameters which have been selected by the sensitivity analysis and the initial concentration for the PAO are given free for the estimation procedure, while at the same time the weight for the $PO_4$ concentration is augmented. A change between different alternatively high weighting factors for the anaerobic reactor or the activated tank is suggested, such that the possibility to end in a local minima is reduced . In opposite to the first two step this is the time consuming part and lasts several hundred repetitions.

### 5.2.5. Influent Characterisation

For the simulation of the pilot plant, experimental influent data are desirable but not available for all model components. The prediction quality of the model is strongly dependent on the accessible influent information which is obtained by a thorough influent sampling campaign during the experiments. During the following presented experiments the wastewater inlet samples were always analysed for filtered COD, total COD, acetate, ammonium, nitrate and phosphate. With help of the measurements and the characterisation of wastewater (Henze *et al.*.) it is possible to approximate the lacking concentrations for alkalinity, soluble inert material and particulate inert material. The incoming micro-organism concentrations are assumed to be negligible while the remaining values for soluble fermentable substrate and slowly biodegradable compounds are calculated from a simple mass balance.

Since the sampling campaign for the influent characterisation is time consuming, it is only performed for special experiments. During the most time of the year the wastewater entering the pilot plant is only analysed for ammonium, phosphate and nitrate concentrations. Therefore, the remaining unknown components must be estimated. For the estimation of readily biodegradable matter and fermentable matter the phosphorus release in the anaerobic reactor can be used. The following approach has been successfully used at the pilot plant and is therefore a specific relation:

$$\hat{S}^*_{A,in} = f_{HAc} \cdot (PO_{4,ANA} - PO_4^\circ) \qquad \text{eq. 5.4}$$

$S^*_A$ is the acetate estimate, $PO_{4,ANA}$ is phosphate concentration in the anaerobic reactor, $PO_4^\circ$ the phosphate concentration at the time $t\text{-}t_{del}$ , $t_{del}$ the hydraulic retention time of the anaerobic reactor and $f_{HAc}$ a constant factor which for most of the available data sets is in the range between 2 and 3.

This approach bases on a mass balance for the phosphorus around the anaerobic reactor. The phosphorus which is leaving the anaerobic reactor is for a stationary case the amount of phosphorus which is entering the plant in the influent and return flow plus the amount of phosphorus which is released due to the uptake of readily biodegradable substrate by PAO minus the amount of phosphorus which is taken up by the DNPAO. It is assumed that the influent concentration of readily biodegradable substrate is reduced by the consumption due to denitrification of the receycled NOx concentration which is assumed to be relatively constant. It is furthermore assumed that all soluble fermentable matter which is entering the plant is used in the fermentation processes and the product is readily biodegradable matter. Finally the relation between the influent readily biodegradable matter and the influent soluble fermentable matter is assumed to be constant. Lysis processes are regarded as negligible. Since this mass balances includes a number of influences the simple approach is used instead, where all dependencies are condensed in the factor $f_{HAc}$. The expected value for this factor is situated around 2 for a constant ratio of 1 between the influent and the return flow.

In the following figure 5.4 the results for the explained relation is demonstrated for different experiments. The top subfigure shows the measurements of acetate in the influent and the estimate with $f_{HAc}$=2.4 during the calibration experiment.

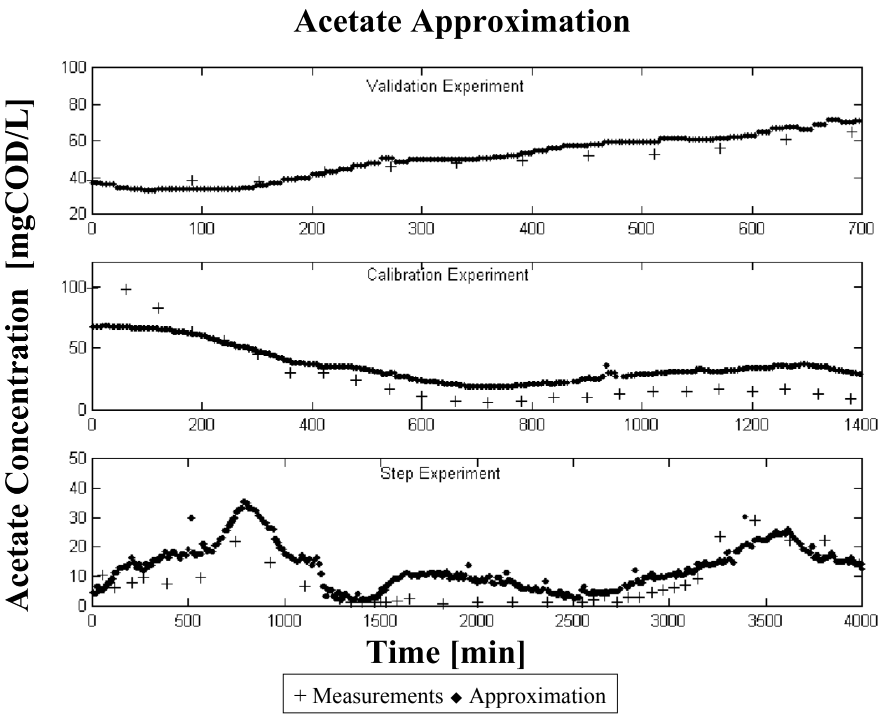


Figure 5.4. Influent acetate approximation as function of the P-release

In the following subfigures the same relationship is used to approximate the acetate concentration for validation and a step experiment. It can be observed that the approach is qualitatively well describing the dynamic behaviour of the influent acetate concentration. Since it is only a rough estimate, there will always be a deviation from the real values. But in many cases this rough estimate is better as if no measurements would be available.

Table 5.3 is summarising the remaining assumed constant factors between the organic soluble components and HAc in order to approximate the missing organic model compounds. These values are based on the available influent information which were gathered during experiments over a time period of two years as well as on the assumption that the influent inert material can be described by the influent characterisation of Henze *et al.*(1995). In figure 5.5 measurements are presented which has been recorded during experiments over the last two years. The measurements of influent soluble COD as functions of the acetate concentrations is presented as white diamonds, while the dependency of the total COD on the soluble COD is presented as black diamonds. Even though the COD measurements are scattered due to the nature of the measurement principle, a general tendency of the relationship seems related except for one sequence of measurements with very little acetate concentrations.

Table 5.3: Influent organic compounds as function of the acetate concentration

| Component | Estimation relationship |
|---|---|
| soluble COD | $5 \cdot S_a$ |
| total COD | 1.5·soluble COD |
| $S_i$ | 0.1·soluble COD |
| Sf | soluble COD-Si-Sa |
| Xi | (total COD-soluble COD)·0.15 |
| Xs | (total COD-soluble COD)-Xi |

In the same figure the total COD concentration is plotted as a function of the soluble COD concentration which is connected by the factor 1.5. This constant relationship between the total and soluble COD must be handled with care since the pilot plant receives the influent wastewater in pre-settled form.

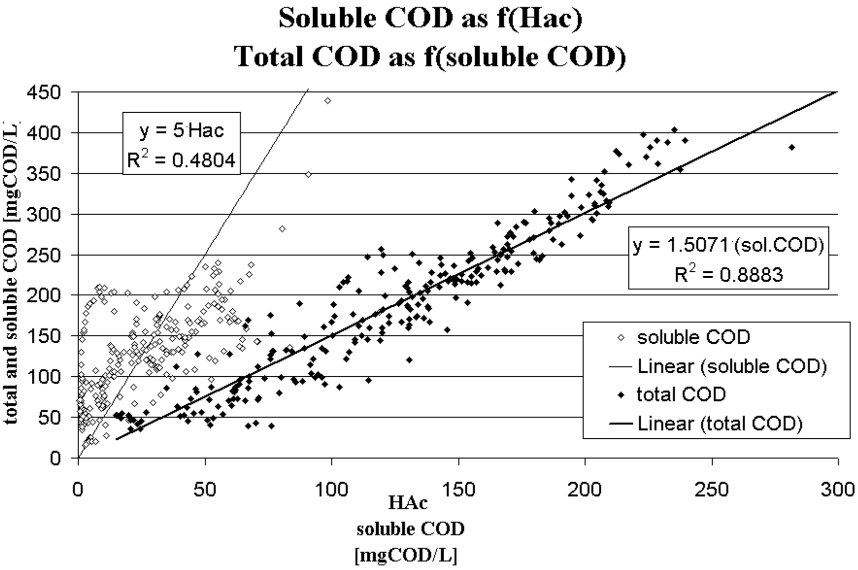


Figure 5.5. Correlation of the soluble and total COD

In summary the proposed influent characterisation demonstrates a reasonable performance and indicates at the same time that it must be used with caution. The thorough analysis of the influent wastewater cannot be replaced in any case by such rough estimates. Furthermore the approximation is only valid for the described specific wastewater at the pilot plant.

## 5.3.Results and Discussion

In this part of the article results of the calibration and validation experiments are demonstrated and discussed and the obtained set of parameters is presented. The presented figures and tables have the intention to increase the confidence into the extended ASM2 model and to encourage potential user to understand the model as a supporting tool for design and control purposes.

### 5.3.1.The Calibration and Validation Experiment

The model is calibrated to pilot plant data collected over a 12 hour period. The calibration is performed with the described evolutionary strategy to determine the set of model parameters and initial conditions, which best fit the calibration data. One third of the available data is employed in the calibration, and the remainder set is used for the model validation. The results are presented in figures 5.6-9. One of the most interesting questions is to evaluate the prediction capacity of the model developed using the determined parameters without further fitting to new data. Therefore a second calibration experiment was performed three month later at approximately the same temperature. The duration of that experiment was 34 hours. The results of measurements and simulation are shown in figures 5.10 -13.

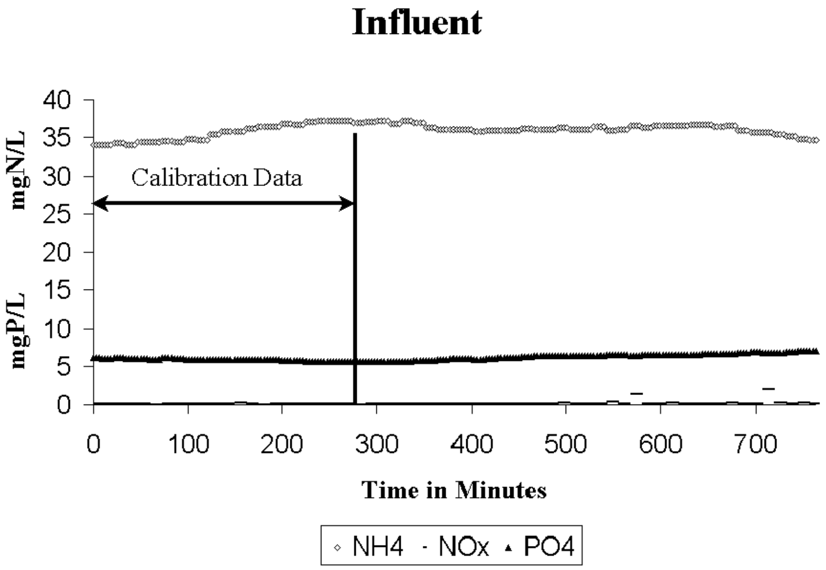


Figure 5.6. Influent concentrations during the calibration experiment

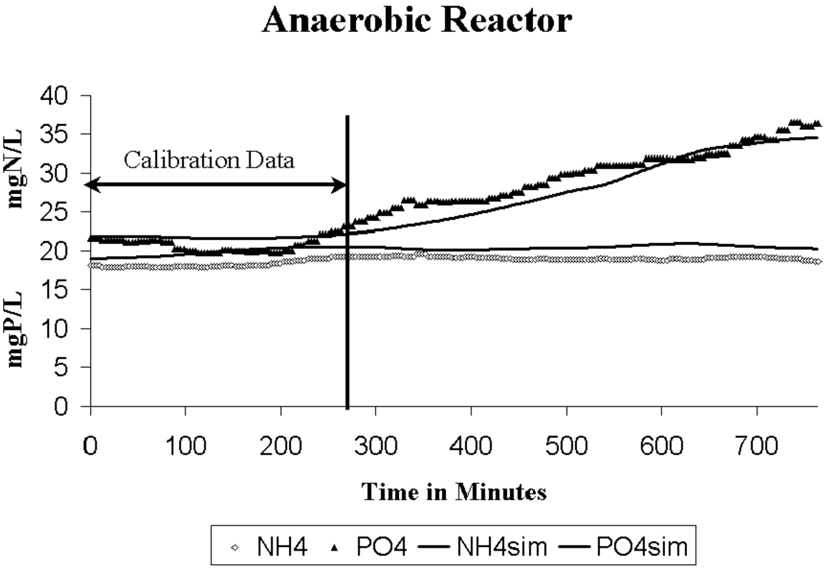


Figure 5.7. The anaerobic reactor concentrations during the calibration experiment

During the first calibration experiment the influent conditions concerning the phosphate and ammonia concentrations are relatively constant (figure 5.6). The increase of phosphate in the anaerobic reactor shows that the incoming load of organic substances is already increasing while the phosphate and ammonium concentrations stays rather stable (figure 5.7). The model is following well the trajectories of phosphate, ammonium and nitrate (figure 5.8 and 5.9). It should be mentioned here that the parameters involved in the nitrogen dynamics are not calibrated. The prediction for the PHA in tank 2 is more of qualitative nature (figure. 5.8) which is expected since the internal storage compounds in the ASM2 model include not only PHA. The aeration time is set to 30 minutes. The aeration is however switched off when the concentration drops below 1mg-N/L.

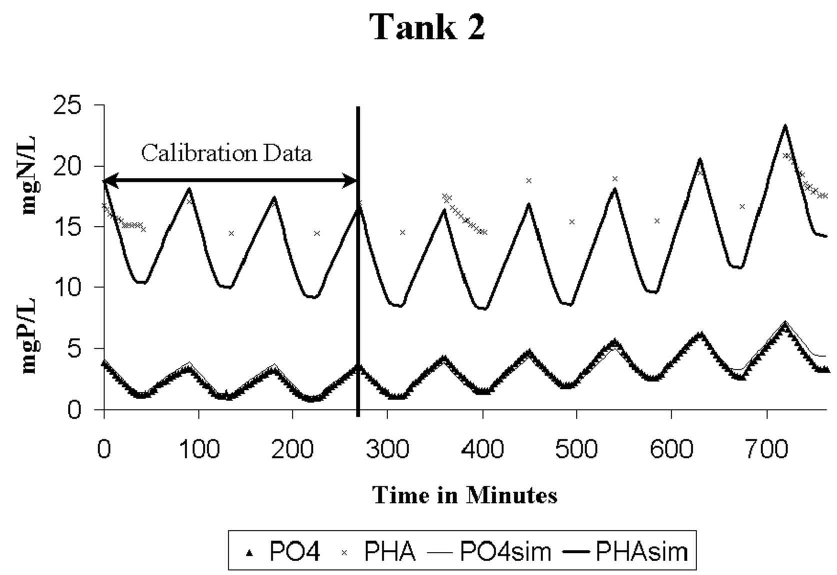


Figure 5.8. The $PO_4$ and PHA concentrations during the calibration experiment in tank 2

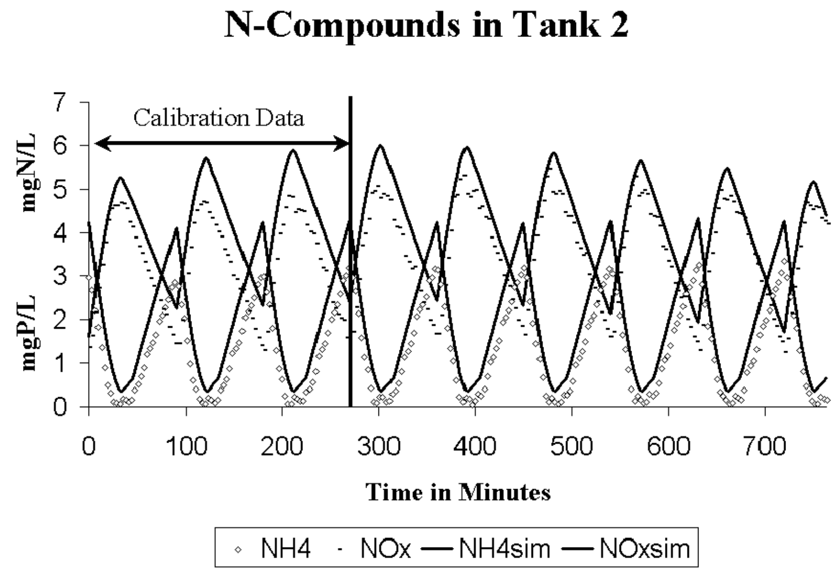


Figure 5.9. The $NH_4$ and NOx concentrations during the calibration experiment in tank 2

In the second experiment (validation) experiment, presented in figure 5.10-13, the incoming wastewater concentration shows a different behaviour than in the first experiment. The phosphate and the ammonium as well as the COD concentrations are strongly varying with time. The drop for the phosphate concentration is not as dramatic as for the ammonium (figure 5.10). The prediction ability for the phosphate and the nitrogen compounds in all reactors demonstrates reasonable quality as shown in figure 5.11 to 5.13.

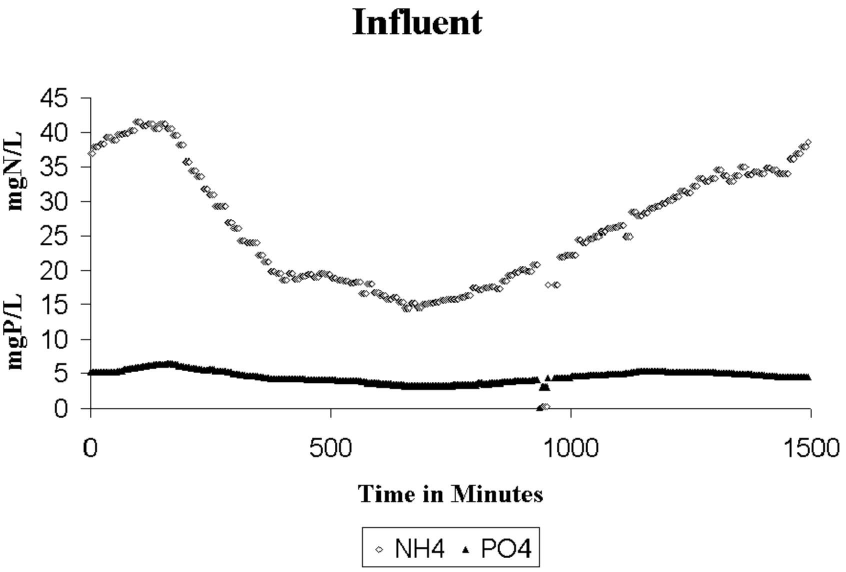


Figure 5.10. Influent concentrations during the validation experiment

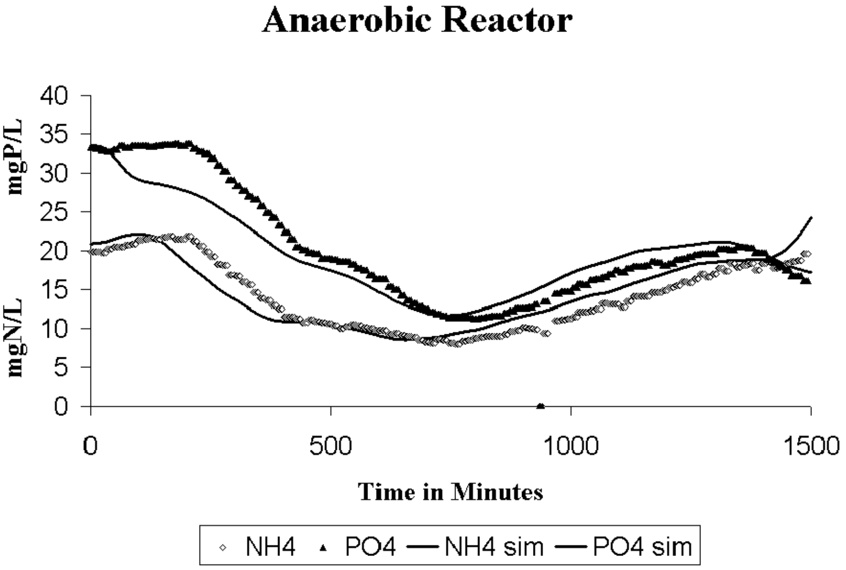


Figure 5.11. The anaerobic reactor concentrations during the calibration experiment

The prediction capacity of the PHA concentrations is relative poor but not out of reasonable range (figure 5.12). For the simulation of the second experimental data the same parameters as determined in the first calibration experiment were used. The initial conditions for the simulation were estimated with the same evolutionary algorithm (not listed here) are different but in the same range as the initial conditions of the first experiment. This is reasonable since the biomass populations will have changed during the three month period.

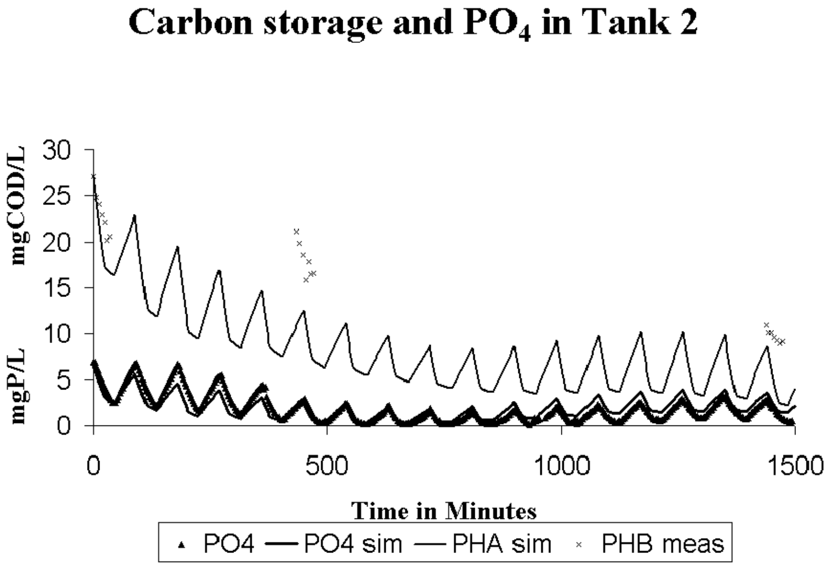

Carbon storage and $PO_4$ in Tank 2

Figure 5.12: The $PO_4$ and PHA concentrations during the calibration experiment in tank 2

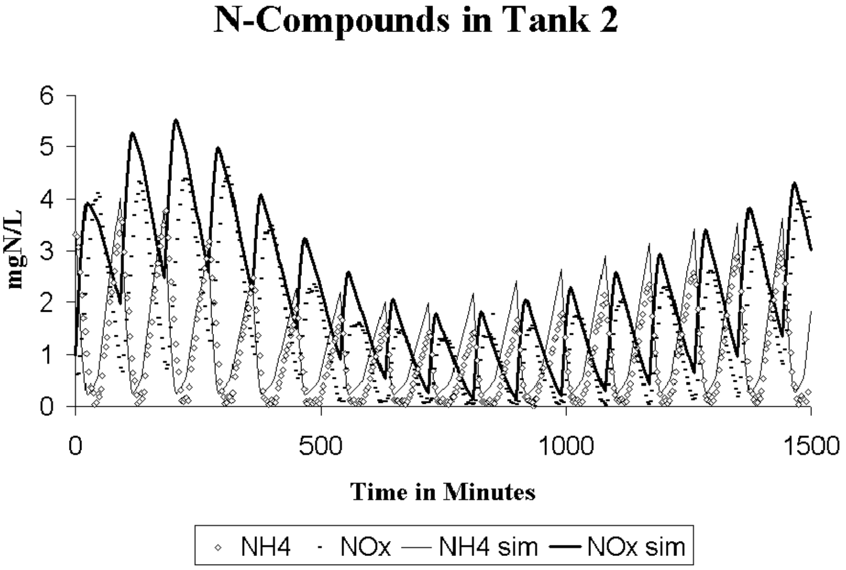

N-Compounds in Tank 2

Figure 5.13. The $NH_4$ and NOx concentrations during the calibration experiment in tank 2

In table 5.4 the deviation between the model and the measurements is presented for both experiments as sum of squares with the weight one for all concentrations (see also equation 1). From the comparison of the SSQ in the anaerobic reactor and the activated tank it becomes clear that the SSQ for the anaerobic case must be weighted in order to reduce the impact on the estimation procedure. Otherwise the determined set of parameter would fit the concentrations in the anaerobic reactor but not in the rest of the plant. As a suitable weighting factor serves the reciprocal value of the mean value of the respective concentration. The comparison of the SSQ for the $PO_4$ concentration in tank 2 makes clear that the evolutionary strategy was focused at the determination of the parameters linked to the BPR process. For the N-compounds the default set of the ASM2 parameters was used and the initial concentrations of the biomass fractions were only determined in some dozens of loops, which explains the higher SSQ for the N-compounds.

Table 5.4. The Sum of Squares for the experiments

| Exp. | SSQ first third of the data | | | | | SSQ last two third of the data | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $PO_{4,T2}$ | $NH_{4,T2}$ | $NOx_{T2}$ | $PO_{4,ana}$ | $NH_{4,ana}$ | $PO_{4,T2}$ | $NH_{4,T2}$ | $NOx_{T2}$ | $PO_{4,ana}$ | $NH_{4,ana}$ |
| | 23.09 | 59.81 | 27.38 | 133.17 | 81.91 | 39.19 | 166.23 | 13.26 | 505.54 | 465.27 |
| 2 | $PO_{4,T2}$ | $NH_{4,T2}$ | $NOx_{T2}$ | $PO_{4,ana}$ | $NH_{4,ana}$ | $PO_{4,T2}$ | $NH_{4,T2}$ | $NOx_{T2}$ | $PO_{4,ana}$ | $NH_{4,ana}$ |
| | 212.46 | 45.26 | 229.72 | 2601.8 | 702.70 | 125.0 | 58.64 | 525.81 | 1330.5 | 1208.5 |

1 is the calibration experiment and 2 is the validation experiment. In case 1 the first third of the data was used for the calibration and the last two third for the validation. In experiment 2 the first third was used for the estimation of the initial concentrations of the biomass and the last two third for the further validation.

For the second experiment, the validation experiment, only the initial concentrations were adapted while the estimated set of parameters was employed in the simulations. In opposite to the fist experiment the SSQ becomes smaller in the second experiment for the validation part. In the first experiment the SSQ in the last two third of the data is at least two times higher than for the set which is used for calibration purposes. This result indicates that the estimated set of parameters deserves the confidence of the reader since the simulation finds after some initial deviations the measurements without further fitting of any parameters.

Altogether it may be concluded that the confidence into the prediction ability of the model was considerably increased. Especially the possibility to use the same set of parameters for the simulation of the pilot plant makes the use of the model very simple The adaptation of the biomass concentrations to the state of the respective conditions of the plant is easily achieved by the evolutionary strategy.

### 5.3.2. Long Term Simulation with an Influent Approximation

Since large amounts of data are available for the ammonium, nitrate and phosphate concentrations measured by the FIA-sytem it is of interest to investigate how precise the estimate for the missing organic compounds would be over a time range which is longer than the here presented experimental horizon. Since no measurements for the organic influent composition were available for a longer time than four to five days, the question must be answered if the behaviour of the plant can be modelled with help of such rough estimates over a long term horizon. Furthermore it is of interest to study how the determined set of parameters can describe the plant behaviour after a period of one year after the calibration experiment.

In Figure 5.14 the simulation and measurements of the pilot plant over a horizon of ten days is shown. The data set which is used, was recorded approximately one year after the first calibration experiment. The first three subfigures demonstrate the $PO_4$, NOx and $NH_4$ concentration in the activated tank, while the last figure presents the $PO_4$ concentration in the anaerobic tank. The data points of the activated tank are plotted with a lower sampling frequency in order to provide a better overview. The sampling frequency is chosen such that only all 90 minutes at the beginning of a new phase the measurement is stored. The alternating behaviour of the activated tank is in this way removed and only the basic trendline is visual. The results in figure 5.13 indicate that the simulation of the behaviour of the specific plant is possible with help of the above described estimate for the influent organic fractions. The $PO_4$ concentrations in the activated tank and anaerobic tank indicates inaccurate estimates of the organic influent fractions over large periods of the observed horizon. Especially the phosphorus release between the start of the data set and the third day is too large, indicating an overestimation of the soluble organic fractions. This overestimation between the fifth and the eighth day is also responsible for the wrong prediction of the phosphorus concentration in tank 2. From the eighth day to the end of the data set the phosphorus release is well predicted indicating a better estimate for the soluble organic compounds. The good qualitative and reasonable quantitative prediction is remarkable not only for the phosphorus components.

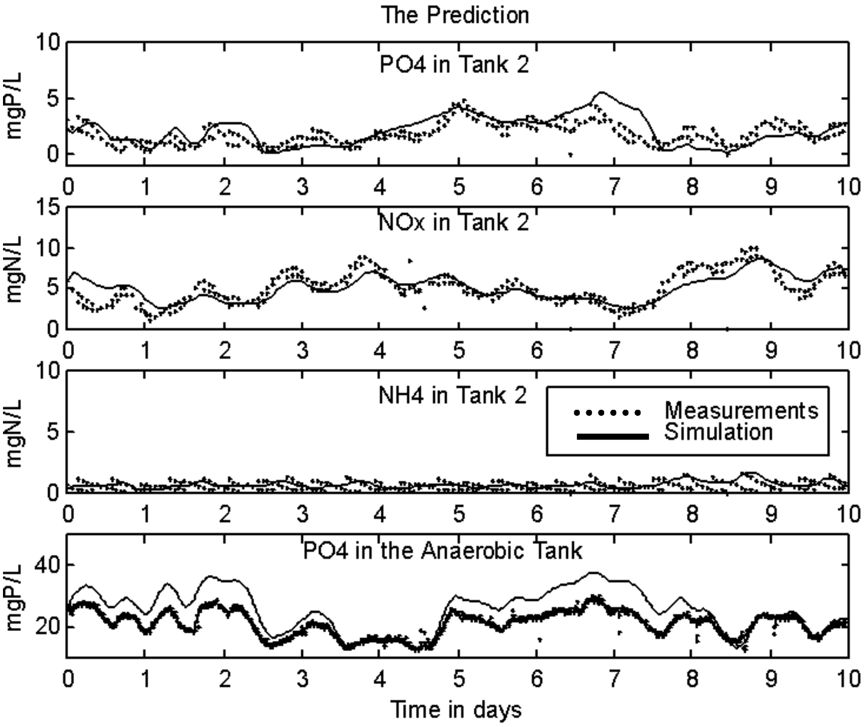


Figure 5.14: The model performance over a period of 10 days. The dots represent the measurement values while the straight lines show the simulation data.

## 5.3.3. The Obtained Set of Parameters

With help of the evolutionary strategy a set of parameters could be found which is valid over a period of more than two years. It should be emphasised, that the investigated pilot plant is placed in a building which ensures almost constant temperatures during summer and winter. Also the pH values can be assumed to be constant which makes the stable set of parameters understandable. The specific numbers for the obtained values can be found in table 5.5. In the first column the determined new parameter is listed while in the second column the proposed default value of the ASM2 can be found. Concerning the obtained values it is remarkable that only the rate constant for storage of $X_{PHA}$, $q_{pha}$ is very much different from the suggested one in the ASM2 and the rate constant for storage of $X_{PP,}$ $q_{pp}$ has a deviation of almost 50% from the default parameter. Nevertheless it is notable that the determined yield coefficients for the PAO and heterotrophic organisms are slightly higher than the default parameters. If the new anoxic rate constants for storage of $X_{PP}$ and growth of $X_{PAO}$ are compared to the aerobic constants, it is notable that the anoxic growth process of $X_{PAO}$ is approximately five times slower than the aerobic while the aerobic uptake of phosphorus is around three times faster than under anoxic conditions.

Concerning the anoxic yield constant for the DNPAO ($Y_{PAOd}$) it should be noted that it has the same value as the aerobic yield coefficient. A possible model parameter reduction could be made at this that it is assumed right from the beginning that the yields (anoxic and aerobic) are the same.

Altogether the result is in conflict with other publications in which the anoxic storage and growth processes are close to 80% of the aerobic constants (literature Kuba, Smolder etc.). At this point the smaller values of the anoxic rate constants reflect the inaccurate structure of the extended model. The work of Meinhold *et al.* (1998) indicates that two groups of PAO are existent, one which is able to store phosphate under aerobic and anoxic addition (DNPAO) and one which is only capable to incorporate phosphate under aerobic conditions. The fraction of DNPAO in the pilot plant was determined by a simple batch test, to be in the range of 40-60%. In the here proposed model all PAO are assumed to be able to denitrify. Therefore the imprecise structure of the model find its consequences in the reduced anoxic rate constants for storage of $X_{PP}$ and growth of $X_{PAO}$.

Table 5.5. The estimated parameter

| Parameter | value | default | |
|---|---|---|---|
| $Y_H$ [gCOD/gCOD] | 0,71 | (0,63) | |
| $Y_{PAO}$ [gCOD/gCOD] | 0,71 | (0,63) | |
| $Y_{PO4}$ [gP/gCOD] | 0,33 | (0,4) | |
| $Y_{PHA}$ [gCOD/gCOD] | 0,21 | (0,2) | |
| $q_{pha}$ [gCOD/gPAOd] | 8,94 | (3) | |
| $q_{pp}$ [gPP/gPAOd] | 0,58 | (1) | |
| $\mu_{PAO}$ [ $d^{-1}$] | 1,14 | (1) | |
| $b_{PAO}$ [ $d^{-1}$] | 0,22 | (0,2) | |
| $b_{PP}$ [ $d^{-1}$] | 0,10 | (0,2) | |
| $b_{PHA}$ [ $d^{-1}$] | 0,16 | (0,2) | |
| $q_{ppno3}$ [ gPP/gPAOd ] | 0,19 | (-) | New Parameter |
| $q_{paod}$ [ $d^{-1}$] | 0,22 | (-) | |
| $Y_{PAOd}$ [gCOD/gCOD] | 0,71 | (-) | |

In table 5.6 the frequently found initial conditions of the biomass fractions are presented. These values reflect the situation of the conditions of the biomass as a function of the influent conditions. Therefore only the concentrations are presented in a draft magnitude. The simulated values for the autotrophic biomass were relatively constant in comparison with the values for PAO and heterotrophic organism.

Table 5.6. Biomass concentrations during the investigated experiments

Initial Conditions

| $X_H$ | $X_{PAO}$ | $X_{AUT}$ |
|---|---|---|
| [ gCOD/$m^3$] | [gCOD/$m^3$] | [gCOD/$m^3$] |
| > 1000 | $200 < X_{PAO} < 500$ | ≈ 100 |

## 5.4.Conclusion

The presented extended ASM2 can be calibrated to an alternating BIODENIPHO™ type pilot plant receiving municipal wastewater. The prediction of the extended model concerning $PO_4$, NOx and $NH_4$ reveals a convincing quality and the set of determined parameters is valid over a long time period including varying scenaria. For the estimation of the parameters and initial conditions of the biomass fractions, an evolutionary strategy has been demonstrated to be a powerful tool. The investigation included observations of the pilot plant over a range of several hours to ten days. The influent conditions of the studied system was changing due to normal daily composition changes as well as due to a rain event. The confidence in the reliability of the model has been established by this investigation. Therefore the model can be used for the investigation of the pilot plant behaviour in order to obtain new control and operational strategies.

As a side effect of this investigation a simple relationship between the organic components of the influent wastewater and the phosphorus release in the anaerobic reactor could be suggested. With help of this relationship the effort for influent sampling campaigns can be reduced and already recorded measurements, where no information about the organic influent compositions is available, can be analysed.

In summary one of the greatest advantages of the here presented model extension is the unique set of estimated parameters which can be used over a time period of more than one year. In this way different influent situations can be analysed with help of the model just by the adaptation of the initial concentrations for the biomass composition without a re-calibration of the whole model. A suitable tool for the determination of such initial conditions is the evolutionary strategy which is very easily brought into a simulation arrangement. The model structure is very similar to the ASM2 model which makes the implementation into existing simulation structures very easy. In the case of the investigated system the quality of the model prediction is impressively good even though the PAO are assumed to be one homogenous group, capable to dentitrify under anoxic conditions. The quality of the model prediction seems not to suffer under the ignoring of internal storage compounds like glycogen. On the other side the size of such deterministic model and the amount of parameters can be regarded as one of the most important disadvantages which will disappear with the increasing progress in the computer developing industry.

# 6. Investigation of an Operational Strategy for the BPR Under Low Influent Concentrations

ABSTRACT

The behavior of a pilot scale biological phosphorus removal process (BPR) of the alternating type was investigated during periods of low influent concentrations and increased hydraulic load. A process disturbance of this type result in an increase in the phosphate concentration level in the anoxic/aerobic reactors and in the plant effluent shortly after the influent wastewater returns to normal strength. The accumulation of phosphorus in the system was avoided by the addition of an external carbon source either to the influent or to the effluent from the anaerobic reactor in form of sodium acetate. With the help of such an addition, the internal carbon storage compounds could be maintained at a high level, which is shown by poly-hydroxy-alcanoates (PHA) measurements. Several levels of acetate addition were investigated experimentally in order to determine a minimal amount of internally stored carbon, which could ensure the stabilization of BPR during such dynamic influent conditions. Identification of such an optimal level was however not possible. The failure of the BPR process was observed even when high concentrations of PHA could be detected. Furthermore reduction of aeration time during periods of low influent concentrations was investigated. It was observed that BPR was stabilized by combining a reduction of aeration time with carbon source addition, which maintained the internal stored carbon at a higher level. This combined control action resulted in a desired high BPR activity when the normal strength of the influent wastewater was re-established.

KEYWORDS

Biological phosphorus removal, external carbon source addition, internal carbon storage compounds, low influent concentrations, operational strategies, wastewater treatment.

## 6.1.Introduction

Occasional failure of biological phosphorus removal processes (BPR) during normal operating conditions of an activated sludge treatment system can render the chemical precipitation of phosphate necessary. A relevant field for close investigation is therefore the behavior of BPR processes after disturbances in the inlet wastewater loading (Temmink *et al.*, 1996, Teichfischer, 1995, Carruci *et al.*, 1999). In particular, dilution of the load by rain events and periodic changes in composition are of interest since the subsequent return to normal wastewater strength frequently results in an increase of the phosphate concentration in the anoxic/aerobic reactors and hence in the plant effluent. This phenomenon is thought to be caused by different recovery times for anoxic/aerobic P-uptake and anaerobic P-release (Temmink *et al.*, 1996). During a period of low inlet wastewater strength the PHA stores in the bacteria are depleted due to the reduced amount of soluble organic components in the influent wastewater. After re-establishment of normal conditions the PHA storage must first be replenished before P-uptake is fully recovered, while the recovery of P-release takes place instantaneously (Brdjanovic *et al.*, 1998). One possibility to overcome this problem could be the addition of an external carbon source to the influent (Teichfischer 1995 and Temmink 1996) in order to maintain the internally stored carbon at a high concentration level. The addition of carbon is only reasonable when an inexpensive carbon source is available and the time of addition is limited to short periods. A different strategy would be the reduction of aeration time, which would limit the unnecessary consumption of PHA during such disturbed influent conditions (Brdjanovic et al 1998 and Temmink (1996).

Some of the essential questions about such an external carbon source addition (ECSA) are in which amount i.e. concentration and time interval it should be added and at which location in the process the addition should take place. Basically both the addition to the influent of the anaerobic reactor and to the anoxic operated tank is reasonable. The efficiency in case of anaerobic addition would be expected to be higher as the polyphosphate accumulating organisms (PAO) will not compete with the other heterotrophic organisms for the added carbon. The benefit of an anoxic addition of carbon will be more significant for the PAO since they can already incorporate the supplied carbon while the denitrifying polyphosphate accumulating organism (DNPAO) still take up phosphate by use of nitrate or nitrite as electron acceptor. A part of the carbon will be lost to favour of the remaining non-PAO heterotrophic organisms. The experimental investigations of Meinhold *et al.* 1999 revealed strong indications that the DNPAO are present in the examined pilot plant. Therefore a largest PHA storage is expected during anaerobic addition and hence less carbon can be additional supplied. A further question is how anoxic additions would influence the development of PAO and DNPAO for additions over a period of several weeks. Under such conditions the heterotrophic organisms could be favoured by the additional substrate and a wash out or decrease in amount of the PAO or DNPAO could be the consequence. Furthermore it is well known that the BPR activity is established by the addition of an anaerobic reactor upstream of a nitrification/denitrification process. In this way the PAO are able to accumulate in the system due to the release of phosphorus and storage of easily biodegradable substrate in the form of e.g. PHA and the subsequent uptake of the released phosphorus under aerobic or anoxic conditions. In this way the PAO obtain a competitive advantage compared with other heterotrophic organisms. The purpose of this work is to perform an experimental investigation of both external carbon source addition (ECSA) and the influence of aeration time upon BPR.

## 6.2.Material and Methods

### 6.2.1.Pilot Plant

An alternating BIODENIPHO™ pilot plant process was employed in this study. The plant and the basic alternating operation is shown in figure 6.1 and is described in e.g. Isaacs *et al.* (1992), Einfeldt (1992), Arvin (1985) and Pedersen *et al.* (1990). This is an activated sludge process for biological C, N and P removal incorporating cyclic changes in flow and aeration. Ammonium nitrogen ($NH_4$-N), nitrate plus nitrite nitrogen ($NO_x$-N) and ortho-phosphate ($PO_4$-P) were measured automatically by flow injection analysis (FIA) as described in Isaacs *et al.* (1992) at the sample points 1-4, which are located in the inlet wastewater, the exit of the anaerobic tank, the aeration tank 2, and the effluent stream respectively (see figure 6.1). PHA were measured as described in Smolders *et al.* (1994) with minor modifications. MLSS was determined according to Standard Methods of the APHA (1985).

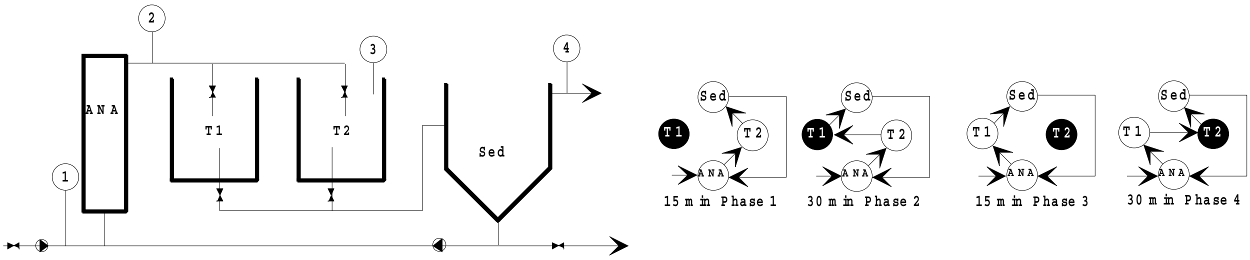


Figure 6.1. The pilot plant and the flow and aeration pattern during a 90 min cycle, black circles indicate aeration periods

### 6.2.2. Pilot Plant Experiments

Altogether ten experiments, simulating a rain event, were performed with variation in the amount of COD added, the place of addition and the aeration time. A summary of the experiments is presented in table 6.1:

Table 6.1: Experimental conditions

|  | ref 1 | ref 2 | anox 15 | anox 30 | ana 15 | ana 22.5 | ana 30 | ana 45 | roxana 15 | roxanox 15 |
|---|---|---|---|---|---|---|---|---|---|---|
| addition location | – | – | 2 | 2 | 1 | 1 | 1 | 1 | 1 | 2 |
| acetate added [mgCOD/L] | – | – | 15 | 30 | 15 | 22.5 | 30 | 45 | 15 | 15 |
| aeration time | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 15 | 15 |

Location 1 = anaerobic addition [ana], 2 = anoxic addition [anox] (see fig. 1)

Each experiment was performed during a time period of approximately three days. The first day the plant received the normal influent wastewater from the Lundtofte wastewater treatment plant in Denmark, which is located close to the pilot plant. During the second day of the experiment the influent wastewater was diluted in a 1:3 ratio with tap water which was stored in a big storage tank. The tank was filled the day before with the intention to warm the tap water up to equal the temperature of the wastewater to avoid a temperature shock of the plant. The hydraulic load was increased from 2.16 to 4.32 m$^3$/d when the dilution took place. The return sludge flowrate was kept constant at 2.16 m$^3$/d. At the third day the normal influent strength was re-established and the flowrate was decreased to its original value.

The influent wastewater was analysed every hour during the day and every three hours during the night for total COD, soluble COD and acetic acid. The samples, taken during the night, were pumped by an automatic sampling device into sample bottles and were prepared for the analysis the next morning. Additional samples were taken manually to determine the concentration of poly-β-hydroxy-butyrate (PHB) and poly-hydroxy-valerate (PHV) which are stored in the sludge. The sum of these components will be denoted as poly-hydroxy-alcanoates (PHA). The samples were collected at the effluent of the anaerobic reactor with a sampling frequency of 1/hour and the activated tank 2 at the beginning and end of one half-cycle (every 45 minutes). The $NH_4$-N, NOx-N and $PO_4$-P concentrations were sampled and analysed with the FIA system approximately every three minutes in the activated tank and every 12 minutes in the other tanks.

Two of the experiments with the lowest amounts of ECSA were repeated with reduced aeration time from 30 to 15 minutes. The intention of these experiments called oxana15 and oxanox15 was to compare the different operational approaches and to study the impact of the aeration time on the PHA concentrations.

In the case of experiment ana 15 a disturbance occurred. During the artificial dilution of the influent wastewater a real rain event was taking place which decreased the influent concentrations even more. No correcting control action could be performed. Therefore it was decided to increase the added amount of COD to 30 mgCOD/L and to maintain the addition also after the re-establishment of normal wastewater composition and flow. Since the addition pump flowrate was maintained and the influent flowrate was reduced to 2.16 m$^3$/d the total added amount was 60 mgCOD/L after the re-establishment of normal influent conditions.

## 6.3. Results and Discussion

The general overview over the performed experimental results is given, followed by the measurements of the internal carbon storage compounds. At the end of this section the impact of the reduction of the aeration time will be shown. For reasons of simplicity the term “failure of BPR” is introduced, which means that an accumulation of phosphorus occurred after the re-establishment of normal wastewater influent strength and flow.

### 6.3.1. Overview of the Experiments

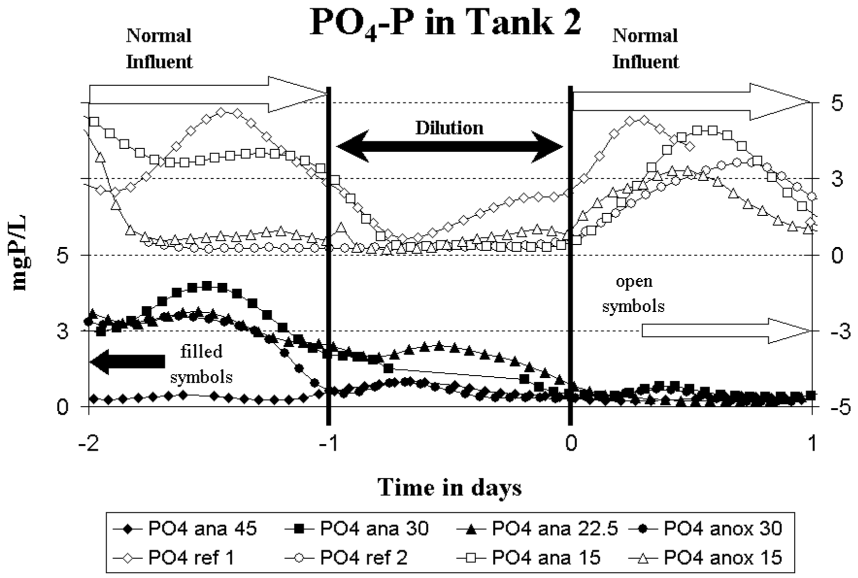
The addition of external carbon to the system stabilised the BPR process in six of the ten cases as presented in table 6.2. Figures 6.2a and 6.2b survey experiments, which have been performed, with a fixed aeration time of 30 minutes. The curves in the upper part of figure 6.2a (open symbols) represent the experiments where the acetate addition was not successfully stabilising the system. In the lower part the filled symbols show the results for the cases where the operational strategy was successful. As shown in the figures, it is obvious that the initial conditions were different, depending on the influent wastewater composition and the current state of the system. Only in three of the cases (anox 15, ana 45 and ref 2) the phosphorus concentrations were at a satisfactory low level before the addition.

Table 6.2. Experimental results

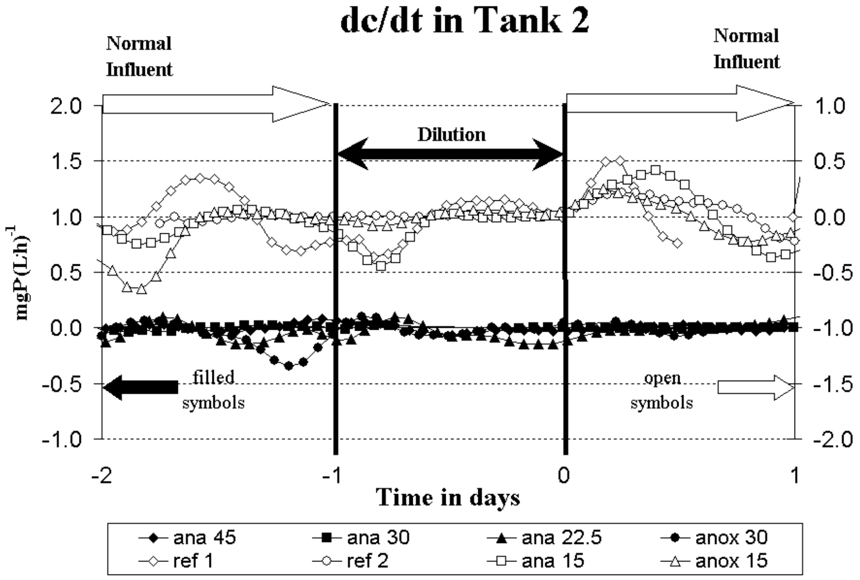
| Name | ref 1 | ref 2 | ana 15 | ana 22.5 | ana 30 | ana 45 | anox 15 | anox 30 | roxana 15 | roxanox 15 |
|---|---|---|---|---|---|---|---|---|---|---|
| result | - | - | - | + | + | + | - | + | + | + |

+ No phosphorus accumulation, - phosphorus accumulation

The derivative of the phosphorus concentration, which is equal to the accumulation in the activated tank, is presented from cycle to cycle in figure 6.2b. For all experiments of BPR failure the characteristic increase of the $dc_{PO4}/dt$-curve after the re-establishment of normal influent composition can be observed. For three of the experiments the slope of the curve, just after the re-establishment of normal influent conditions, is similar. Only the experiment ref 1 shows a higher initial slope. In the cases where the operational strategy worked the curve stays as expected close to zero.



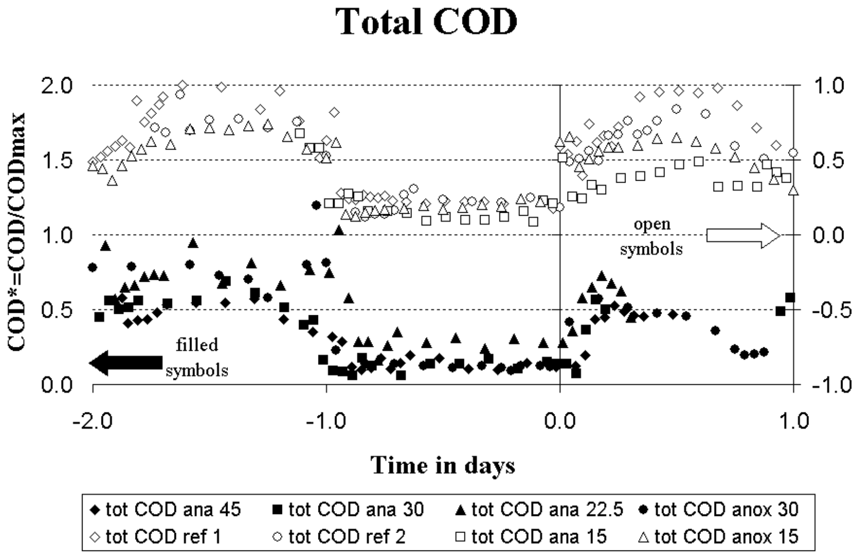
a



b

Figure 6.2. a) $PO_4$-P concentration in the activated tank, sampled every 90 minutes at the beginning of a new cycle, b) Accumulation of concentrations in the activated tank (white symbols = failure of BPR)

Since the influent phosphorus concentration was similar throughout all experiments it is of interest to compare the influent organic compounds. To make the graphs directly comparable and more clear the influent values are all related to the highest average total COD concentration in experiment ana 22.5 which was 400 mgCOD·$L^{-1}$. The dimensionless influent concentrations of soluble COD and total COD are presented in figure 6.3a and 6.3b.

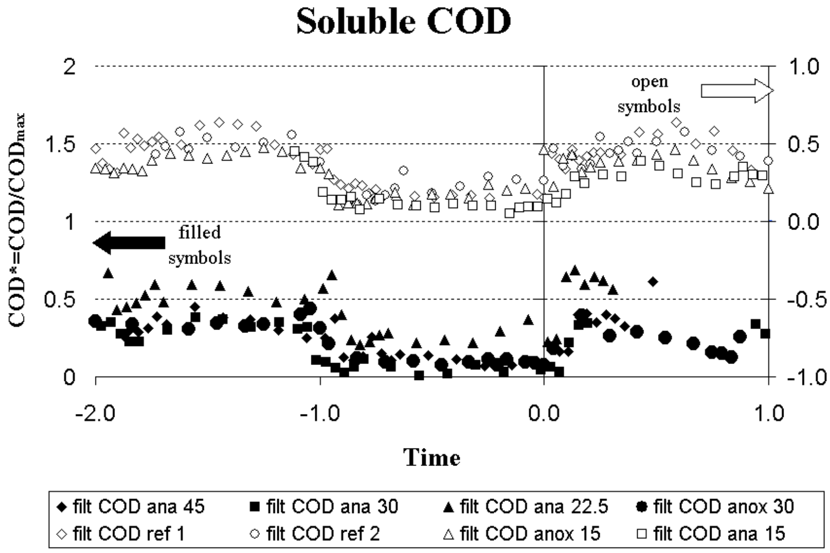


a

Figure 6.3. a) Dimensionless total COD influent concentrations during the experiments (open symbols = failure of BPR. CODmax = 400 mgCOD/L)

From figures 6.3a and 6.3b it can be recognised that the concentration ranges are comparable even though, e.g. in the case of the two reference experiments, a deviation of more than 50 % occurs. But even though such strong differences between the influent conditions exist, the behaviour following such dilutions (days 0-1) is still the same and the phosphorus accumulation takes place. The study of figures 6.2 and 6.3 illustrate that the accumulation of phosphorus is relatively independent of the absolute values of the influent concentrations of organic matter.

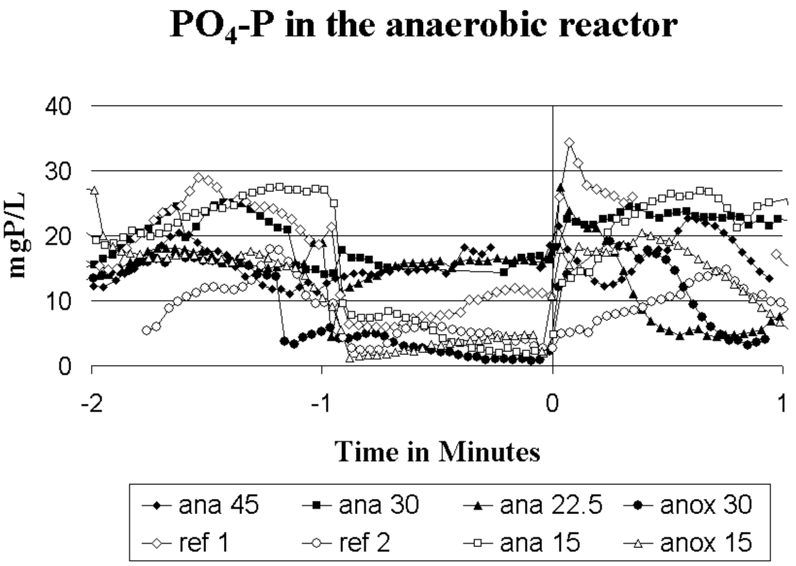
The alternating influent conditions from normal wastewater strength to diluted conditions back to normal influent strength seem to be of more significant relevance.



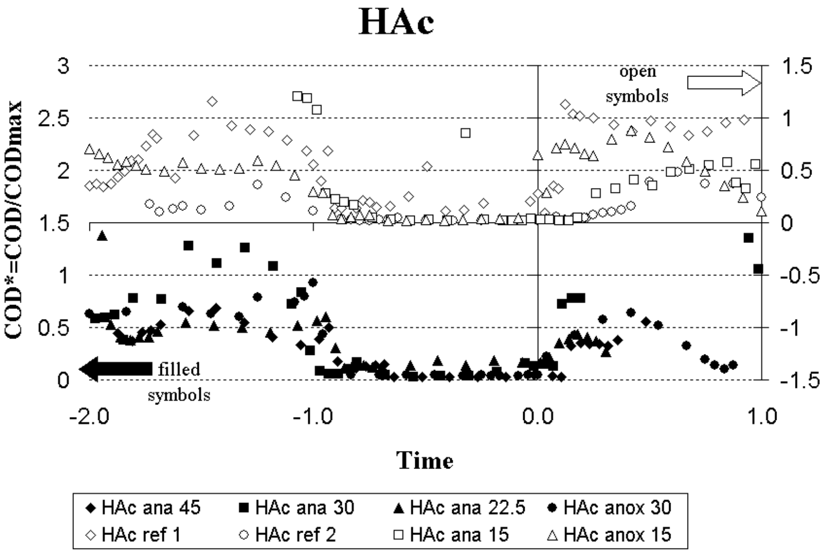
b

Figure 6.3. b) Dimensionless soluble COD influent concentrations during the experiments (open symbols = failure of BPR. CODmax = 400 mgCOD/L)

The phosphorus release in the anaerobic reactor is not only dependent on the influent concentration of readily degradable substrate. The fermentation processes in the anaerobic reactor also convert soluble fermentable compounds into readily degradable substrates. The phosphorus release is therefore mainly a function of these two influent characteristics. In order to compare the load situation of all experiments the phosphorus concentrations of the anaerobic reactor are of significant interest. In figure 6.4a the $PO_4$–P concentrations at the end of the anaerobic reactor for all experiments are presented.



a



b

Figure 6.4. a) $PO_4$–P concentrations in the anaerobic reactor, b) HAc concentrations in the influent (white symbols imply failure of BPR)

Figure 6.4a demonstrates that the highest and lowest P-releases take place during the reference experiments. The build up of the anaerobic phosphorus concentration for the experiment ref 2 develops slowly while in all other experiments the increase of the $PO_4$-P concentration takes place immediately. Nevertheless the characteristic accumulation or release of phosphorus from the sludge can be found in figure 6.2. The maximum of $PO_4$-P is reached later than in the other experiments due to this slower build up. The tendencies that are found in the $PO_4$-P concentrations in the anaerobic reactor are also present in the influent acetate concentration as shown in figure 6.4b. The acetate concentrations are like the COD concentrations presented dimensionless and are related to 60 mgCOD/L, the highest average observed concentration. The failure of BPR takes place for high as well as for low HAc concentrations. The comparison of the influent organic load confirms that the failure of BPR is not dependent on a minimum organic load, since the failure takes place over the whole presented concentration range.

As a preliminary summary it can be concluded that the ECSA as an operational strategy supports maintaining the BPR process. The lowest anaerobic addition of sodium acetate which stabilised the BPR after a rain event was 22.5 mgCOD/L, which corresponds under consideration of the MLSS concentration in the plant, to 8.5 kgCOD/kgMLSS. The anoxic addition of carbon was also successful and an amount of 30 mgCOD/L could achieve results comparable to the anaerobic addition with 22.5 mgCOD/L. In the cases were the BPR process could not be improved it can be concluded that the characteristic accumulation of phosphorus after such disturbance occurs at both high and low organic loading.

### 6.3.2. Internal Storage

For the comparison of the internal carbon storage compounds the eight experiments with 30 minutes aeration are presented in units of mgPHA/gSS. In figure 6.5a the PHA concentration (the sum of PHB and PHV) is shown related to the amount of biomass in the system. It is to notice that the level of PHA concentrations between the failed and the stabilised cases are not differing very much from each other. Especially in the experiments ana 15 and ana 45 the difference between the PHA concentrations is only marginal. Particularly during the dilution (second measurement clusters) the stabilised cases have a positive slope while the reference experiments show a decreasing tendency. The difference between the absolute values is relatively small.

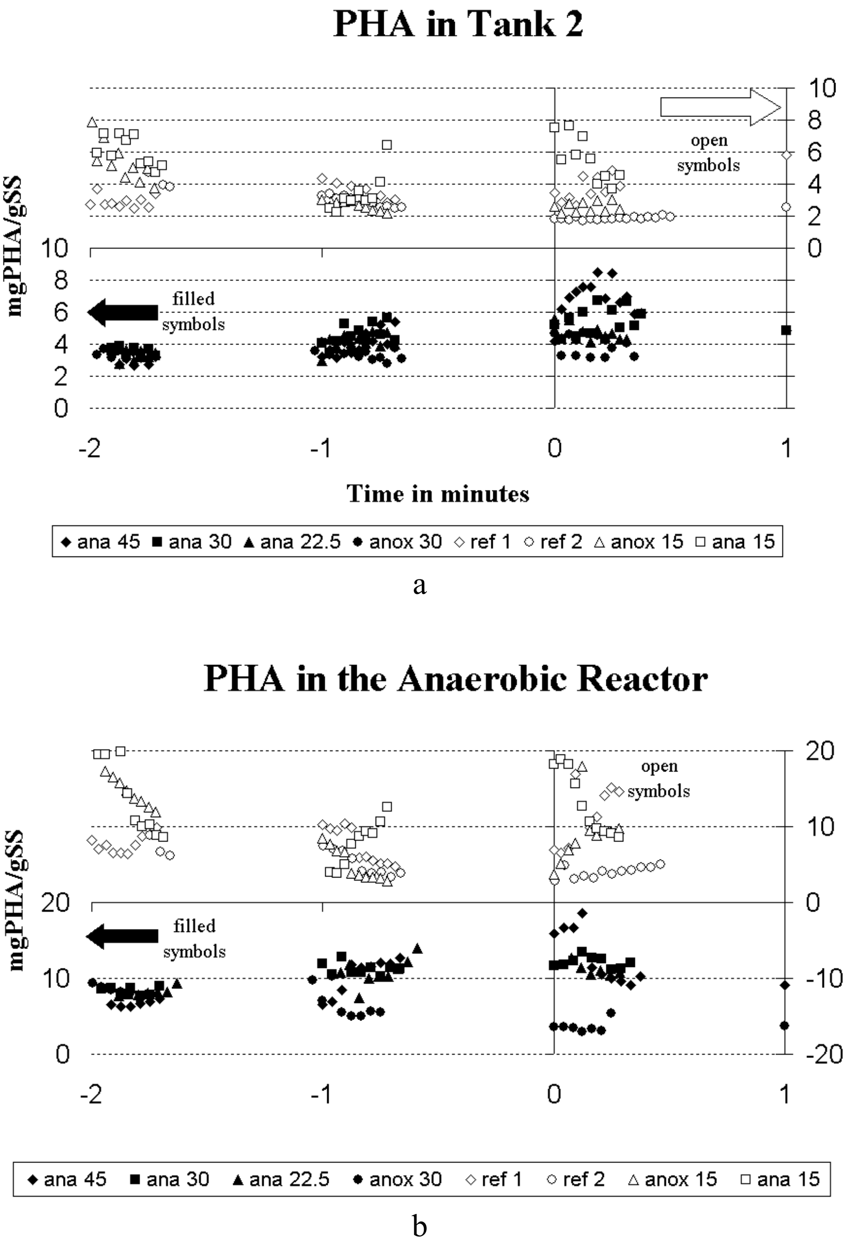


Figure 6.5. a) PHA concentration in the activated tank, b) PHA concentration in the anaerobic tank (open symbols imply failure of BPR)

In the case of stabilised BPR the lowest amount of internal stored PHA was obtained for the anoxic addition with ~3 mgPHA/gSS. This value is approximately three times larger than the observed concentrations in investigations of Brdjanovic (1998) and Temmink (1995) where the depletion of PHA during excessive aeration or periods of diluted inflow compositions is studied. Compared with the cases of failed BPR stabilisation, the anoxic addition of 30 mgCOD/L could stabilise the BPR process even though the lowest PHA concentrations have been in a range where the other experiments failed. A comparison of the process ana 15 in the upper part of figure 6.5a with ana 45 in the lower part of figure 6.5a shows that one of the process failed while the other performed well after the re-establishment of normal operating conditions. For these experiments the PHA values are comparably high with around 8 mgPHA/gSS at the maximum of the tank dynamics. Even though the PHA concentrations of the ana 15 experiment are comparably high, an accumulation of phosphorus in the bulk liquid occurs after the dilution period. The main difference between ana 15 and ana 45 seems to be that PHA continues to rise for several hours after the dilution period in ana 45, whereas it decreases relatively rapidly in ana 15.

It is remarkable that the levels of PHA concentrations in tank 2 are not differing very much during the time of dilution (second cluster). For the stabilised cases the majority of the measurements are slightly higher than for the non-stabilised cases (~3-6 mgPHA/gSS in the stabilised case and ~2-4 mgPHA/gSS in the non-stabilised experiments). After the return to normal inlet conditions, the level of the PHA concentrations are varying according to the received amounts of COD. In the cases of stabilised BPR the lowest values are observed for the anoxic addition while the highest belong to the ana 45 experiment. Also for the non-stabilised cases the anoxic addition show the lowest stored amounts while the ana15 experiment has the highest.

The low amounts of stored PHA for the anoxic cases seems to be reasonable since it was expected that a part of the additionally available COD will be used during denitrification processes of heterotrophic organisms. The surprising result is that even though only small values of internal stored carbon are observed during experiment anoxic 30, the BPR is stabilised, while in other cases the characteristic imbalance between release and uptake of phosphorus occurs. One possible explanation for such results could be the low amount of PAO in the system, which would lead to a higher amount of PHA per PAO. Such low concentrations could be caused by a longer time of low influent concentrations of easily degradable carbon. In case that the amount of PAO is considerable high a different uptake behaviour could be the consequence, since the PHA concentrations per unit biomass could become rate limiting, while in the other case no limitation occurs. The measurement of the PAO fraction in the system is unfortunately not possible since it is not yet known which of the organism or organisms are responsible for the uptake in activated sludge systems.

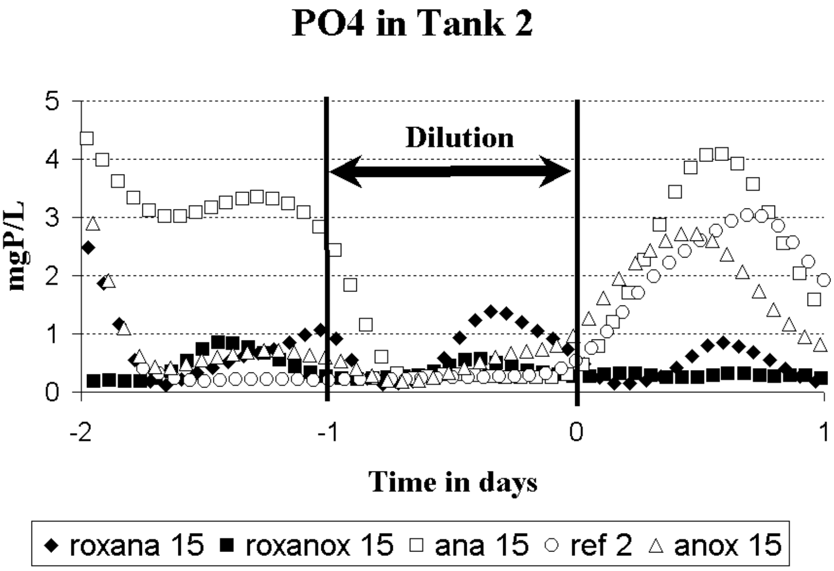
In the presentation of the PHA concentrations of the anaerobic reactor in figure 6.5b the levels between the stabilised and non-stabilised cases are more different than as for the activated tank. With exception of the anoxic 30 experiment all PHA concentrations during the disturbance are situated around ~10-14 mgPHA/gSS while for the non-stabilised cases the values lie between 4 and 10 mgPHA/gSS. When normal influent conditions are re-established the values for the stabilised cases stay in the region of 10~14 mgPHA/gSS while in the other experiments the levels are slowly increasing. The experiment anox 30 demonstrates again a different behaviour since the PHA level is even decreasing after the step back, while the BPR process is performing surprisingly well.

The conclusion from this part is that the actual level of PHA concentration itself is not sufficient information to indicate whether the process will be stabilised or not but an increase of the PHA level seems to have a positive effect on the BPR process.

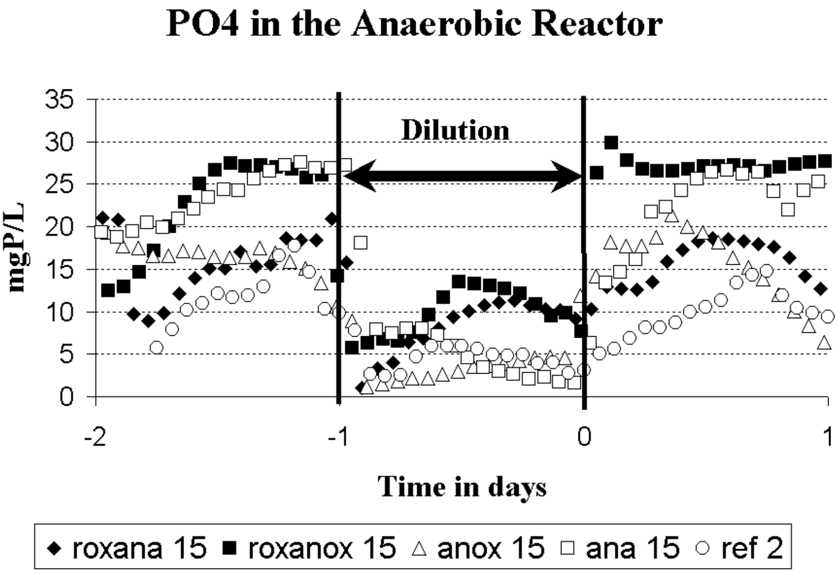
### 6.3.3. Reduction of the Aeration Time

The above-presented experimental results indicate the possible stabilisation of the BPR process by the means of an external carbon source addition. The carbon source supports during the periods of low organic influent concentrations the BPR process such that in most of the cases the PHA concentration can be maintained at a higher level than without addition. During these type of disturbances the $NH_4$-N and $PO_4$-P concentrations are reduced as well as the influent organic concentrations. Due to this reduction the necessary aeration time for the nitrification process and the biological phosphorus uptake is also reduced. Many wastewater treatment plants are operated nevertheless by constant aeration time schedules just as performed during the first eight experiments. The usage of excessive aeration will lead to unnecessary high consumption of PHA due to static aeration control strategy. A flexible reduction of the aerated periods in the plant is assumed to reduce or even avoid the undesired consumption of PHA. Therefore this reduction of aeration is investigated on the two experiments with acetate addition which could not stabilise the BPR process (ana 15 and anox 15). The results of these experiments are together with a reference experiment (ref 2) and the original experiments presented in figure 6.6.

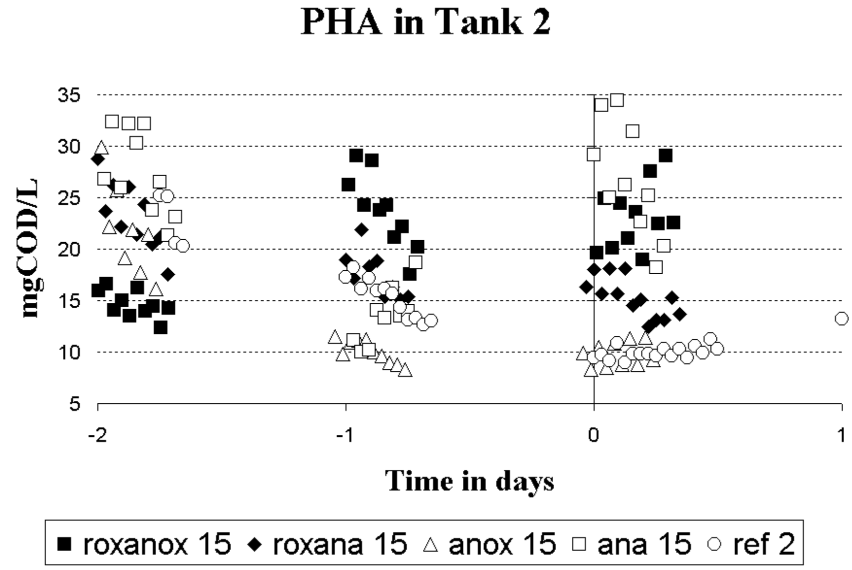
In figure 6.6a the $PO_4$-P concentrations demonstrate that the permanent reduction of aeration time could stabilise the BPR process in combination with an acetate addition. While in the reference experiment and the previous experiments with an addition of 15 mgCOD/L the phosphorus accumulates in the system, the $PO_4$-P concentration stays for the reduced aeration time experiments at the desired levels.


PO4 in Tank 2

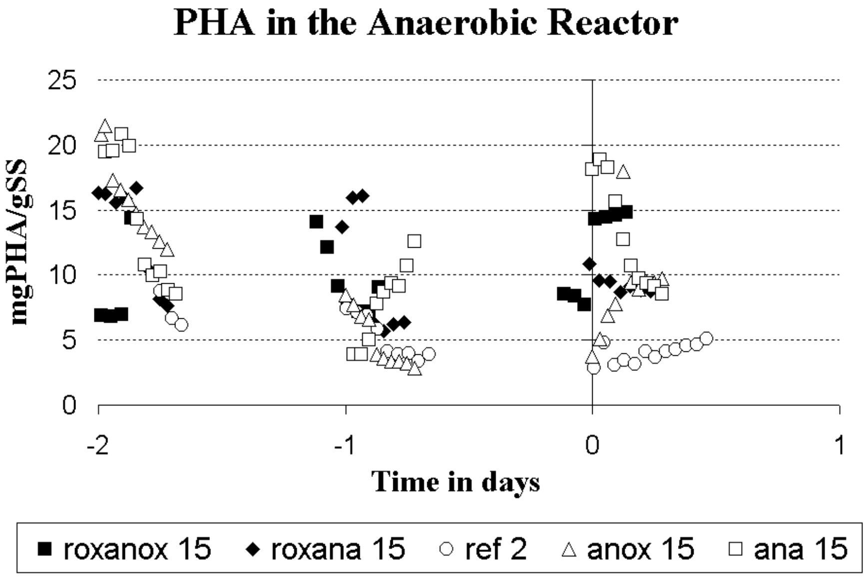
a


PO4 in the Anaerobic Reactor

b



c



d

Figure 6.6. Influence of aeration time on BPR recovery. roxana15 = anaerobic addition of 15 mgCOD/L, reduced aeration time, roxanox15 = anoxic addition of 15 mgCOD/L, reduced aeration time. Open symbols = failure of BPR.

The $PO_4$-P concentration of the anaerobic reactor is shown in figure 6.6b in order to relate the influent organic load to the system during the disturbances. The phosphorus release in the anaerobic reactor depends mainly upon the soluble influent organic concentrations, therefore it can be concluded that the strongest organic influent composition was entering the pilot plant during experiment oxanox 15 while the weakest composition occurred during the reference experiment ref 2. In figures 6.6c and 6.6d the impact on the PHA concentrations is shown. While in the cases of combined addition and reduced aeration time the level can be increased the concentrations of the experiments ref 2 and anox 15 remain at a lower level. The PHA concentration of experiment ana 15 is as for the previously presented experiments relatively high but rapidly decreasing when the normal influent composition is re-established. This behaviour is probably caused by the inappropriate high addition rate during this part of the experiment. It demonstrates that the BPR process can fail even though high concentrations of PHA are available. A possible explanation for the failure of BPR during this period of high PHA concentrations can be a low concentration of PAO in the process. The use of a model could be most useful in further interpretation of the experimental results.

## 6.4.Conclusion

The dilution of the influent wastewater composition by rain events causes an increase of the phosphorus concentration in an alternating pilot plant when the normal inlet wastewater composition is re-established. The reason for this behaviour of the BPR process is assumed to be an imbalance between the phosphorus release in the anaerobic zone and the phosphorus uptake in the aerobic/anoxic zone. The P-uptake rate is assumed to be limited by the internal carbon storage compound PHA, which normally is depleted during a rain-event.

It is demonstrated experimentally that the BPR process could be improved by the addition of an external carbon source during such changing influent conditions. The improvement was established by the addition of sodium acetate in the influent to the anaerobic reactor or into the anoxic phase of the process. In case of anaerobic addition an improvement of the BPR was obtained from 22.5 mgCOD/L during the whole dilution period. With increasing sodium acetate addition the phosphorus release during the disturbances was enhanced and the amount of PHA in the biomass was augmented as well. In case of anoxic addition the stabilisation could be achieved with 30 mgCOD/L. The increase of the PHA concentration during the disturbance could be observed but with a smaller magnitude than in the anaerobic cases.

Even though the level of PHA concentration during recovery to normal conditions was expected to be crucial, no minimum value, which ensures the performance of the BPR process, could be observed. In cases of the anoxic addition the BPR process was stabilised at low internal stored PHA levels while in case of the anaerobic addition the BPR process failed even though high amounts of PHA were available. The lowest amount of PHA (3 mgPHA/gSS) during a stabilised case was observed during the anoxic carbon addition of 30 mgCOD/L. This observation is possibly caused by low concentration of PAO.

As a second operational strategy, which supports the stabilisation of the BPR process during low influent concentrations, the reduction of the aeration time in the process was successfully used. With a combination of a low external carbon source addition and a reduced aeration time it was possible to stabilise the BPR process, while the sodium acetate addition alone could not prevent the accumulation of phosphorus after a disturbance. Thus development of further operational or control strategies should have the intention to maintain the PHA concentration at a level that does not limit the phosphorus uptake. The assistance of biological models can be of major importance for further interpretation of these experimental results and for subsequent development of an operation or control strategy to handle rain events in order to discriminate between the limiting influence of the PHA concentration or other causes.

# 7. Model Assisted Investigation of an Operational Strategy for the BPR at Low Influent Concentrations

ABSTRACT

An operational strategy to support the biological phosphorus removal (BPR) process during situations of low influent concentrations and increased hydraulic load such as rain events was investigated. A process disturbance of this type can result in an increase in the phosphate concentration level in the anoxic/aerobic reactors and in the plant effluent shortly after the influent wastewater once again achieves normal strength. The increase of phosphorus in the effluent was avoided by the addition of an external carbon source in form of sodium acetate to the influent or the effluent of the anaerobic reactor.. In this way the internal carbon storage compounds in the form of poly-hydroxy-alcanoates are during the disturbance maintained at a high level and a possible PHA limitation is avoided when the normal influent composition is re-established. The identification of a minimum concentration of PHA necessary to ensure BPR was not possible and a dependency of the PHA concentration on the location of the addition was observed. The failure of the BPR process was sometimes observed even when comparatively high concentrations of PHA could be detected. During this investigation an extended version of the activated sludge model No.2 (ASM2), which includes denitrification by phosphate accumulating organisms (PAO), is used for the detailed analysis of the experiments. The model predicted the phosphorous build-up after the process disturbance as well as the performance during the stabilized experiments. Assisted by the model, the investigations indicate that a PHA limitation is not the only factor affecting the recovery of the BPR process during periods of low influent concentrations.

KEYWORDS

ASM2, biological phosphorus removal, external carbon source addition, internal carbon storage compounds, operational strategies, wastewater treatment.

## 7.1.Introduction

The examination of the biological phosphorus removal (BPR) process under dynamic inlet wastewater compositions is most relevant since such disturbance often results in an undesired increase of effluent phosphorus concentrations. In particular, dilution of the organic load by rain events is of significance (Temmink *et al.*, 1996; Teichfischer, 1995, Carruci *et al.*, 1999). This phenomenon is thought to be caused by different recovery times for anoxic/aerobic P-uptake and anaerobic P-release (Temmink *et al.*, 1996). During the period of low inlet wastewater strength the PHA stores in the bacteria are depleted due to the reduced amount of soluble organic components in the influent wastewater. After re-establishment of normal conditions the PHA storage must first be replenished before P-uptake is fully recovered, while the recovery of P-release takes place instantaneously (Brdjanovic *et al.*, 1998). Teichfischer (1995) suggests to overcome this problem by an addition of an external carbon source to the influent in order to maintain the internal stored carbon on a high concentration level.

In a previous investigation such external carbon source addition (ECSA) was studied with the intention to obtain information about a optimum level of PHA which has to be maintained in the system to avoid phosphorus accumulations (Krühne *et al.* 1999) and to minimize the ECSA. As a second operational alternative reduction of aeration time was investigated to avoid an unnecessary consumption of PHA during such disturbed operational periods. Even though a general dependency of the PHA concentration on the added amount of carbon could be observed, the phosphorus uptake was sometimes limited despite a relatively high amount of internal stored carbon was detected in one case. As reason for this phenomenon a too short aeration time after the disturbance or a general low amount of polyphosphate accumulating organisms (PAO) was suggested.

A comparison of the PHA concentrations obtained during anaerobic additions with those obtained during anoxic addition show much lower PHA levels for the anoxic cases. Under the assumption that denitrifying polyphosphate accumulating organisms (DNPAO) are present in the investigated sludge (Meinhold *et al.* 1999), the addition under anoxic conditions would favour only PAO or the remaining heterotrophic organisms. The DNPAO are still incorporating phosphate by use of nitrate or nitrite (Meinhold *et al.* 1998) as electron acceptor. Therefore storage of more PHA is expected to occur during anaerobic addition and thus less carbon must be supplied. But even if only PAO are present in the system, lower amounts of PHA would be expected due to the competition for substrate with non-PAO heterotrophic organisms. The anoxic addition was nevertheless able to support the BPR process during such low influent conditions. Even though the absolute amounts of PHA were comparatively low, no phosphorus accumulation occurred, when normal inlet wastewater conditions were re-established.

If the PHA concentration is high during the and failure of BPR occurs, another limiting mechanism must be responsible. The purpose of the present paper is to investigate further the possible mechanisms behind failure of BPR during periods of low inlet wastewater concentrations. This investigation is assisted by the application of an extended and calibrated version of the activated sludge model no. 2 (ASM2, Henze *et al.* 1995 and Krühne *et al.* 1998). The objective of the performed investigation is also to verify if the model can describe the pilot plant behaviour with an adequate precision for control purposes.

## 7.2.Material and Methods

### 7.2.1.The Experiments

Altogether ten experiments, reproducing a rain event were performed. The experiments varied in the amount of COD added, the place of addition and the aeration time. A summary of the experiments is presented in table 7.1:

Table 7.1: The experiments

| | ref 1 | ref 2 | anox 15 | anox 30 | ana 15 | ana 22.5 | ana 30 | ana 45 | roxana 15 | roxanox 15 |
|---|---|---|---|---|---|---|---|---|---|---|
| addition location | – | – | anox | anox | ana | ana | ana | ana | ana | anox |
| acetate added [mgCOD/L] | – | – | 15 | 30 | 15 | 22.5 | 30 | 45 | 15 | 15 |
| aeration time | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 30 | 15 | 15 |

Each experiment was performed during a time period of approximately three days. The first day the plant received the normal influent wastewater from the Lundtofte wastewater treatment plant in Denmark, which is located close to the pilot plant. During the second day of the experiment the influent wastewater was diluted in a 1:3 ratio with tap water. The hydraulic load was increased to 200 % at the same time the dilution took place. The return sludge flowrate was kept constant. For the third day the normal influent strength was re-established and the flowrate was decreased to its original value. The detailed description of the experiments and measurements are given in Krühne and Jørgensen (1999).

### 7.2.2. Numerical Methods

For the simulation of the pilot plant an extended version of the ASM2 model including denitrification by the PAO was introduced into a Matlab/Simulink simulation platform. The model was earlier calibrated to the pilot plant (Krühne *et al* 1998) using a simple evolutionary strategy and the same set of model parameters were used for the simulations of all experiments. The determined set of parameters was found to be reasonably valid during a time period of more than two years and is, with exception of the phosphorus release rate $q_{pha}$, similar to the default values of the ASM2 (Krühne *et al.* 1999). The initial conditions of the biomass concentrations ($X_{AUT}$, $X_H$ and $X_{PAO}$) had to be estimated in order to predict the behaviour of the plant via the model. This estimation was performed by a simple manual adjustment of the initial values. The dynamics of the BIODENIPHO™ process for the $PO_4$-P, $NH_4$-N and NOx-N concentration is supporting such a manual adjustment since the uptake rates can be determined without much effort, based on the concentration profiles observed in the tanks.

For the influent organic concentrations the influent wastewater was analysed for the total COD concentration, the soluble COD concentration and for the acetic acid ($S_A$) concentration. The wastewater was assumed to correspond to the characterisation method as presented in Henze *et al.* 1995. The fraction of inert soluble matter was assumed to be 10% of the influent soluble organic fraction while the amount of particulate inert matter was assumed to be 15% of the influent particulate matter.

## 7.3. Results and Discussion

The experimental results concerning the internal stored carbon in form of PHA are discussed in detail in Krühne and Jørgensen (1999). A summary of the observations are presented in figure 7.1:

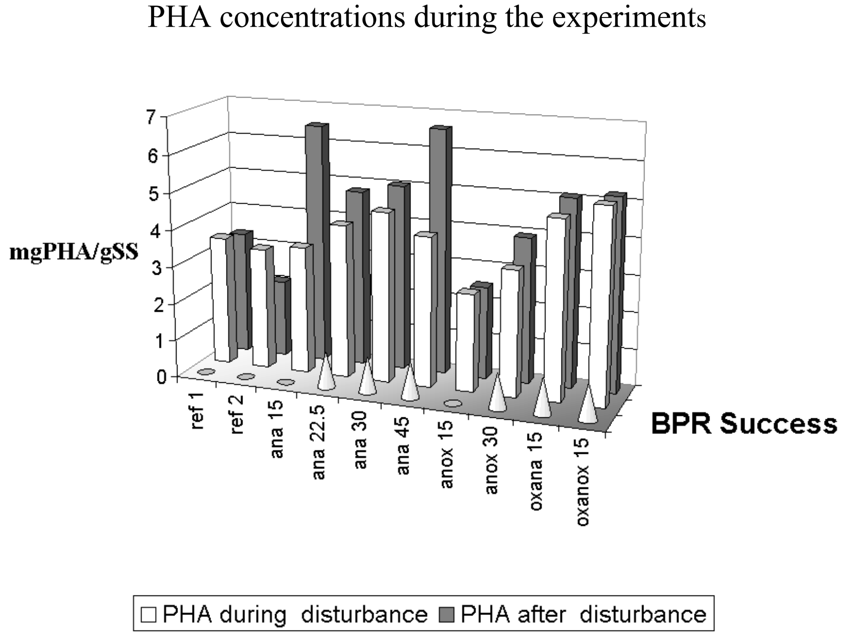

PHA concentrations during the experiments

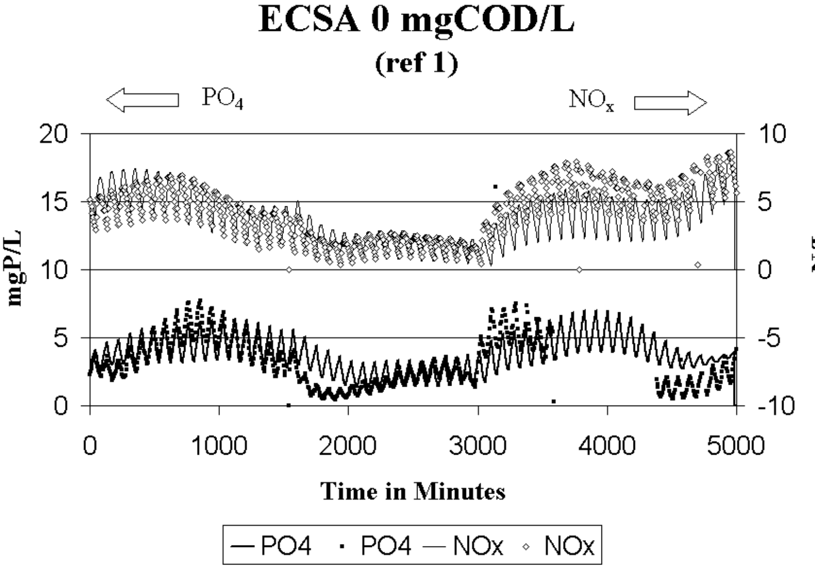
Figure 7.1. Experimental results for PHA. The cones symbolise no phosphorus accumulation, the PHA concentrations are measured in the aerated tanks (average values during the disturbance and the first six measurements after end of the disturbance)

With exception of experiment ana 15, the BPR process performance was improved with increasing amounts of carbon added. From an anaerobic addition of 22.5 mgCOD/L the accumulation of phosphorus could be avoided. For the anoxic addition 30 mgCOD/L had to be added to avoid the accumulation of phosphorus. During anoxic addition the PHA concentrations were, as expected, lower than under anaerobic carbon addition. In experiment ana 15 it was not possible to avoid an accumulation of carbon even though high PHA concentrations could be observed after the re-establishment of normal influent concentrations. In comparison to ana 15 the addition of 45 mgCOD/L enabled similar PHA concentrations to be achieved after the disturbance but here an accumulation of phosphorus could be prevented.

### 7.3.1. Comparison between Model Prediction and Measurements

In order to verify the performance of the model, the $PO_4$-P and NOx-N concentrations of the eight experiments are compared with simulation results. In cases where the sampling frequency of the influent organic compounds was too low an approximation of the influent was used as described in Krühne *et al.* 1999.

In figure 7.2 the results of the reference experiments and the addition of 15mgCOD/L under anaerobic and anoxic conditions are shown.



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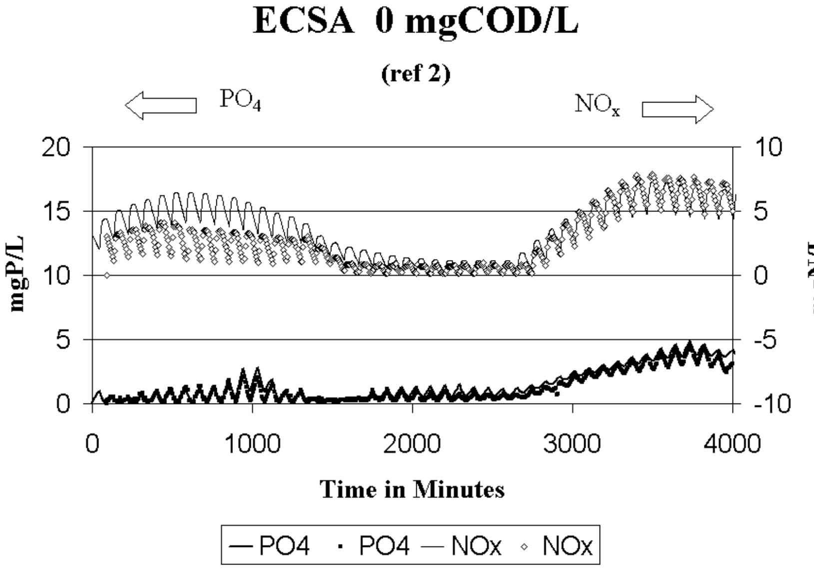

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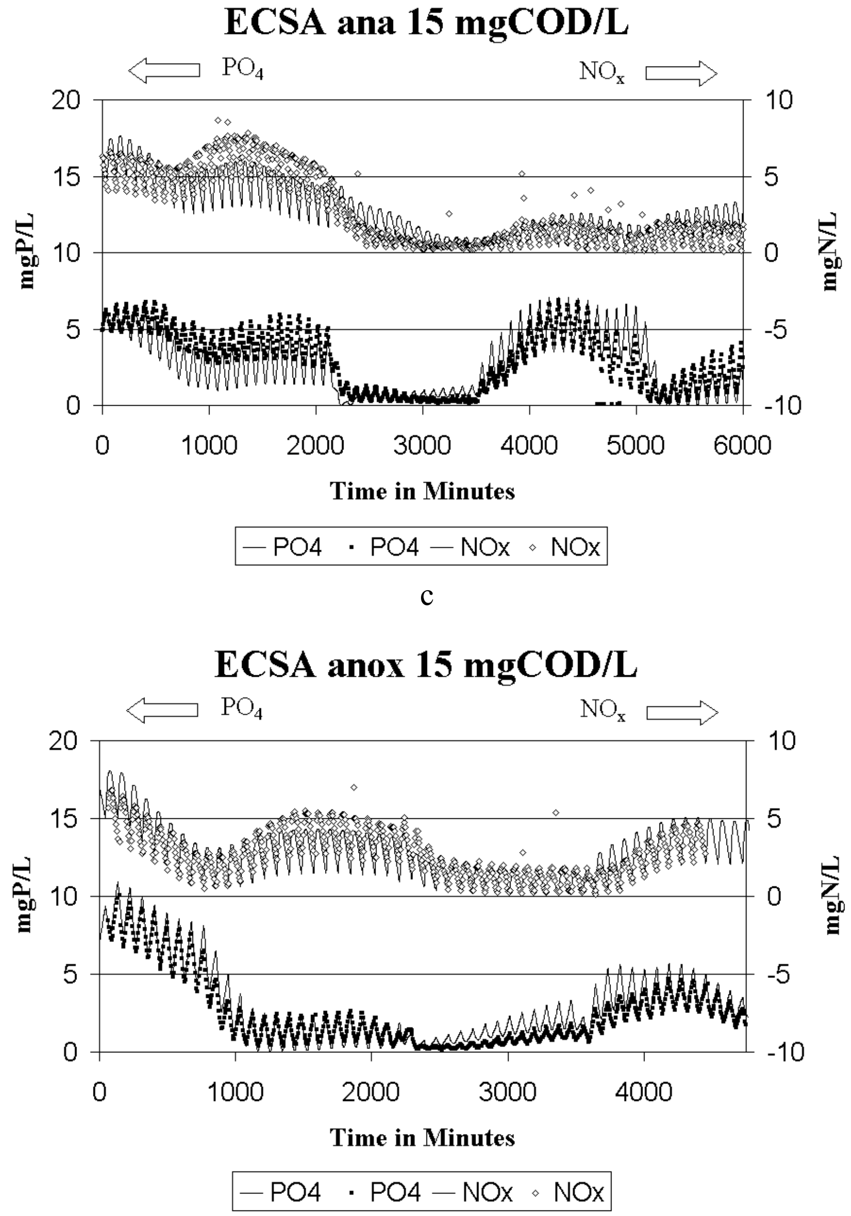

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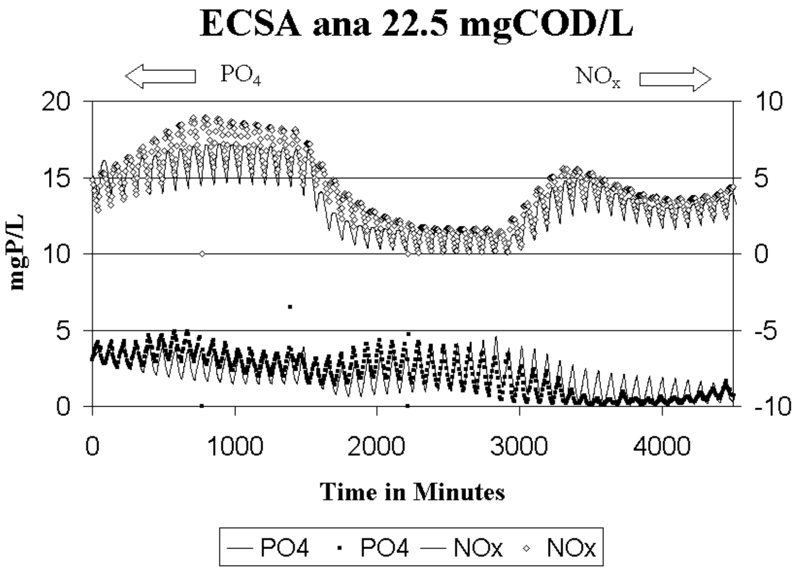
Figure 7.2. Comparison of the simulation prediction and measurements for NOx-N and $PO_4$-P-P. a) ref 1, b) ref 2, c) ana 15, d) anox 15. Simulation results are shown as solid lines.

In all cases an increase of phosphorus is observed after re-establishing of the normal inlet conditions. The model predicts well the dynamics of the $PO_4$-P and the NOx-N concentrations. The deviations between the predicted and measured $PO_4$-P concentrations and NOx-N concentrations are probably caused by an incorrect estimation of the initial conditions and are only a few mg/L. The qualitative prediction of the behaviour is nevertheless described well and the quantitative representation is satisfactory.

The good agreement between the model prediction and the measurements is of interest since some of the definitions in the extended ASM2 model are simplified, compared to what is known about the metabolism. The model component $X_{PHA}$ is assumed to be the sum of internal stored carbon, including glycogen. $X_{PHA}$ is to be understood as a key model component, which is not expected to be observable on an analytical basis. The reason for the incorporation of glycogen into this component is to keep the model simple. A second weak point in the extended ASM2 model might be the assumption that only one group of PAO is present. The PAOs are assumed to be capable to take up phosphorus under anoxic conditions with a reduced uptake rate, compared to aerobic conditions. This assumption might not be true for the investigated pilot plant since a previous investigation (Meinhold *et al*. 1998) suggested the presence of both DNPAO and PAO in this sludge. A more reasonable model representation should therefore include such organisms with their respective internal storage compounds into the model structure. The objective of the performed investigation is also to verify if the less complex model can describe the pilot plant behaviour with a precision adequate for control purposes.

Further examples of model predictions are demonstrated in figure 7.3, where the model prediction and measurements are shown for the experiments with external carbon source addition (ECSA).



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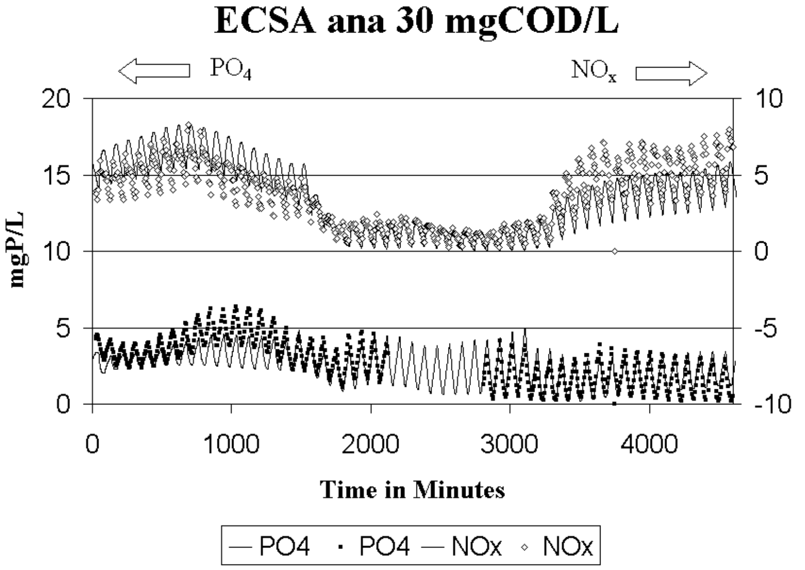

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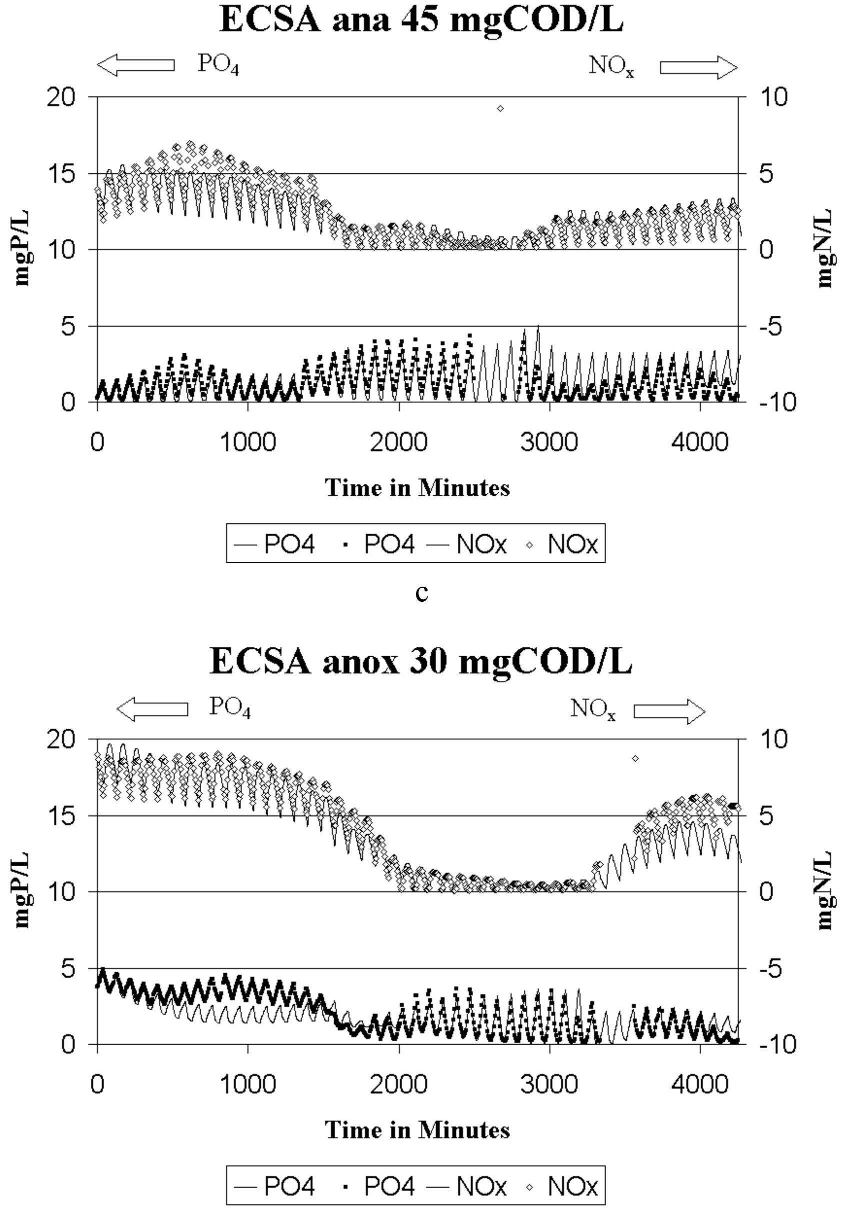


c

d

Figure 7.3. Comparison of the simulation prediction and measurements for NOx-N and $PO_4$-P-P. a) ana 22.5, b) ana 30, c) ana 45, d) anox 30

The model predicts with minor deviations between the measured data points and the calculated values, the observed behaviour in all cases. For all four experiments it is observed that no accumulation of the phosphorus occurs and the level of phosphorus concentration stays, after the re-establishment of normal inlet wastewater composition, below a desired level of 1 mgP/L at the cycle end.

### 7.3.2. General Considerations

The model prediction of $PO_4$-P and NOx-N concentrations are in good agreement with the measurements while the simulated PHA concentrations during all the experiments fit the measured data only qualitatively (not shown here). Those results are not unexpected and support the assumption that the model can be used only for a qualitative analysis of the PHA concentration variations during the experiments. Under the assumption that the main reactions involved in the phosphorus removal process are reasonably well described, the model may be used for the investigation of the failure of BPR, since high PHA concentrations have been predicted as well. In order to investigate this phenomenon, the phosphorus uptake rate for the aerobic uptake of ortho-phosphate is:

$$r = qpp \cdot \frac{S_{O_2}}{S_{O_2} + K_{O_2}} \cdot \frac{S_{PO_4}}{S_{PO_4} + K_{PO_4}} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot \frac{X_{PHA}/X_{PAO}}{X_{PHA}/X_{PAO} + K_{PHA}} \cdot X_{PAO} \qquad \text{eq. 7.1}$$

If the model correctly represents the uptake of phosphorus, several components can be limiting during the uptake process such as oxygen, $PO_4$-P, alkalinity, polyphosphate or the PAO. The alkalinity of the investigated wastewater is not considered as limiting, since most of the water used in Denmark has a high buffering capacity. Furthermore if the alkalinity would be limiting it would be observed for the nitrification processes as well. Since the concentration of PAO cannot be determined by analytical measures the measured concentrations of PHA leave much room for speculation. The internally stored carbon compounds can become limiting when a high concentration of $X_{PAO}$ has been build up in the system and simultaneously low absolute concentrations of PHA are present. On the other hand it is also possible to have sufficiently internally stored carbon but insufficient amounts of $X_{PAO}$ available to take up the released phosphorus. A rough estimation of the maximal amount of phosphorus, which can be taken up, is neglecting the Monod terms in the kinetic expressions, which means that no limitation occurs. Such estimates are presented in figure 7.4:

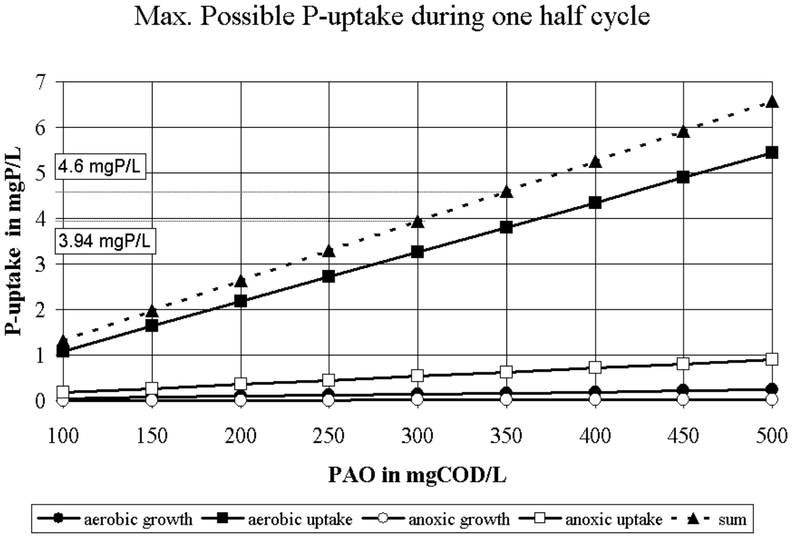


Figure 7.4. Maximal possible contribution of the uptake rates

| | |
|---|---|
| $r_{\text{aerobic uptake}} = q_{pp} \cdot i_{TSSBM} \cdot X_{PAO} \cdot \frac{d}{1440min} \cdot 30min$ | $r_{\text{anoxic uptake}} = q_{ppNOx} \cdot i_{TSSBM} \cdot X_{PAO} \cdot \frac{d}{1440min} \cdot 15min$ |
| $r_{\text{aerobic growth}} = \mu_{PAO} \cdot i_{PBM} \cdot X_{PAO} \cdot \frac{d}{1440min} \cdot 30min$ | $r_{\text{anoxic growth}} = \mu_{PAO,NOx} \cdot i_{PBM} \cdot X_{PAO} \cdot \frac{d}{1440min} \cdot 15min$ |

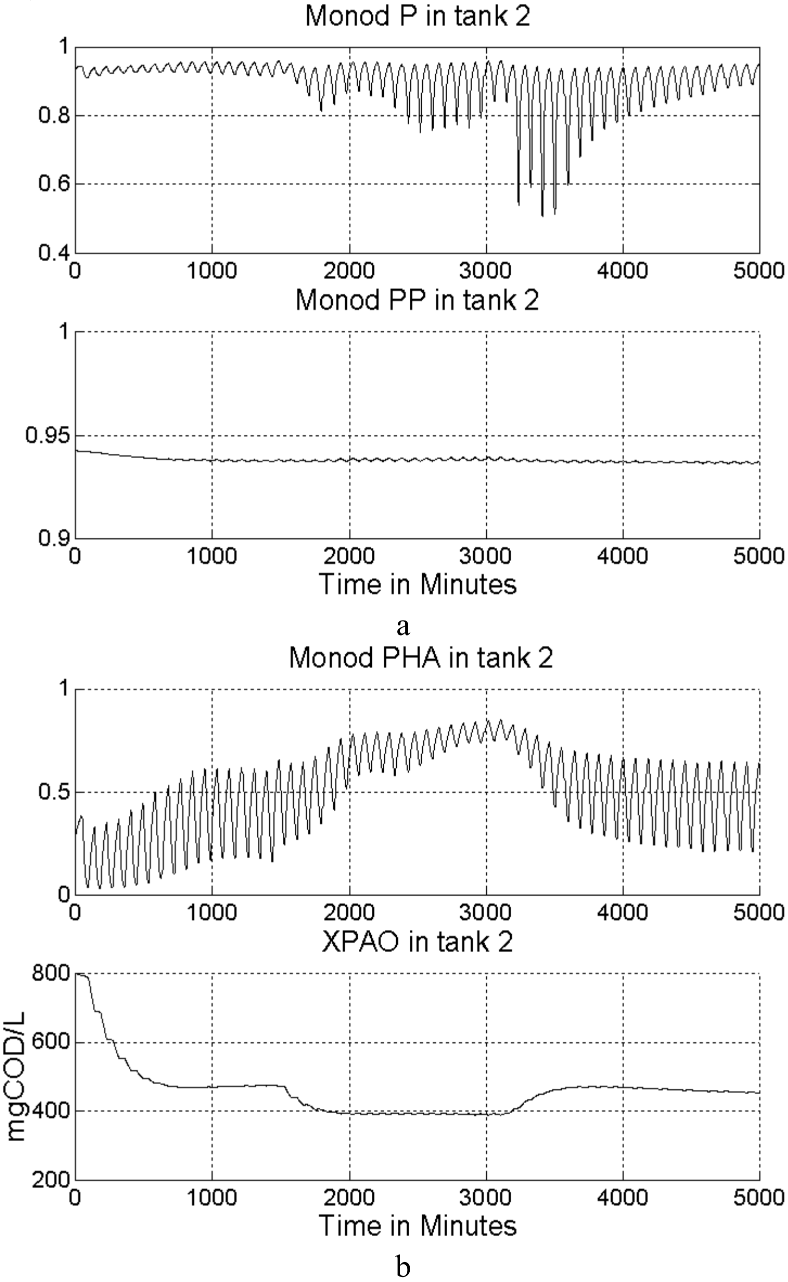
(Values: $q_{pp}$=0.58, $\mu_{PAO}$=1.13, $q_{ppNOx}$=.19, $\mu_{PAONOx}$=0.22, $i_{TSSBM}$=0.9, $i_{PBM}$=0.02),

Concerning figure 7.4 it must be noticed that the stoichiometric coefficients, conversion factors and the aeration time are included in the calculations. From this simple overview it can be seen that during an investigated situation with low levels of $X_{PAO}$ such as 300 mgCOD/L maximally 3.94 mgP/L could be taken up. When the released phosphorus in the anaerobic reactor, which upon entering the activated tank, increases the phosphorus concentration above this 3.94 mgP/L, the accumulation of phosphorus will occur without PHA limitation. In such cases the aeration time should be extended in order to take up the surplus phosphorus.

### 7.3.3. Investigation of Further Limitations

As shown in the previous simple calculations other limitations than the PHA limitation are possible during the accumulation of phosphorus after a rain event. Therefore an investigation was performed with help of the model, where the possible limiting kinetic Monod expressions were investigated during two experiments. The influence of the oxygen concentration and alkalinity were excluded since the DO concentration is well controlled and as explained in a previous the alkalinity was not considered likely to be a limiting factor.

In figure 7.5 simulation results of experiment ana 30 are presented. All simulations with the title Monod X in tank 2 are the Monod terms in the reaction rates calculated as described in equation 1 for the aerated tanks. The saturation coefficients are the default parameters of the ASM2 (Krühne *et al.* 1999).



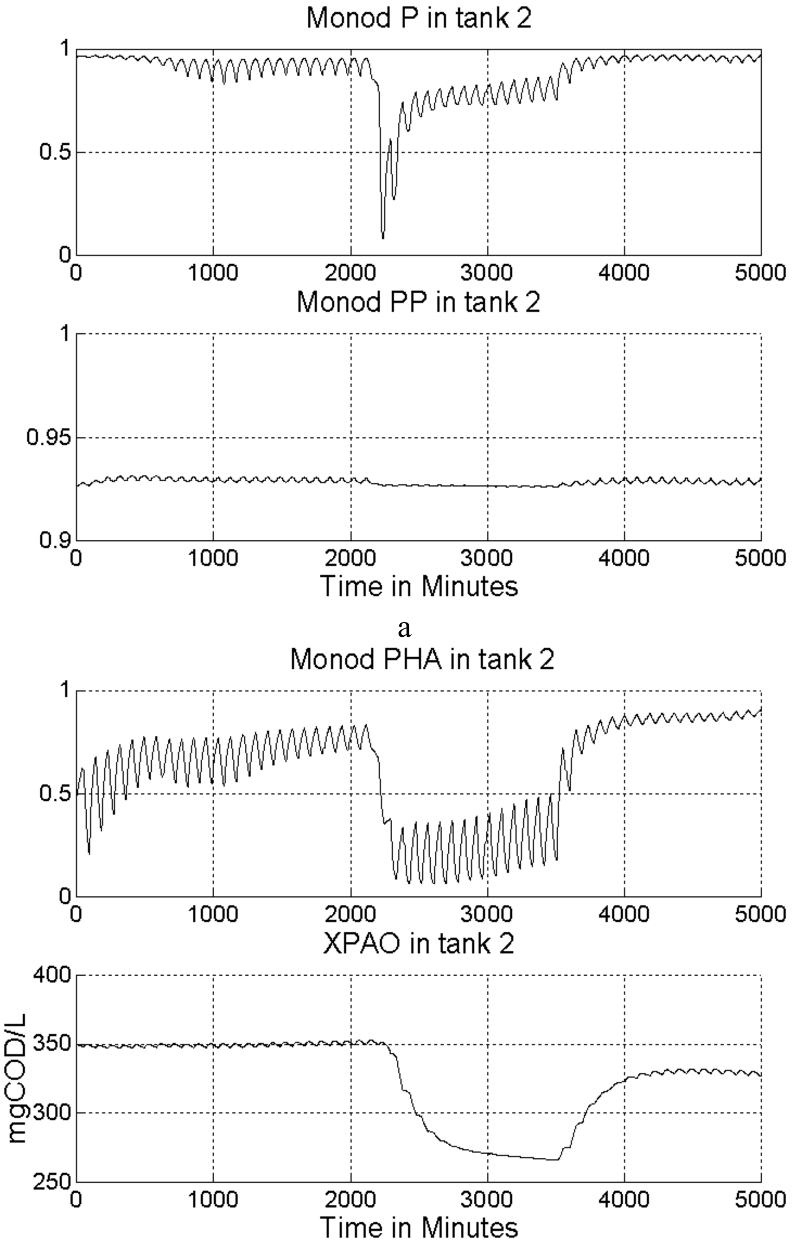
a

b

Figure 7.5. Simulation of two possible limitations during experiment ana 30. a) $PO_4$-P and polyphosphate, b) PHA and $X_{PAO}$

The left part of the figure 7.5 reveals that the phosphorus concentration and the polyphosphate concentration are not identified as the rate limiting components since their values are above 0.9

during the periods of importance. In the upper plot of figure 7.5b it is demonstrated that during the first part of the experiment the Monod terms of the PHA concentration were below 0.5 which explains why the $PO_4$-P concentration during the starting phase of the experiment could not be completely taken up. During the carbon addition the P-uptake-rate is improved and is stabilised after the addition at a higher level than before. If the measurements of the $PO_4$-P concentration during this experiment (illustrated in figure 7.5b) are compared with this Monod term it can be recognised that the uptake of phosphorus was improved from t = 1000 minutes. After this point in time the phosphorus concentration decreased towards the desired level of 1 mgP/L and remained there even though the disturbance took place. In the lower part of figure 7.5b the simulated concentration of PAO is shown. The crude manual fitting of the initial conditions gives rise to the initial transient, which however is insignificant for the above discussion.



a

b

Figure 7.6. Simulation of two possible limitations during ana 15. a) $PO_4$-P and polyphosphate, b) PHA and $X_{PAO}$

In case of the experiment ana 15, presented in figure 7.6, the circumstances were different. In figure 7.6a the same result as in ana 30 could be observed. No $PO_4$-P or polyphosphate limitation (only for a short period) could be observed. In the upper part of figure 7.6b the Monod term for the PHA concentration was initially at a relative high level. Especially the disturbed period caused a decrease of the PHA Monod-term and a strong impact of the PHA concentration. Towards the end of the disturbance, i.e. from ~2700 minutes, the ECSA was increased to 30 mgCOD/L (for details see Krühne *et al.* 1999) and consequently the Monod term increased. The accumulation of phosphorus occurred due to low PAO in the system, even though the limiting Monod term was at the highest level.

The concentration of PAO in tank 2 during the ana 15 experiment was approximately 25% smaller than in the experiment ana 30 according to the simulation results shown in figure 7.5 and 7.6. The absolute value of 350 mgCOD/L results according to figure 7.4 in a maximal uptake of 4.6 mgP/l. Considering the Monod term for PHA (~0.8), the Monod term for PP (~0.93) and the Monod term for $PO_4$-P (~0.95) the maximal value is reduced to $0.95 \cdot 0.93 \cdot 0.8 \cdot 4.6$ mgP/L=3.25 mgP/L which can be taken up under these conditions. The maximum measured $PO_4$-P concentration at t=4275 minutes is 7 mgP/L and the minimum value is ~3.9 mgP/L at t=4320 minutes, which matches the simulation quite accurately.

During this phase of the experiment it was difficult to take up all the released phosphorus which was entering from the anaerobic reactor. But instant help under such conditions would have been the extension of the aeration time, since sufficient PHA was available during this situation. The strong accumulation directly after the end of the disturbance can be explained by the smaller amount of PAO, which need as shown in figure 7.6b a certain time to reach a higher level.

## 7.4.Conclusion

The accumulation of phosphorus in a BPR process, which is exposed to a period of diluted influent concentrations can be avoided by the addition of external carbon in form of sodium acetate. The addition of carbon supports the maintenance of the internally stored carbon in the form of PHA at a higher level than without addition. When the normal influent conditions are re-established and the phosphorus release is immediately taking place, a possible PHA limitation is avoided. In the majority of the experiments, the balance between the phosphorus release rate in the anaerobic reactor and the phosphorus uptake rate in the activated tank is obtained. As a result no phosphorus accumulation occurs.

Experimental results have demonstrated that, in most of the investigated cases, the PHA concentration is the rate-controlling component in the BPR process. However one experiment demonstrated that the accumulation of phosphorus could occur despite the measurement of a considerable concentration of PHA. The experimental results were investigated with help of an extended and calibrated version of the ASM2, with the intention to identify further limiting phenomena.

The simulations demonstrate that the model could predict the behaviour of the process before, during and after the dilution disturbance. Even though the concentration of internal carbon storage products is only a model component, it is possible to perform an analysis of the impact of the ratio of PHA/PAO. The model could confirm the experimentally observed phosphorus accumulation during the experiments where high PHA concentrations were observed. The limitation during this high PHA concentration period was, according to the model, mainly caused by a low concentration of PAO in the system and not predominantly by PHA limitation.

The simulation analysis demonstrated that it is possible that, even if PHA concentrations are high enough, the PAO concentration might be limiting and other actions should be considered such as the extension of the aeration period.

# 8. Model Predictive Control for a Biological Phosphorus Removal System Under Low Influent Concentrations

ABSTRACT

The biological phosphorus removal (BPR) process was previously studied during situations of low influent concentrations and increased hydraulic load. Such disturbance results in a subsequent increase in the phosphate concentration level in the anoxic/aerobic reactors and hence in the plant effluent shortly after the influent wastewater returns to normal strength. It was demonstrated that the accumulation of phosphorus can be avoided or significantly reduced when an external carbon source was added prior to the anaerobic reactor. Since the design of such addition is dependent on many influencing variables which are difficult to access by analytical measurements the design of a model-based observer can improve the robustness operation of the addition significantly. This article investigates both the design of a receding horizon observer that estimates the unmeasured influent soluble organic concentrations and the design of different control strategies. A non-linear predictive control law, based on a calibrated and validated version of an extended version of the ASM2 incorporating denitrification by the PAO, has been developed. The non-linear model predictive control law is investigated in simulation studies where different reference concentrations are used in order to stabilize the BPR process during such disturbance. The simulation results illustrate the performance of the advanced control system. The model predictive control performance is compared to a simple feed-forward control law, which also is based on the estimated organic influent concentrations. It is shown that the simple feed-forward as well as the more advanced control strategies can improve the BPR without major interference with the nitrogen removal processes. With increasing complexity of the control strategy the amount of external added carbon could be significantly reduced while the $PO_4$-P concentration could be kept below the concentration of 1 mgP/L. The best performance was obtained with a model predictive control strategy, which used the internal PHA concentration as reference signal, which was coupled with a $PO_4$-P setpoint control in the aerated tanks permitting a flexible aeration time.

KEYWORDS

ASM2, biological phosphorus removal, external carbon source addition, model predictive control, receding horizon observer, wastewater treatment.

## 8.1. Introduction

The activated sludge process is, due to its non-linear, time varying and multivariable nature, difficult to control such that ammonia, COD, nitrate and phosphorus concentrations simultaneously are maintained below the permitted effluent levels. A network of complex bio-reactions takes place, which are carried out by a complex and partly unidentified symbiotic culture of micro-organisms. Since the benefit of an improved effluent wastewater quality can only be seen from an environmental point of view and not on an direct economical background, the efforts in the control of wastewater treatment plants are only growing with the demand which is dictated by the society and their politicians.

The development of mathematical models, which consider the key-processes of biological phosphorus removal (BPR), took place relatively late (Smolders et al 1994, Henze et al 1994, Dold et al 1995). This late progress explains why there are many investigations about dissolved oxygen control or nitrogen removal reported in literature, while the control of biological phosphorus removal itself is scarce, e.g. Larose *et al.* 1997, Lee *et al.* 1999 and Sasaki *et al.* 1993. A reason for this late development is the successful use of chemical precipitation of phosphorus, which is easy and inexpensive to achieve, and the absence of reliable measurement equipment for most of the relevant components.

With the recent efforts in sensor development connected with the increasing demands for such measurement devices in the biotechnology industries, the level of process monitoring has increased in wastewater treatment plants. Corresponding with this development the complexity of applied control strategies has increased and will in future meet model-based control strategies as well. The breakthrough for the application of BPR control strategies will therefore be connected with the development of inexpensive measurement devices for phosphorus measurements and improved understanding of the key-phenomena involved in the BPR processes.

The focus of the presented work is development of an advanced control strategy, which may have for the moment mainly an academic value. It is established on a model based receding horizon observer, which estimates the current not-measured influent composition of the wastewater. With the help of these estimates an optimisation procedure is invoked, which designs the manipulated variable, an external carbon source addition. The optimisation procedure is either based on a model predicted design law or a simple linear and proportional relationship. At the present state such control strategy has mainly an academic value but the more practical benefit will develop with the time and the increasing request for BPR control strategies. With the increasing number of investigations of such control strategies the call for this technology will increase. A proper control of the BPR process can lead to a minimisation of external added precipitation salts as well as to a minimisation of aeration efforts and hence a reduction of energy consumption.

## 8.2.Material and Methods

### 8.2.1.Model Implementation and Performance

For the simulation of the pilot plant an extended version of the ASM2 model including denitrification by polyphosphate accumulating organism (PAO) was introduced into a Matlab/Simulink simulation platform. The model was earlier calibrated against real data collected at a BIODENIPHO™ pilot plant, (Krühne *et al.* 1998), using a simple evolutionary strategy. The determined set of parameters was found to provide reliable predictions even after a time period of more than two years and is, with exception of the phosphorus release rate $q_{pha}$, similar to the default values of the ASM2 (Krühne and Jørgensen 1999).

The model consists of 17 state variables and a set of 19 Monod type or first order kinetic reaction rates forming a system of 17 coupled ordinary differential equations. Due to the non-linear kinetic expressions and coupling, the resulting system is a non-linear multivariable process. The influent wastewater composition is due to the seasonal, weekly or daily influences of alternating nature.

In figure 8.1 the model prediction is demonstrated during two similar experiments performed with approximately one-year time difference. The background for these experiments was to investigate how the dilution of the influent wastewater influences the pilot plant behaviour. In the both experiments the influent wastewater is diluted with tap water in the ratio 1:3 and in the upper figure the hydraulic load to the plant is increased by factor 2, while in the right case the influent hydraulic load is kept constant.

The decrease of the inlet concentration and the increase of the hydraulic load can be caused by a rainfall, while the second case could result from the temporary closure of an industrial plant in the catchment area, for a short time period. Both types of scenaria result in an accumulation of phosphorus after the re-establishment of normal influent conditions and are quite well predicted by the model.

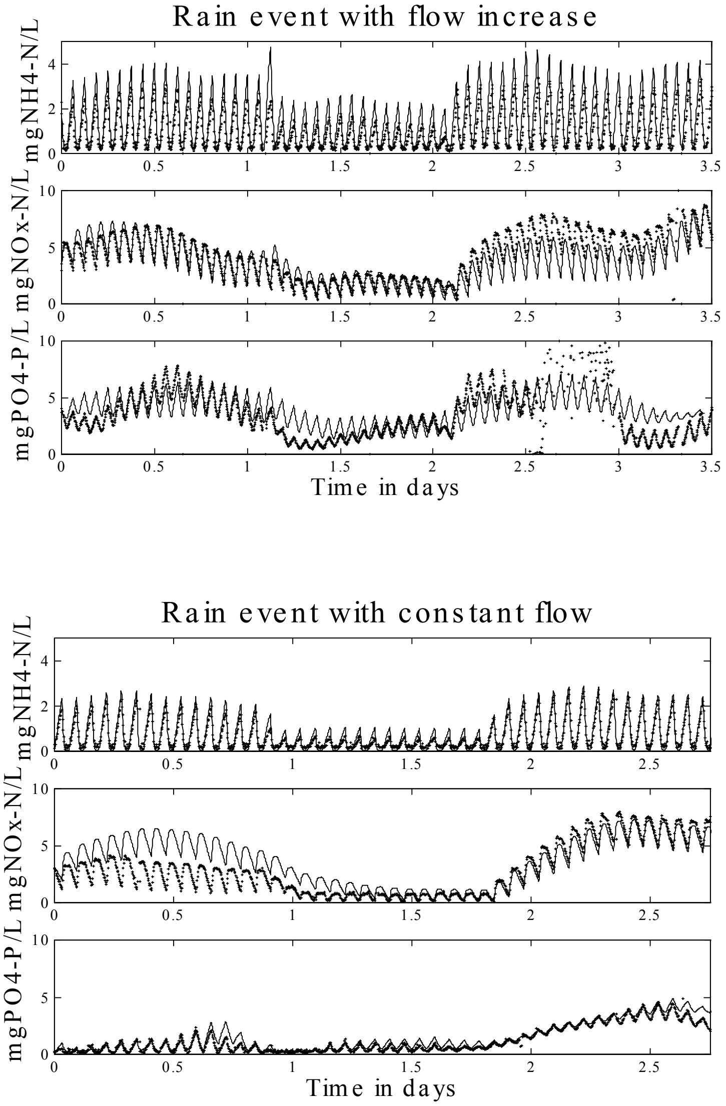


Figure 8.1. Model prediction during two experiments with a dilution of the influent wastewater composition (solid lines = model simulation, points = measurements)

### 8.2.2. The Operational Strategy

The influent composition of municipal wastewater treatment plants is highly variable. The composition changes due to seasonal, weekly or daily influences and has therefore different consequences for the BPR process. In particular the dilution of the concentrations by rain events or periodic changes in composition are of interest since the subsequent return to normal wastewater strength results frequently in an increase of the phosphate concentration in the anoxic/aerobic reactors and hence in the plant effluent. This phenomenon is thought to be caused by different recovery times for anoxic/aerobic P-uptake and P-release (Temmink et al. 1996). During the period of low inlet wastewater strength the PHA stores in the micro-organism are depleted due to the reduced amount of soluble organic components in the influent wastewater. After re-establishment of normal conditions the PHA storage must first be replenished before P-uptake fully recovers, while the recovery of P-release takes place instantaneously (Brdjanovic et al. 1998).

One operational strategy to overcome such starvation periods is of an external carbon source addition (ECSA) during the period of low influent concentrations and high hydraulic load. The addition supports the phosphorus accumulating organisms (PAO) during such periods by the maintenance of a high level of internal carbon storage compounds in form of poly-hydroxy-alconoates (PHA). The improvement of the process by such ECSA is illustrated in figure 8.2 where the $PO_4$-P concentration of the activated tank is shown. The alternating behaviour of the BIODENIPHO™ process would make the presentation of the results confusing, therefore the concentrations at a cycle start are shown only. In this way the continuous transition of the concentrations are obtained.

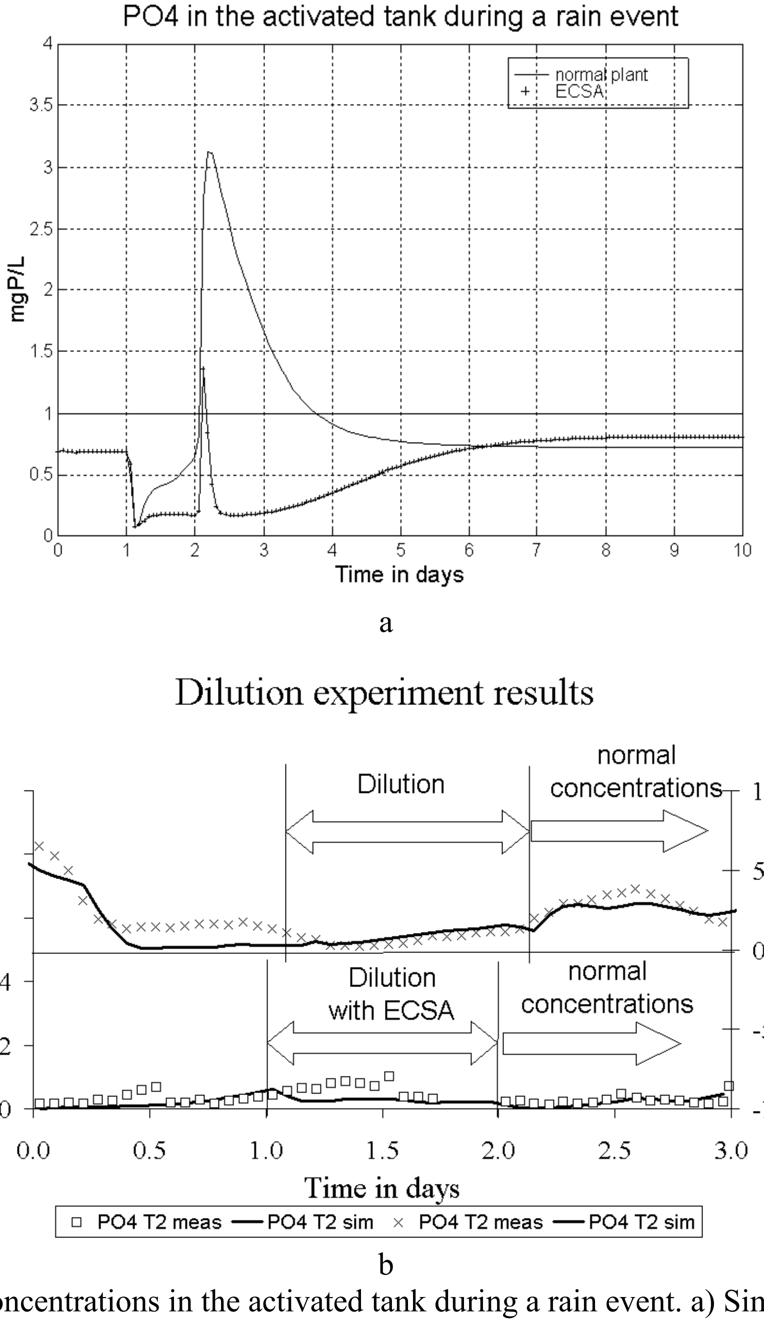


Figure 8.2. $PO_4$ concentrations in the activated tank during a rain event. a) Simulated experiment from steady state, with addition of 30 mgCOD/L during the dilution b) Measured and simulated experiment with low (15 mgCOD/L) and high (45 mgCOD/L) ECSA during dilution.

In figure 8.2a it can be observed, that in the normal case where no ECSA was implemented phosphorus accumulates in the system and approximately two days are needed to obtain the desired concentration below 1 mgP/L. In the stabilised case (ECSA) the $PO_4$ concentration stays with except for a short period directly after the re-establishment of normal influent conditions, below the desired value. The peak in the concentration after the re-establishment of the normal conditions is caused by an increase of the phosphorus release, which lasts for a short time period.

In figure 8.2b measurement results are shown together with simulation results for two dilution experiments. In both cases a dilution in the ratio 1:3 was established with simultaneous increase of the hydraulic load by the factor 2. In the upper subfigure the experiment was performed with a low carbon addition rate while in the lower case the ECSA was sufficient to stabilise the BPR after the re-establishment of normal operating conditions. From these results it can be seen that the operational strategy, which supplied sufficient external carbon, could avoid the accumulation of phosphorus in the tank. The detailed information about this experimental investigation can be found in Krühne and Jørgensen 1999. It should be however considered that measurements below 0.5 mg/L have to be treated with caution since the accuracy of the FIA measurements is rather poor in this region.

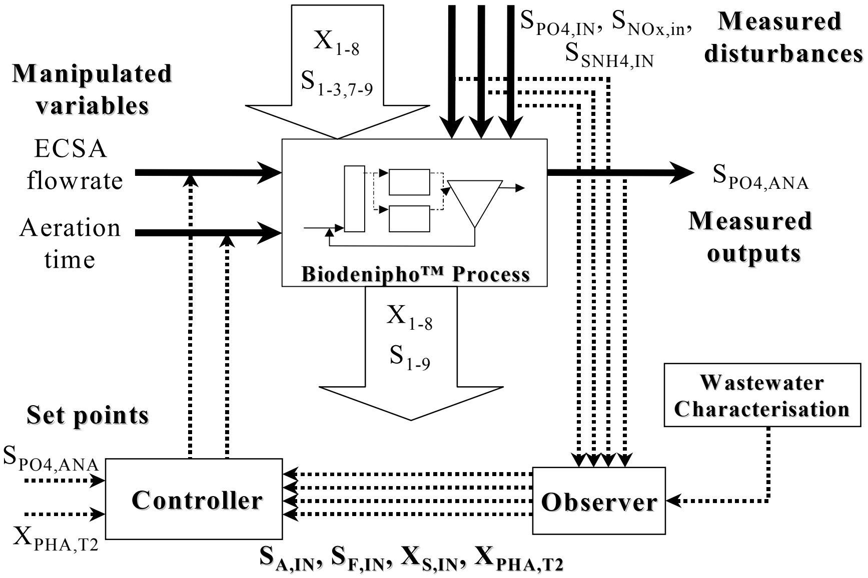
Under the assumption that an appropriate carbon source is economically available, a straight forward control strategy is to keep the phosphorus release in the anaerobic reactor on a suitable level, for example the steady state concentration. In this way it could be ensured that the PHA stores are not depleted during or after the disturbed period of operation. The implementation of an easy control strategy like the use of a PID controller is, without measurements of the readily soluble organic concentration $S_a$ in the influent, not possible for such purposes since the phosphorus release in the anaerobic reactor takes place with a delay of approx. 45 minutes.

### 8.2.3. The Non-Linear Model Predictive Control Strategy

If the difference between the actual $PO_4$ concentration and a reference signal is used as the driving force of a PID controller, the system will arrive at an oscillatory behaviour or will react sluggishly. For a compensation of the delay a model of the process is necessary which can predict the behaviour of the anaerobic reactor in dependence of the measurable influent components. Since no continuous measurements of the influent organic compounds are available at most wastewater treatment plants a model-based observer can be used for such purposes. The control action for the manipulated variable (ECSA) can then be designed by use of a simple linear model of the anaerobic reactor or by use of a more complex multivariable model predictive control algorithm.

In the model predictive control strategy presented in figure 8.3 an observer uses the input information (u) of an observed and controlled plant together with the output measurements (y) to estimate process states ($\hat{x}$), which are used in an control law for the calculation of new input values of the manipulated variables. The main elements of the proposed model predictive controller are presented in figure 8.3a. The observer uses the measured disturbances from the influent concentrations of $PO_4$-P, $NH_4$-N, NOx-N and the anaerobic effluent concentration of phosphorus in combination with the wastewater characterisation as previously described. The observer estimates the missing influent concentrations for the organic components ($S_A$, $S_f$ and $X_S$) and the internally stored carbon as $X_{PHA}$ in tank 2. Dependent on the applied control strategy the controller uses different control laws in order to obey the set point reference signal and manipulates the ECSA flowrate and or the aeration time. Since the investigated system is equipped with an continuous flow injection analysis (FIA) system, the $PO_4$-P, $NH_4$-N and NOx-N concentrations were chosen as measured variables.

Based on the current state estimate classic prediction algorithms can be employed to predict the behaviour of the process outputs over some output horizon $H_p$ when the manipulated inputs u are changed over some input horizon $H_c$ (figure 8.3b). The intention of this model predictive control is to design the present and future moves of the manipulated input variable such that the prediction of the outputs follows a reference signal in a desirable manner, considering possible constraints on the inputs or outputs of the system.



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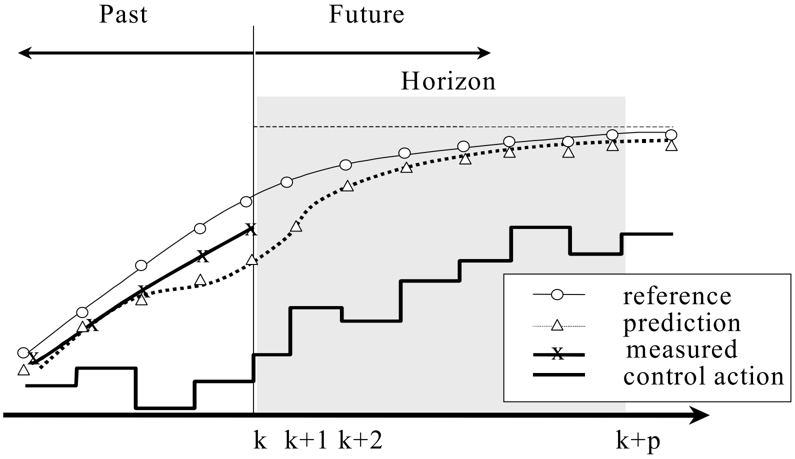


b

Figure 8.3. The MPC structure

Instead of the model predicted control law it is also possible to use knowledge based or even simple proportional control algorithms that design the next move of the manipulated input variable. In this way the necessary time consuming computational effort can be reduced when sufficient knowledge about the process behaviour is available.

### 8.2.4. Receding Horizon Observer

The influent wastewater consists of miscellaneous compounds of various importance for the treatment plant performance. Most of the key-components like the influent organic compounds can not yet be economically analysed. To overcome this problem a model-based observer can be used.. The observer used is of the receding horizon type, which principle is demonstrated in figure 8.4:

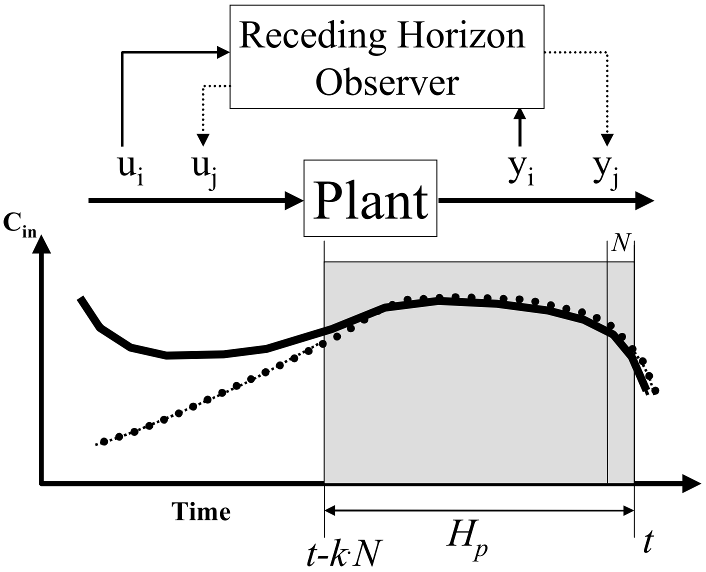


Figure 8.4. The receding horizon observer. Subscript i and j denote measurable and non-measurable components respectively

In this type of observer the input (u) and output (y) variables are divided into measurable (i) and non-measurable (j) components. The classification into the group of non-measurable components can be due to economical or physical/chemical/biological reasons. The non-linear extended ASM2 model receives parallel to the plant the measurable influent and effluent state variables. With a sample frequency of every N minutes and a observation horizon of $H_p=t\text{-}kN$ minutes the model minimises an objective function describe in equation 1:

$$\min J(t,\hat{u}_0) = \min \sum_{k=1}^{N} (y(t-k\cdot N) - y_{obs}(t-k\cdot N|\hat{u}_0))^2 \qquad \text{(eq. 8.1)}$$

The objective function is defined as the squared difference between the measured $PO_4$-P concentration values during the observation horizon and the model predicted $PO_4$-P concentration values in dependence of different assumed input soluble organic concentrations $S_f$ and $S_a$. With J as objective function, t = time, $\hat{u}_0$ = assumed input for $S_a$ and $S_f$, k = sample interval, N = number of samples, y = measured $PO_4$-P concentrations and $y_{obs}$ = model predicted $PO_4$-P concentrations.

The basic sequence for the receding horizon observation is presented in figure 8.5:

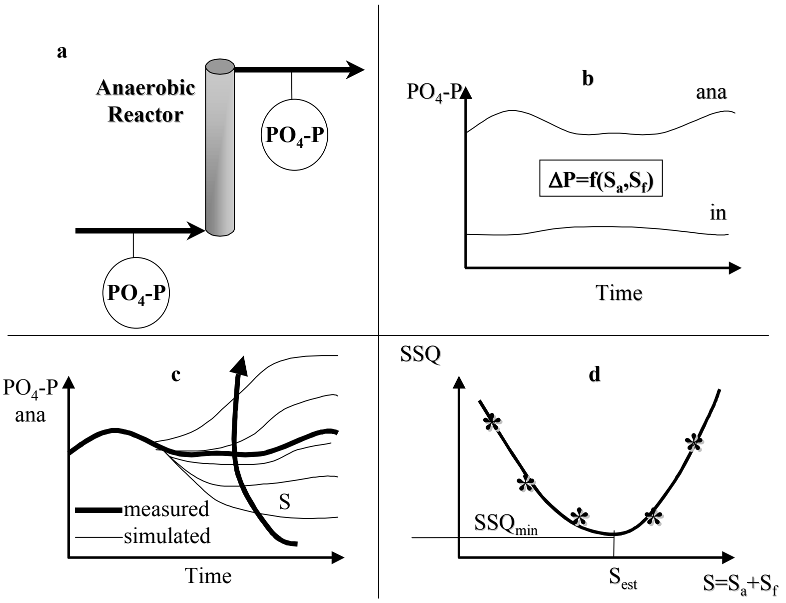


Figure 8.5. Estimation sequence for the observer

The measurements used are the effluent and influent phosphorus concentration of the anaerobic reactor (figure 8.5a). The phosphorus release in the anaerobic reactor is proportional to the soluble organic components in the system (figure 8.5b). The measured $PO_4$-P concentration during the prediction horizon is simulated with different compositions of soluble organic influent (figure 8.5c). Finally the objective values of the predicted and measured phosphorus concentrations (sum of squares = SSQ), in dependence of the influent soluble organic concentration, are fitted with a second order polynomial (figure 8.5d). The minimum of this function represents the estimated organic concentration for this time step. The procedure is repeated at the next sampling step.

Basically the three organic compounds $X_s$, $S_f$ and $S_a$ have an impact on the phosphorus release in the anaerobic reactor. Since only one measurement is used for the observation it may not be possible to identify the three components. In previous investigations (Krühne and Jørgensen 1999) it was shown that the influent wastewater at the investigated pilot plant follows a certain composition pattern for the characteristics are summarised in table 8.1.

Table 8.1. Influent organic components and their relationship

| $S_a$ | S | $S_i$ | $S_f$ | CODtot | X | $X_i$ | $X_s$ |
|---|---|---|---|---|---|---|---|
| Measured | $5 \cdot S_a$ | $0.1 \cdot S$ | $S-S_a-S_i$ | $1.5 \cdot S$ | CODtot-S | $X \cdot 0.15$ | $X-X_i$ |

In this way it is possible to express all organic influent components of the model via measurements or estimation of the concentration of the readily degradable components. This behaviour is used during the receding horizon observer sequence.

### 8.2.5. Control Laws

During *the linear controller (LIN $PO_4$ SP)* routine it is considered that the phosphorus release in the anaerobic reactor is not only dependent on the influent concentration of readily biodegradable substrates. The fermentation processes in the anaerobic part of the plant convert soluble fermentable compounds into readily degradable substrates. The phosphorus release is therefore mainly a function of these two influent concentrations. When simulations with the calibrated model are conducted the linear relationship between the phosphorus release and the soluble organic influent concentrations as presented in figure 8.6 can be observed:

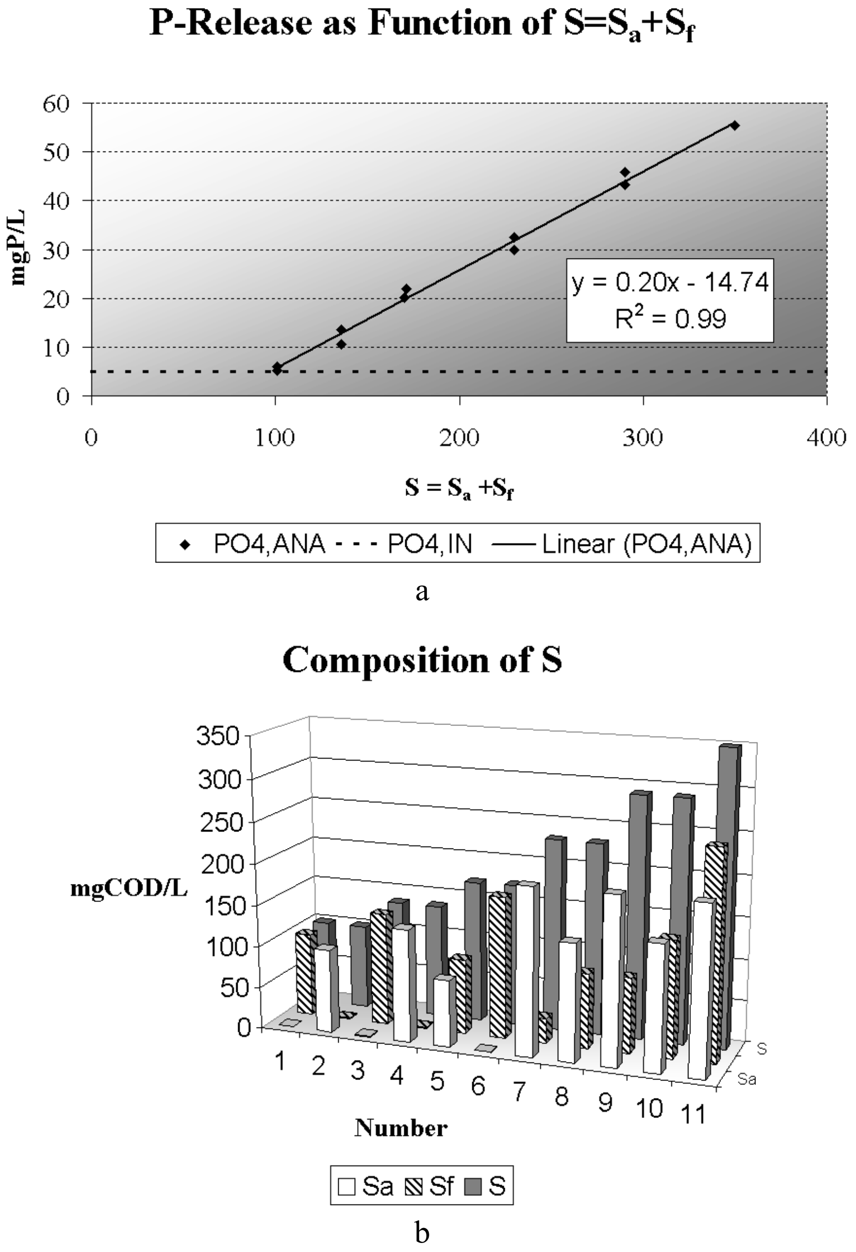


Figure 8.6. Relationship between the phosphorus release and the non-inert soluble organic concentrations a) The phosphorus release as function of the soluble organic compounds, b) the composition of the influent soluble organic concentration $S=S_a+S_f$

The constant dashed line at 5 mgP/L represents the $PO_4$ assumed average influent concentration to the plant. During this simulation different compositions of organic fractions have been used to create the influent concentration of $S=S_a+S_f$. The influent concentrations used for the simulations are illustrated in figure 8.6b. The phosphorus release occurs for influent concentrations of S>100 mgCOD/L and follows an almost linear relationship. Per 5 mgCOD/L slightly more than 1 mgP/L is released. The calculations were performed with the same hydraulic inflow conditions and the same amount of particulate organic substrate. It is only an approximation for the case that no complex model prediction shall be used. This behaviour of the process can be used under the assumption that a target influent load is known and the influent organic concentration ($S_a+S_f$) is measured or estimated. The missing amount of the desired level is added via a controller, which follow this linear dependency for the desired organic amount of $PO_4$ in the anaerobic reactor. In other words it is always the missing of carbon added which is needed in order to keep the desired setpoint concentration of phosphorus in the anaerobic reactor.

In the *model predictive controller (MPC*) two possible operation modes are investigated. In the first mode (MPC $PO_4$ SP) the $PO_4$ concentration in the anaerobic reactor is used as reference concentration under the same conditions as in the linear approach (1). In the second case (MPC PHA SP) it is investigated if the change of the reference concentration from phosphorus to PHA will influence the performance of the controller (2). In both cases the whole strategy is based on the idea to keep the internal stored carbon at a high level. The selection of this concentration promises the best results for the stabilisation of BPR since the depletion of the PHA stores in the PAO is causing the deterioration of BPR after such disturbed periods. It is therefore expected that the use of the PHA concentration as controlled variable will increase the performance of the controller. The PHA concentration in the activated tank serves as reference signal. The controller is designed such that the PHA concentration is kept on a setpoint level of 11 mgCOD/L, a concentration that has been chosen since it is close to the steady state value. Additional on the setpoint concentration change, the operational strategy is changed such that the aeration is stopped when the phosphorus concentration in the activated reactor sinks below 1 mgP/L. In that way it can be examined if the reduction of the aeration time has a positive effect on the PHA consumption and therefore on the acetate addition rate.

An overview about the control strategies and their controller parameters are given in table 8.2:

Table 8.2: Control strategies and controller parameter

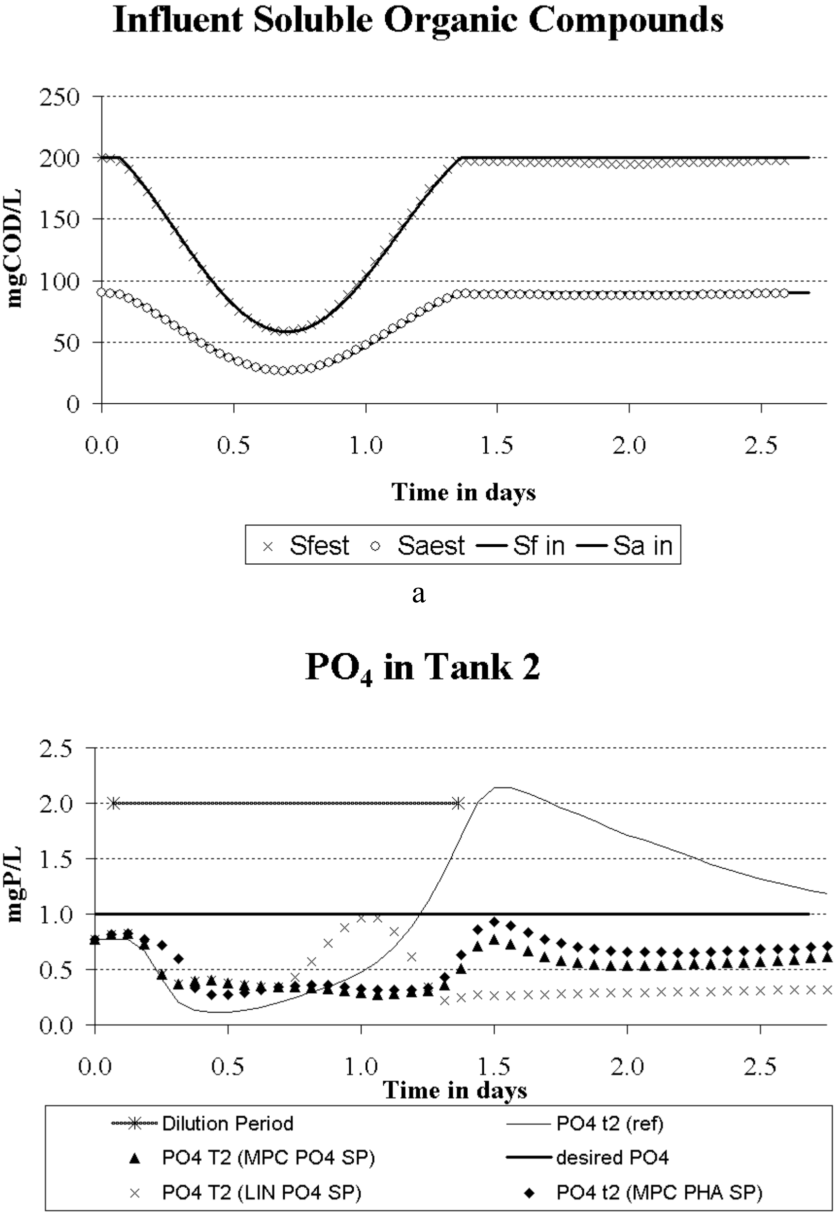
| Strategy | Prediction Horizon | $PO_4$-P setpoint | PHA setpoint |
|---|---|---|---|
| LIN PO4 SP | 610 min | 30 mgP/L | - |
| MPC PO4 SP | 610 min | 30 mgP/L | - |
| MPC PHA SP | 610 min | - | 11 mgCOD/L |

The prediction horizon was set to 610 min due to a simulation study in which the impact of different prediction horizons on the controller performance was tested.

## 8.3.Results and Discussion

The primary purpose of the control system is to support the PAO during periods of low organic loading. This is achieved by an external carbon source addition to the anaerobic reactor during the disturbance, this addition ensures that the internal stored carbon compounds are kept at a sufficient high level. A possible setpoint for such disturbances is to obtain a phosphorus release in the anaerobic reactor, which has 2/3 of the value obtained during the steady state or normal operation (~45mgP/L). From steady state simulations a minimum value of 30 mgP/L was chosen for this purpose. The purpose of the control unit is therefore to maintain the anaerobic $PO_4$ concentration as close as possible to the desired minimum value of 30 mgP/L despite the disturbances.

As a disturbance the reduction of all concentrations of the influent wastewater has been chosen. The influent concentrations of micro-organism have been assumed to be negligible. The influent hydraulic flowrate was assumed to be constant which might conflict with the reality of such disturbances. A possible scenario could be the existence of a plant with different units, which treat wastewater diluted by a rain event. In one of the units the flow is kept constant and treated during constant hydraulic conditions, while in the others the remaining wastewater will be treated or stored. A reason for the chosen hydraulic load is to show that such accumulation problems can occur with changing influent concentrations only. The influent concentrations for $S_a$ and $S_f$ are presented together with the observer estimated values in figure 8.7a.

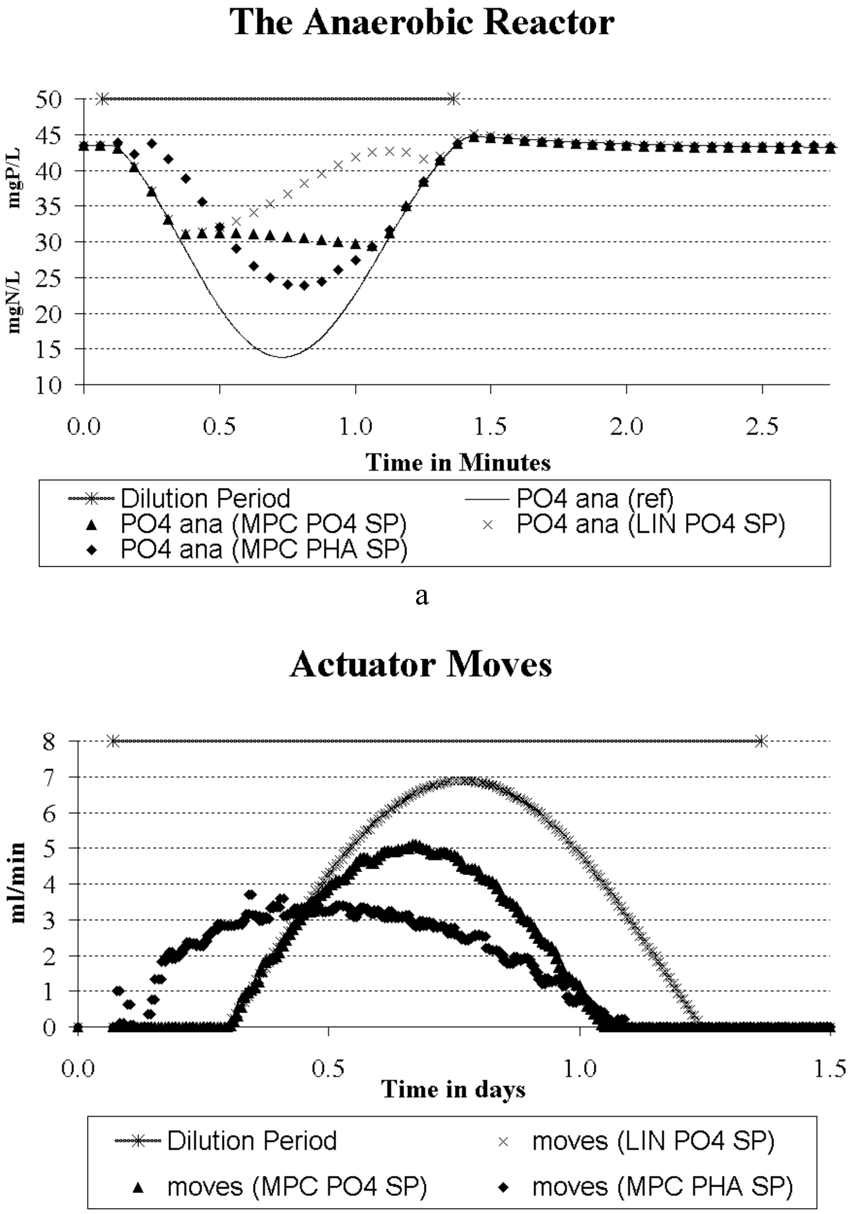


a

b

Figure 8.7. Simulation results. a) Influent soluble organic compounds fit of estimations b) $PO_4$ concentration in the activated tank

In figure 8.7b, the phosphorus concentration is shown in the activated tank for the uncontrolled and the controlled cases. The solid line at 1 mgP/L symbolises the desired value of phosphorus that should not be exceeded in order to obey the effluent limits. The uncontrolled case (labelled as reference experiment ref) shows the typical accumulation of phosphorus while the controlled cases stay as expected inside the desired region. The MPC controlled case with $PO_4$ setpoint and the proportional controlled case stay during the disturbed and the undisturbed time clearly below 1 mgP/L while the proportional $PO_4$-P controlled case with $PO_4$-P setpoint is close to the limit value. This phenomenon occurs during the disturbance, which indicates that the chosen setpoint for $PO_4$-P might be inappropriate and should be reduced for the proportional case. In this way external added carbon could be saved and the operating costs for such control strategy would decrease.



a

b

Figure 8.8. Simulation results. a) $PO_4$-P concentrations in the anaerobic reactor, b) the flow rate of the external carbon source

The transients of the phosphorus concentration in the anaerobic reactor are presented in figure 8.8a. As previously stated the objective was to follow the reference signal, which is 30 mgP/L, as closely as possible. The non-controlled case has a drop of the concentration down to approximately 14 mgP/L while in the $PO_4$ setpoint controlled cases the phosphorus release is kept at a high level. In the case where the model predictive control algorithm is used, the objective is fulfilled with minor deviations. In the case where the linear design is used the phosphorus concentration in the anaerobic reactor exceeds the desired reference signal, which results in a high phosphorus concentration in the activated tanks during the disturbance. The reason for the unnecessarily high addition rate might be found in the simplification of the phosphorus release to a linear design law, which is only valid within a narrow region. Steady state simulations determined this linear dependency where only the soluble organic load was perturbed. Since the process is highly non-linear and multivariable inputs can result in multivariable outputs, this linear dependency may be different for changing influent conditions for components like $PO_4$ or $NH_4$.

The transition of the phosphorus concentration in the anaerobic reactor for the PHA setpoint controlled case has a different shape. The concentration is reduced to 22.5 mgP/L, which indicates that the addition of acetate was smaller than in the other cases. This observation is confirmed by figure 8.8b, which presents the actuator moves of the addition pump. It can be seen that the addition starts much earlier than in the $PO_4$ SP controlled cases. The maximum of the addition rate is approximately 3 ml/min for the PHA setpoint controlled experiment while for the linear case a maximum value of ~7 ml/min is reached. In the MPC $PO_4$ setpoint experiment a maximum value of 5 ml/min is observed.

The amount of COD added per litre of wastewater is shown in figure 8.9 a).

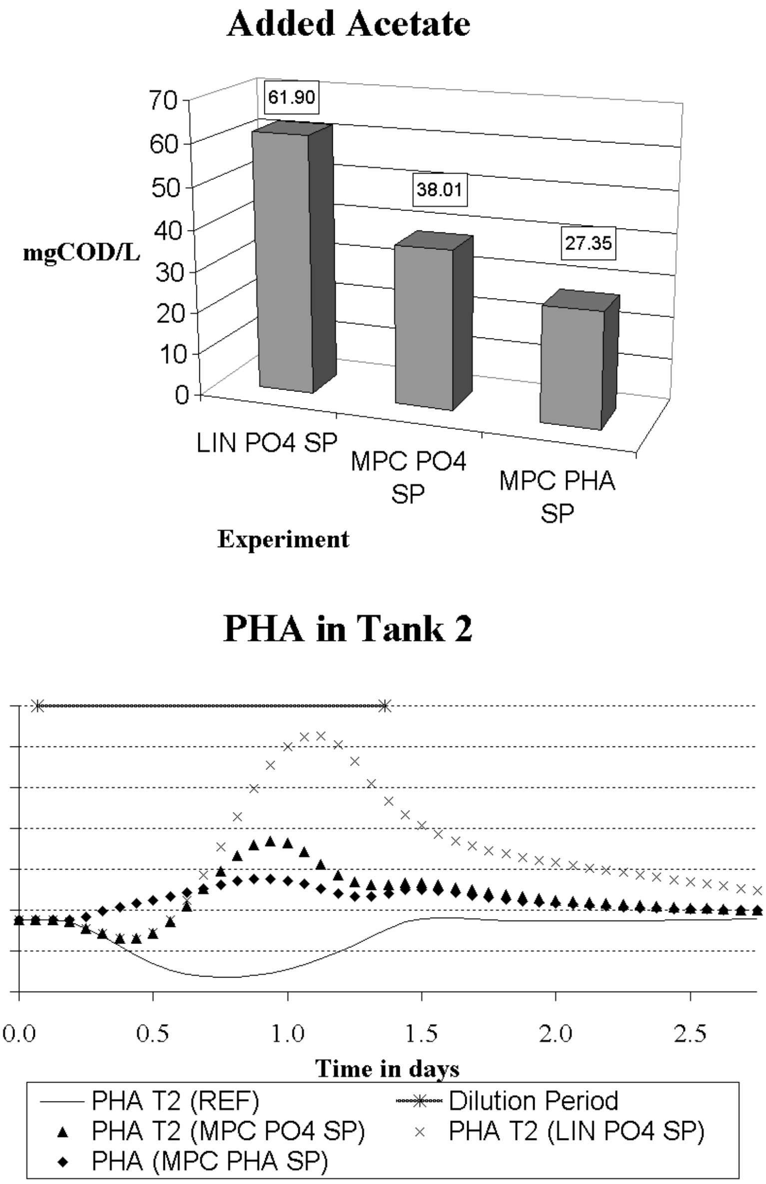


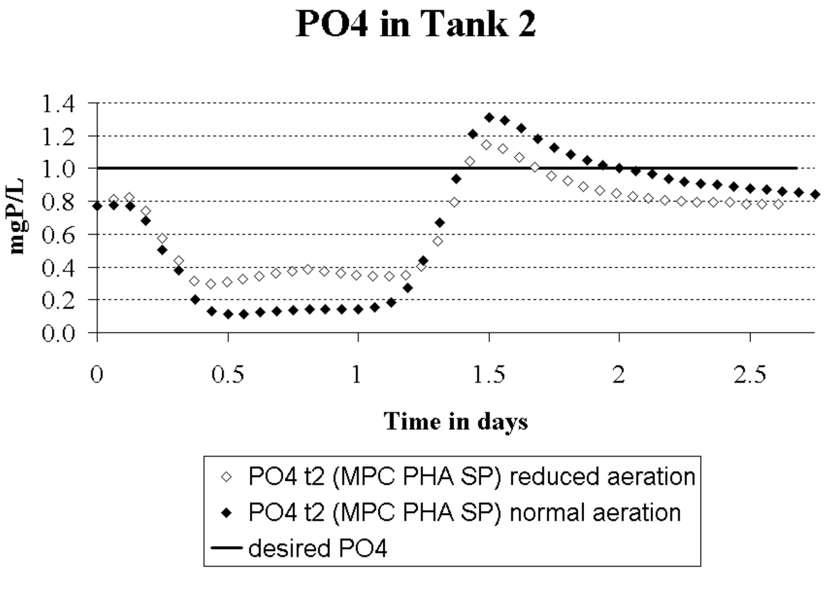
Figure 8.9. Consumption of the added acetate and its impact on PHA. a) Average acetate in mgCOD/L used per experiment b) PHA concentrations in the activated tank

If the amount of acetate added in experiment LIN $PO_4$ SP is assumed to be 100 %, the saving of acetate in MPC $PO_4$ SP case is 38.9 % while the PHA setpoint controlled case 56 % less carbon is used for the stabilisation. The model predictive controlled case with PHA setpoint is therewith from an economical point of view the most effective control strategy.

The objective of the observer is to provide an estimate design of the manipulated variable such that the PHA concentration is sufficient in order to ensure complete phosphorus uptake while the supplied amount of acetate should be minimised to reduce costs. The optimiser that uses the PHA concentration as reference signal is therefore the most suitable optimiser. In figure 8.9 b) the PHA concentration during the experiments is illustrated. The amount of internally stored carbon is highest for the linear controlled experiment and lowest for the non-controlled experiment. In case of the PHA setpoint controlled experiment the lowest amount of carbon is used and the PHA level is maintained during the disturbance around the desired setpoint of 11 mgCOD/L.

Even though the quality of the MPC controlled situation is much higher and less carbon is used, the implementation of the simple linear control law might be attractive, when the carbon source is available on an inexpensive basis. In combination with a sensor, which gives information about the organic load, a feed forward control can be combined with such simple control law.
The *impact of reduced aeration* during the disturbance is demonstrated in figure 8.10. In the case of the model based control strategy with PHA setpoint control a second variable is manipulated in order to support the control of the disturbed situation. The aeration time during one cycle was changed from the fixed aeration time of 30 minutes to flexible time periods, which lasts as long as the phosphorus and ammonium concentration in the activated tank are below the desired value of 1 mg/L. In other words an additional setpoint control was introduced which interrupted the aeration as soon as the PO$_4$ level has dropped below 1 mgP/L, provided that the NH$_4$-N is smaller than 1 mg/L. This change has a major impact on the internal stored PHA concentration and therewith on the performance of the BPR process. The influence is rather fast compared with the addition of acetate since neither the delay of the anaerobic reactor nor mixing times are involved.

In figure 8.10a the impact of the reduction in the aeration time is demonstrated for the phosphorus concentration. The phosphorus concentrations in the experiment with normal aeration (filled symbols) exceed the desired value in contrast to the reduced aeration experiment more clearly after the re-establishment of normal inflow concentrations, while lower values are reached during the disturbance. The normal aeration time is in the case of disturbance inappropriate since the phosphorus concentration due to the low influent concentrations of readily biodegradable substrate is low in the activated tanks. The reduction of the aeration time in this particular case is not only supporting the BPR process but also saving energy and hence reducing costs.



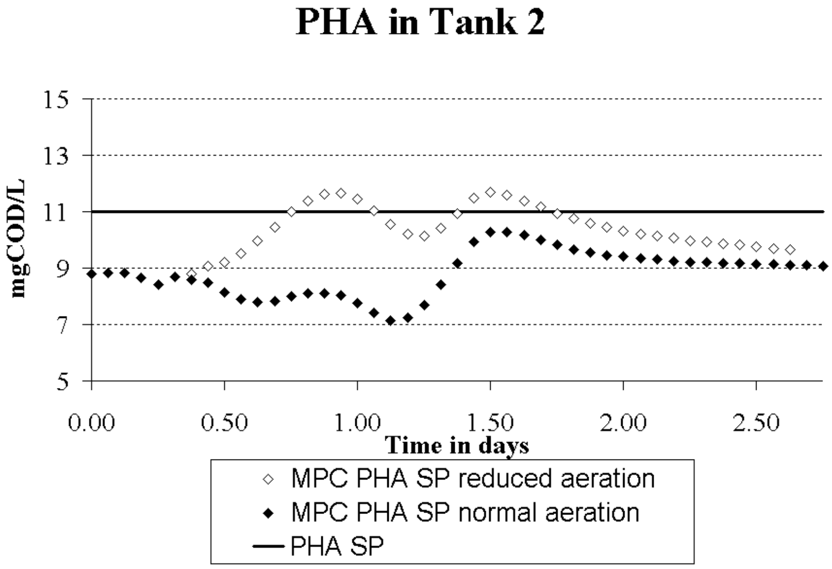


Figure 8.10. Impact of reduced aeration time. Phosphorus (a) and PHA (b) concentrations in the activated tank with (open symbols) and without (filled symbols) aeration reduction

The impact of the PHA setpoint control strategy on the PHA level in the activated sludge is more significant for the case where also the aeration time is controlled as demonstrated in figure 8.10. The desired setpoint region of 11 mgCOD/L PHA can be maintained while in the normally aerated case the level drops to approximately 7 mgCOD/L. It is remarkable that the setpoint, which has been chosen for the disturbance, is slightly higher than the steady state value during normal operations. The reason for this choice of setpoint was to guarantee a suitable high PHA concentration that avoids a PHA limitation. The simulation results show that even a higher setpoint can be chosen in order to avoid exceeding 1 mgP/L in the activated tanks.

The difference between the desired setpoint for the PHA concentration and the obtained values makes clear that the procedure has still the demand for improvements. This difference is mainly caused by the influent information, which is available for the model-based optimiser. Even though the estimation of the present influent concentrations are accurate their future development is not known. Therefore the last values of the estimates are extrapolated. The prediction horizon may not be dimensioned too short, since the delay times of the anaerobic reactor must be considered in the prediction of the possible actuator moves. In this study a prediction horizon of 610 minutes has been chosen in order to consider the involved complexity. This limitation could be improved by combining known periodic variations with weather forecasts to predict future influent characteristics.

If the reduced aeration time is applied to the control strategies where the phosphorus concentration in the anaerobic reactor is used as setpoint the impact will be negligible. The explanation can be found in a simple mass-balance of the phosphorus component in the anaerobic reactor. The accumulation of phosphorus in the anaerobic reactor is mainly the sum of the released phosphorus and the flow induced transported phosphorus entering and leaving the system. All other reactions will be neglected since they are relatively small. The reduction of the aeration time will have an impact on the phosphorus concentration in the activated tank such that the concentration level can be between 0 and 1 mgP/L. Under the assumption that this concentration is the recycled phosphorus concentration, which is mixed in a ratio 1:1 with the influent flow, the biggest concentration difference between the full aeration and a reduced concentration case will be 0.5 mgP/L or less. For the linear setpoint controlled case where approximately 5 mgCOD/L is used in order to obtain a release of 1 mgP/L a value of 2.5 mgCOD/L would be the resulting acetate addition difference. If this value is converted into the difference in the actuator move for the worst case the difference between the flow-rates would be 0.125 ml/min.

## 8.4.Conclusion

The intention of the presented work was to implement high performance control to a biological phosphorus removal system that includes long delay times. A non-linear model predictive control law and a simplified linear control law have been established which are based on an extended version of the ASM2 model including denitrification by PAO. Both strategies use external carbon source addition rate as manipulated variable. The investigated system is equipped with a continuous measurement system, which analyses only a fraction of the state variables ($PO_4$, $NH_4$ and NOx). A receding horizon observer was designed in order to access the unmeasured states. Since the model is rather complex and needs computation time, the observer and the model predictive control law, are based on an optimisation formulation. Process knowledge, which is based on numerical system investigations, is used for the design of setpoints in the control law. All investigated strategies are based on the intention to maintain the internal stored carbon compounds in form of PHA at a high level.

The linear and the non-linear control law were tested in simulations for a disturbed influent composition that is known to cause an accumulation of phosphorus in BPR systems. The results are very promising since both control strategies could prevent the accumulation of phosphorus. The model predictive control strategy shows however a more effective performance and much less carbon addition. The combination of the non-linear model predictive optimiser which hold the PHA concentration in a setpoint region and a $PO_4$-P setpoint control which reduces the aeration time during the disturbed situation, show the best performance.

Future investigations should focus on the verification of the control strategy on a pilot plant scale or full-scale basis. Since the operational strategy is confirmed in several experiments in pilot-scale investigations the coupling of continuous measurements of the influent organic concentration and the model-based optimisation procedure for the design of the external carbon source addition rate can be an attractive intermediate step in the application of feed-forward control. Independent from future applications of such an advanced control strategy the reduction of aeration during times of low organic loading should be applied. The benefit of such aeration reduction would yield in cost reduction since the accumulation of phosphorus nevertheless would occur. The maintenance of a sufficiently high level of internal stored carbon should be, besides the effluent limiting values for nutrients, the focus of operation during such disturbed operational periods. The addition of external carbon in form of readily biodegradable matter can support the BPR process and should be used when a source is available on a reasonable economical basis.

# 9. Conclusions and Future Work

Experimental investigations have been performed in order to study the failure of BPR at an alternating pilot plant, receiving municipal wastewater. The process was investigated during periods of low influent concentrations and increased hydraulic load, with subsequent re-establishment of normal conditions. A process disturbance of this type result in an increase in the phosphate concentration level in the effluent, shortly after the wastewater returns to normal strength. The performed work was mainly structured into three parts. In the first part a model was calibrated to the investigated pilot plant with the intention to develop further operational and control strategies. In the subsequent part the operational strategy was experimentally tested and in the final part of the thesis an advanced control strategy was investigated by simulations.

## 9.1. Parameter Estimation

It was examined if an extended version of the activated sludge model No. 2 (ASM2) including denitrification by phosphate accumulating organism (PAO) can be calibrated and validated to the existing system. The prediction of the extended model concerning $PO_4$, NOx and $NH_4$ reveals a convincing quality and the set of determined parameters is valid over a long time period (two years) including varying scenaria. The investigation included observations of the pilot plant over a range of hours to several days. The confidence in the reliability of the model has been established by this investigation. Therefore the model can be used for the investigation of the pilot plant behaviour in order to obtain new control and operational strategies.

As a side effect of this investigation a simple relationship between the organic components of the influent wastewater and the phosphorus release in the anaerobic reactor could be suggested. With help of this relationship the effort for influent sampling campaigns can be reduced and already recorded measurements, where no information about the organic influent compositions is available, can be analysed

In summary one of the greatest advantages of the here presented model extension is the unique set of estimated parameters which can be used over a time period of more than two years. In this way different influent situations can be analysed with help of the model just by the adaptation of the initial concentrations for the biomass composition without a re-calibration of the whole model.

## 9.2. Operational Strategy

The dilution of the influent wastewater composition by rain events causes an increase of the phosphorus concentration when the normal inlet wastewater composition is re-established. The reason for this behaviour of the BPR process is assumed to be an imbalance between the phosphorus release in the anaerobic zone and the phosphorus uptake in the aerobic/anoxic zone. The P-uptake rate is assumed to be limited by the internal carbon storage compound PHA, which normally is depleted during a rain-event. Based on the model simulations during such experiments an external carbon source addition (ECSA) was designed in order to overcome the process failure.

It is experimentally demonstrated that the BPR process could be improved by the addition of an external carbon source during such changing influent conditions. The improvement was established by the addition of sodium acetate in the influent to the anaerobic reactor or into the anoxic phase of the process. With increasing sodium acetate addition the phosphorus release during the disturbances was enhanced and the amount of PHA in the biomass was augmented as well. In case of anoxic addition the stabilisation could be achieved with higher amounts of added COD. The increase of the PHA concentration during the disturbance could be observed but with a smaller magnitude than in the anaerobic cases.

As a second operational strategy, which supports the stabilisation of the BPR process during low influent concentrations, the reduction of the aeration time in the process was successfully used. With a combination of a low external carbon source addition and a reduced aeration time it was possible to stabilise the BPR process, while the sodium acetate addition alone could not prevent the accumulation of phosphorus after a disturbance.

The experimental results have demonstrated that, in most of the investigated cases, the PHA concentration is the rate-controlling component in the BPR process. The experimental results demonstrated however that the accumulation of phosphorus could occur despite that a considerable concentration of PHA could be observed. The experimental results were investigated with help of the extended and calibrated version of the ASM2, with the intention to identify further limiting phenomena.

The simulations demonstrate that the model could predict the behaviour of the process before, during and after the dilution disturbance. Even though the concentration of internal carbon storage products is only a model component, it is possible to perform an analysis of the impact of the ratio of PHA/PAO. The model could confirm the experimentally observed phosphorus accumulation during the experiments where high PHA concentrations were observed. The limitation during this high PHA concentration period was, according to the model, mainly caused by a low concentration of PAO in the system and not predominantly by PHA limitation.

The simulation analysis demonstrated that it is possible that, even if PHA concentrations are high enough, the PAO concentration might be limiting and other actions should be considered such as the extension of the aeration period.

## 9.3.Advanced Control Strategy

In the last part of the thesis the gained comprehension by the operational investigations was used for the design of a model predictive control (MPC) strategy for the BPR system under low influent concentrations. The strategy is based on the addition of an ECSA keeping the internal stored carbon products at a high level. A model-based observer estimating the unmeasured influent soluble organic or internal PHA concentrations was used and could improve the robustness operation of the addition significantly. The MPC control performance was compared to a simple feed-forward control law, which also was based on the estimated organic influent concentrations.

The linear and the non-linear control law were tested in simulations for a disturbed influent composition that is known to cause an accumulation of phosphorus in BPR systems. The results are very promising since both control strategies could prevent the accumulation of phosphorus. The model predictive control strategy shows however a more effective performance and much less carbon addition. The combination of the non-linear model predictive optimiser which hold the PHA concentration within a setpoint region and a $PO_4$-P setpoint control which reduces the aeration time during the disturbed situation, show the best performance.

## 9.4.Further Work

Thus development of further operational or control strategies should have the intention to maintain the PHA concentration at a level that does not limit the phosphorus uptake. The assistance of biological models can be of major importance for further interpretation of these experimental results and for subsequent development of an operation or control strategy to handle rain events in order to discriminate between the limiting influence of the PHA concentration or other causes.

Future investigations should focus on the verification of the control strategy on a pilot plant scale or full-scale basis. Since the operational strategy is confirmed in several experiments in pilot-scale investigations the coupling of continuous measurements of the influent organic concentration and the model-based optimisation procedure for the design of the external carbon source addition rate can be an attractive intermediate step in the application of feed-forward control. Independent from future applications of such an advanced control strategy the reduction of aeration during times of low organic loading should be applied. The benefit of such aeration reduction would yield in cost reduction since the accumulation of phosphorus nevertheless would occur. The maintenance of a sufficiently high level of internal stored carbon should be, besides the effluent limiting values for nutrients, the focus of operation during such disturbed operational periods. The addition of external carbon in form of readily biodegradable matter can support the BPR process and should be used when a source is available on a reasonable economical basis.

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# Appendix

# List of Abbreviations

## List of Abbreviations

| | |
|---|---|
| ANA | Anaerobic Reactor |
| ANOX | Anoxic Conditions |
| APHA | American Public Health Association |
| ARMAX | Auto Regressive Moving Average Model |
| ASM1 | Activated Sludge Model No.1 |
| ASM2 | Activated Sludge Model No.2 |
| ASP | Activated Sludge Process |
| ATP | Adenosine Triphosphate |
| BM | Biomass |
| BNR | Biological Nutrient Removal |
| BOD | Biological Oxygen Demand |
| BPR | Biological Phosphorus Removal |
| C | Carbon |
| C-NMR | Carbon Nuclear Magnetic Resonance |
| COD | Chemical Oxygen Demand |
| DNPAO | Denitrifying Phosphate Accumulating Organism |
| DO | Dissolved Oxygen |
| ECSA | External Carbon Source Addition |
| ED | Entner-Doudoroff Pathway |
| EMP | Embden Meyerhof Parnas Pathway |
| FIA | Flow Injection Analysis |
| GDPMC | Genetic Distributed Parameter Model-Based Control |
| HAc | Acetate Concentration |
| IAWQ | International Association of Water Qualitiy |
| ITAE | Integral Time Absolute Error |
| LIN | Linear |
| MIMO | Multivariable Input Multivariable Output |
| MLSS | Mixed Liquor Suspended Solids |
| MLVSS | Mixed Liquor Volatile Suspended Solids |
| MPC | Model Predictive Control |
| N | Nitrogen |
| NADH | Reduction equivalent (Nicotin Adenin Dinucleotid Hydrogen) |
| $NH_4$-N | Ammonium Concentration |
| Non-PAO | Non Phosphate Accumulating Organism |

| | |
|---|---|
| NOx-N | Nitrate-Nitride Concentration |
| ORP | Oxidation Reduction Potential |
| OUR | Oxygen Utilisation Rate |
| P | Phosphorus |
| PAO | Phosphate Accumulating Organism |
| PHA | Poly Hydroxy Alcanoates |
| PHB | Poly-Hydroxy-Butyrate |
| PHV | Poly-Hydroxy-Valerate |
| PID | Proportional Integral Differential |
| PLC | Programmable Logical Controller |
| $PO_4$-P | Ortho-Phosphate Concentration |
| PP | Polyphosphate |
| RHO | Receding Horizon Observer |
| RHOC | Receding Horizon Observed Control |
| rRNA | Ribo Nucleic Acid |
| SED | Sedimentation Tank |
| SP | Setpoint |
| SRT | Sludge Retention Time |
| SS | Suspended Solids |
| SSQ | Sum of Squares |
| T1 | Tank 1 |
| T2 | Tank 2 |
| TCA | Tricarboxylic Acid |
| UCT | University of Capetown |
| VSS | Volatile Suspended Solids |
| WAS | Waste Activated Sludge Rate |
| WRC | Water Research Commission |
| WWTP | Wastewater Treatment Plant |

# List of Symbols

# List of Symbols

| Symbol | Declaration | Units |
|---|---|---|
| $S_A^*$ | Acetate estimate | $mgL^{-1}$ |
| $\hat{x}$ | Estimate process state | Respective unit |
| $\theta$ | Parameter vector | - |
| $\varphi$ | Regression vector | - |
| $\hat{y}(t_k)$ | Predicted output measurements | $mgL^{-1}$ |
| $\mu$ | Growth rate | Unit/time |
| $\mu_{PAONOx}$ | Anoxic PAO growth rate | $d^{-1}$ |
| $a_i$ | Constant | 1 |
| $b_i$ | Constants | 1 |
| $C_{18}H_{19}O_9N$ | Organic substrate | $mmol\ L^{-1}$ |
| $C_5H_7NO_2$ | Biomass concentration | $mmol\ L^{-1}$ |
| $Ca^{2+}$ | Calcium Concentration | $mmol\ L^{-1}$ |
| $c_i$ | Constants | 1 |
| $CO_2$ | Carbon dioxide concentration | $mmol\ L^{-1}$ |
| $C_S$ | Substrate Concentration | $mgL^{-1}$ |
| e | Process and measurement noise | - |
| $f_{HAc}$ | Constant factor for estimation of SA | 1 |
| $H^+$ | Hydrogen concentration | $mmol\ L^{-1}$ |
| $H_2CO_3$ | Carbonic acid | $mmol\ L^{-1}$ |
| $H_2O$ | Water | $mmol\ L^{-1}$ |
| $H_3PO_4$ | Phosphoric acid | $mmol\ L^{-1}$ |
| Hc | Input Horizon | Minutes |
| $HCO_3^-$ | Bicarbonate | $mmol\ L^{-1}$ |
| Hp | Prediction Horizon | Minutes |
| $i_{PBM}$ | P content of biomass $X_H$, $X_{PAO}$ and $X_{AUT}$ | $gPgCOD^{-1}$ |
| $i_{TSSBM}$ | TSS to biomass ratio for $X_H$, $X_{PAO}$ and $X_{AUT}$ | $gTSSgCOD^{-1}$ |
| J | Objective function | - |
| $K^+$ | Potassium Cooncentration | $mmol\ L^{-1}$ |
| $K_S$ | Saturation concentration | $mgL^{-1}$ |
| $LINPO_4SP$ | Linear phosphorus setpoint control law | - |
| $Mg^{2+}$ | Magnesium concentration | $mmol\ L^{-1}$ |
| minJ(t,u0) | Minimised objective function | - |
| MLSS | Mixed Liquor Suspended Solids | $mgL^{-1}$ |

| | | |
|---|---|---|
| MLVSS | Mixed Liquor Volatile Suspended Solids | $mgL^{-1}$ |
| Mo(V) | Molybdenium (V) ion | $mmolL^{-1}$ |
| Mo(VI) | Molybdenium(VI) ion | $mmol\ L^{-1}$ |
| $Mo_{12}O_{40}$ | Molybdeniumoxide | $mmol\ L^{-1}$ |
| $MoO_4$ | Molybdeniumoxide | $mmol\ L^{-1}$ |
| MPCPHASP | Model predictive control PHA setpoint control law | - |
| MPCPO4SP | Model predictive control phosphorus setpoint control law | - |
| $N_2$ | Molecular nitrogen concentration | $mmol\ L^{-1}$ |
| $N_2O$ | Dinitrogen oxide | $mmol\ L^{-1}$ |
| $NH_3$ | Ammonia | $mmolL^{-1}$ |
| $NH_4^+$ | Ammonium concentration | $mmol^{-1}$ |
| $NH_4$-N | Ammonium Concentration | $mgNL^{-1}$ |
| NO | Nitric oxide | $mmol\ L^{-1}$ |
| $NO_2^-$ | Nitride concentration | $mmol\ L^{-1}$ |
| $NO_3^-$ | Nitrate concentration | $mmol\ L^{-1}$ |
| NOx-N | Nitrate-Nitride Concentration | $mgNL^{-1}$ |
| $O_2$ | Oxygen concentration | $mmol\ L^{-1}$ |
| $OH^-$ | Hydroxylic group | $mmolL^{-1}$ |
| $PO_4$-P | Ortho-Phosphate Concentration | $mgPL^{-1}$ |
| $q_{PAONO3}$ | Anoxic phosphate accumulation organism growth rate | $d^{-1}$ |
| $q_{PP}$ | Phosphorus uptake rate | $gPPg^{-1}PAOd^{-1}$ |
| $q_{PPNO3}$ | Anoxic phosphate uptake rate | $gPPg^{-1}PAOd^{-1}$ |
| r | Reaction rate | mass/time |
| $S_A$ | Fermentation products, considered to be acetate | $mgCOD\ L^{-1}$ |
| $S_{ALK}$ | Alkalinity of the wastewater | $mol_{HCO3}$-$L^{-3}$ |
| $S_F$ | Fermentable, readily biodegradable organic substrates | $mgCOD\ L^{-1}$ |
| $S_I$ | Inert soluble organic material | $mgPL^{-1}$ |
| $S_i$ | Deviation from the nominal set of parameter = $(J_x/J_n)_i$ | 1 |
| Sn(II) | Tin(II) | $mmol\ L^{-1}$ |
| Sn(III) | Tin(III) | $mmolL^{-1}$ |
| $S_{N2}$ | Dinitrogen $N_2$ | $mgNL^{-1}$ |
| $S_{NH4}$ | Ammonium plus ammonia nitrogen | $mgNL^{-1}$ |
| $S_{NO3}$ | Nitrate plus nitrite nitrogen | $mgNL^{-1}$ |
| $S_O$ | Dissolved oxygen | $mgL^{-1}$ |
| $S_{PO4}$ | Inorganic soluble phosphorus, primarily ortho phosphates | $mgPL^{-1}$ |
| SRT | Sludge Retention Time | Days |

| | | |
|---|---|---|
| $t$ | Time | Days, hours or seconds |
| $u$ | Process input | $mgL^{-1}$ |
| $u$ | Process input | $mgL^{-1}$ |
| $W_i$ | Weighting factor | - |
| $X_{AUT}$ | Autotrophic organsims | $mgCOD\ L^{-1}$ |
| $X_{BM}$ | Biomass concentration | $mgCODL^{-1}$ or $mgL^{-1}$ |
| $X_H$ | Heterotrophic organisms | $mgCOD\ L^{-1}$ |
| $X_I$ | Inert particulate organic material | $mgCOD\ L^{-1}$ |
| $X_{PAO}$ | Phosphate accumulating organisms | $mgCOD\ L^{-1}$ |
| $X_{PHA}$ | Cell internal storage product of phosphorus accumulating organisms PAO | $mgCOD\ L^{-1}$ |
| $X_{PP}$ | Poly-phosphate | $mgPL^{-1}$ |
| $X_S$ | Slowly biodegradable substrates | $mgCOD\ L^{-1}$ |
| $X_{TSS}$ | Total suspended solids | $mgL^{-1}$ |
| $y(t)$ | Process output | $mgL^{-1}$ |
| $y(t_k)$ | Current output measurement | $mgL^{-1}$ |
| $Y_H$ | Heterotrophic Yield coefficient | $gCODg^{-1}COD$ |
| $Y_{PHA,d}$ | Yield | $gCODg^{-1}COD$ |

# Figures of the Pilot Plant

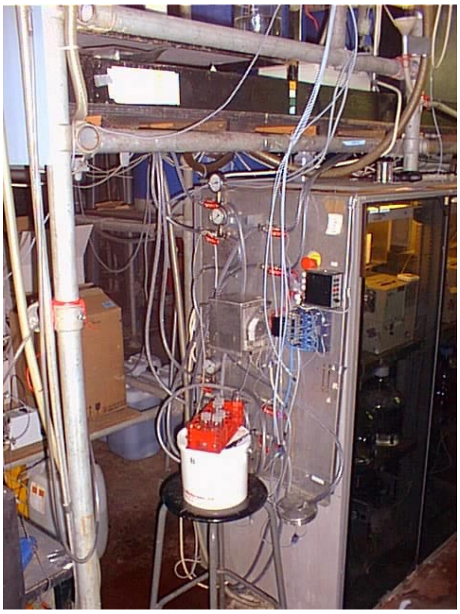
# Appendix A

Pilot Plant Pictures

Anaerobic Reactor with Michael

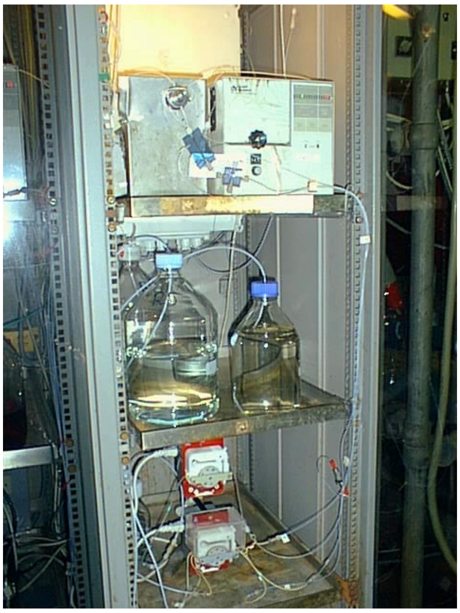
Aerated Tank No.2

FIA Detectors

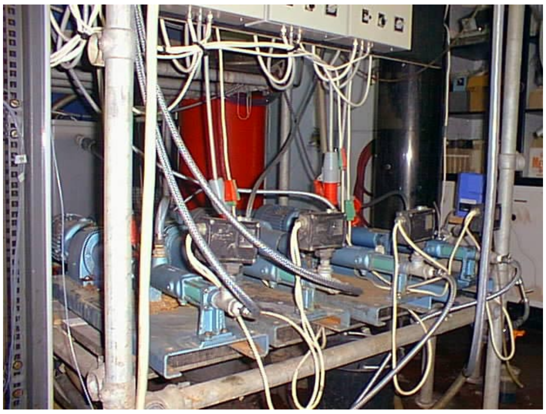


Crossflow Membrane Filtration and Sample Transport Pump


Laboratory


Nitrate Spectrophotometer


Primary Settler


Sample Transport Pumps in upstream the Membrane Filters

# ASM2x Model Formulation

## The Extended ASM2 Model with enitrification by the PAO

| **Process** | $S_O$ | $S_F$ | $S_A$ | $S_{NH4}$ | $S_{NO3}$ | $S_{PO4}$ | $S_I$ | $S_{ALK}$ | $S_{N2}$ | $X_I$ | $X_S$ | $X_H$ | $X_{PAO}$ | $X_{PP}$ | $X_{PHA}$ | $X_{AUT}$ | $X_{TSS}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1. Aerobic Hydrolysis** | | $1-f_{SI}$ | | $\nu_{1,NH4}$ | | $\nu_{1,PO4}$ | $f_{SI}$ | $\nu_{1,ALK}$ | | | -1 | | | | | | $-i_{TSSXS}$ |
| **2. Anoxic Hydrolysis** | | $1-f_{SI}$ | | $\nu_{2,NH4}$ | | $\nu_{2,PO4}$ | $f_{SI}$ | $\nu_{2,ALK}$ | | | -1 | | | | | | $-i_{TSSXS}$ |
| **3. Anaerobic Hydrolysis** | | $1-f_{SI}$ | | $\nu_{3,NH4}$ | | $\nu_{3,PO4}$ | $f_{SI}$ | $\nu_{3,ALK}$ | | | -1 | | | | | | $-i_{TSSXS}$ |
| **4. Aerobic Growth on $S_F$** | $1-\frac{1}{Y_H}$ | $-\frac{1}{Y_H}$ | | $\nu_{4,NH4}$ | | $\nu_{4,PO4}$ | | $\nu_{4,ALK}$ | | | | 1 | | | | | $i_{TSSBM}$ |
| **5. Aerobic Growth on $S_A$** | $1-\frac{1}{Y_H}$ | | $-\frac{1}{Y_H}$ | $\nu_{5,NH4}$ | | $\nu_{5,PO4}$ | | $\nu_{5,ALK}$ | | | | 1 | | | | | $i_{TSSBM}$ |
| **6. Anoxic Growth on $S_F$ (Denitrification)** | | $-\frac{1}{Y_H}$ | | $\nu_{6,NH4}$ | $\frac{-(1-Y_H)}{2.86\cdot Y_H}$ | $\nu_{6,PO4}$ | | $\nu_{6,ALK}$ | $\frac{(1-Y_H)}{2.86\cdot Y_H}$ | | | 1 | | | | | $i_{TSSBM}$ |
| **7. Anoxic Growth on $S_A$ (Denitrification)** | | | $-\frac{1}{Y_H}$ | $\nu_{7,NH4}$ | $\frac{-(1-Y_H)}{2.86\cdot Y_H}$ | $\nu_{7,PO4}$ | | $\nu_{7,ALK}$ | $\frac{(1-Y_H)}{2.86\cdot Y_H}$ | | | 1 | | | | | $i_{TSSBM}$ |
| **8. Fermentation** | | -1 | 1 | $\nu_{8,NH4}$ | | $\nu_{8,PO4}$ | | $\nu_{8,ALK}$ | | | | | | | | | |
| **9. Lysis** | | | | $\nu_{9,NH4}$ | | $\nu_{9,PO4}$ | | $\nu_{9,ALK}$ | | $f_{XI}$ | $1-f_{XI}$ | -1 | | | | | $\nu_{9,TSS}$ |
| **10. Storage of $X_{PHA}$ (phosphorus release)** | | | -1 | | | $Y_{PO4}$ | | $\nu_{10,ALK}$ | | | | | | $-Y_{PO4}$ | 1 | | $\nu_{10,TSS}$ |
| **11. Storage of $X_{PP}$ (phosphorus uptake)** | $-Y_{PHA}$ | | | | | -1 | | $\nu_{11,ALK}$ | | | | | | 1 | $-Y_{PHA}$ | | $\nu_{11,TSS}$ |
| **12. Aerobic Growth of $X_{PAO}$ on $X_{PHA}$** | $1-\frac{1}{Y_H}$ | | | $\nu_{12,NH4}$ | | $\nu_{12,PO4}$ | | $\nu_{12,ALK}$ | | | | | 1 | | $-\frac{1}{Y_{pao}}$ | | $\nu_{12,TSS}$ |
| **13. Lysis of $X_{PAO}$** | | | | $\nu_{13,NH4}$ | | $\nu_{13,PO4}$ | | $\nu_{13,ALK}$ | | $f_{XI}$ | $1-f_{XI}$ | | -1 | | | | $\nu_{13,TSS}$ |
| **14. Lysis of $X_{PP}$** | | | | | | 1 | | $\nu_{14,ALK}$ | | | | | | -1 | | | $\nu_{14,TSS}$ |
| **15. Lysis of $X_{PHA}$** | | | 1 | | | | | $\nu_{15,ALK}$ | | | | | | | -1 | | $\nu_{15,TSS}$ |
| **16. Aerobic Growth of $X_{AUT}$** | $\frac{r_A-4.57}{Y_A}$ | | | $\nu_{16,NH4}$ | $\frac{1}{Y_A}$ | $\nu_{16,PO4}$ | | $\nu_{16,ALK}$ | | | | | | | | 1 | $\nu_{16,TSS}$ |
| **17. Lysis of $X_{AUT}$** | | | | $\nu_{17,NH4}$ | | $\nu_{17,PO4}$ | | $\nu_{17,ALK}$ | | $f_{XI}$ | $1-f_{XI}$ | | | | | -1 | $\nu_{17,TSS}$ |
| **18. Anoxic Storage of $X_{PP}$ (phosphorus uptake)** | | | | | $-\frac{Y_{PHA}}{2.86}$ | -1 | | | $\frac{Y_{PHA}}{2.86}$ | | | | | 1 | $-Y_{PHA}$ | | |
| **19. Anoxic Growth of $X_{PAO}$ on $X_{PHA}$** | | | | | $\frac{-(1-Y_H)}{2.86\cdot Y_H}$ | $-i_{PBM}$ | | | $\frac{(1-Y_H)}{2.86\cdot Y_H}$ | | | | 1 | | $-\frac{1}{Y_{pao}}$ | | |

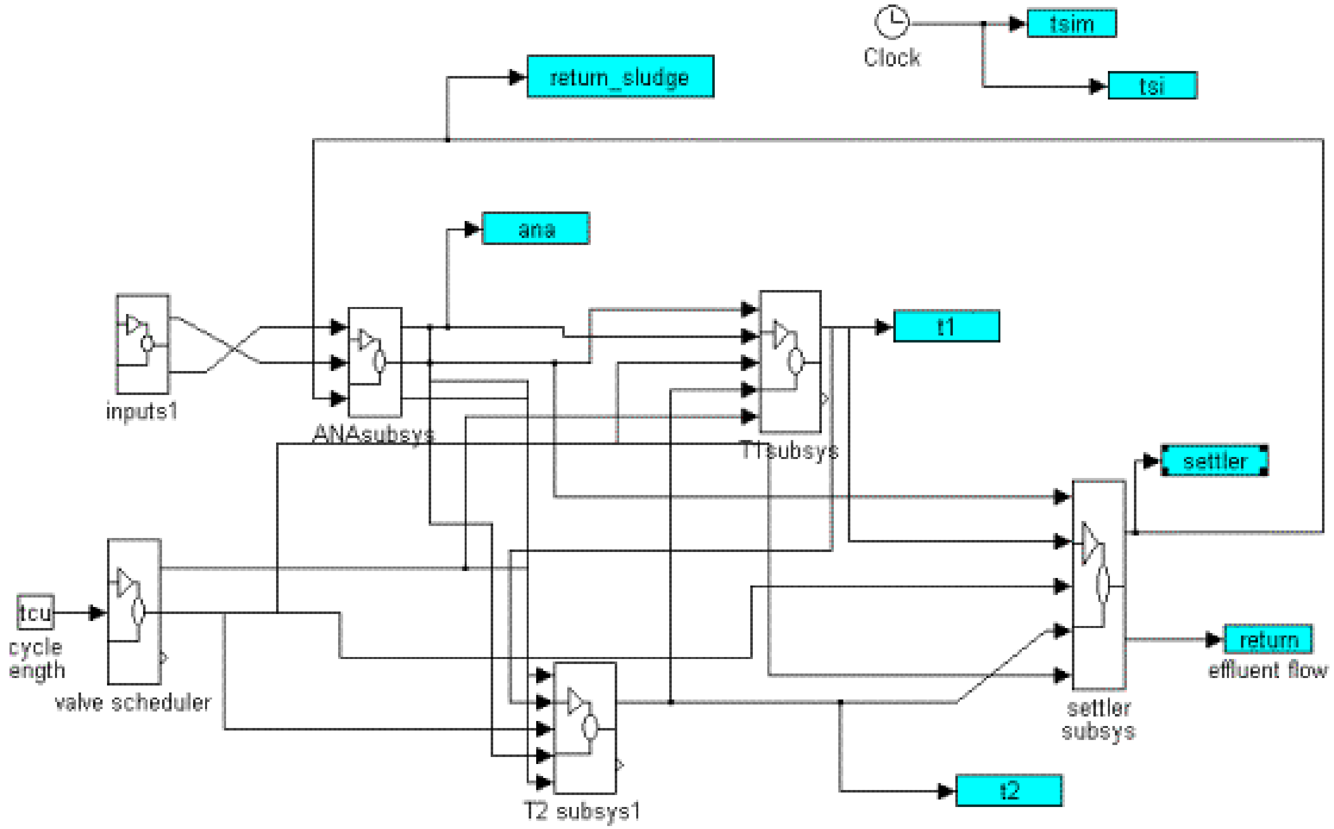
# The Rate vector

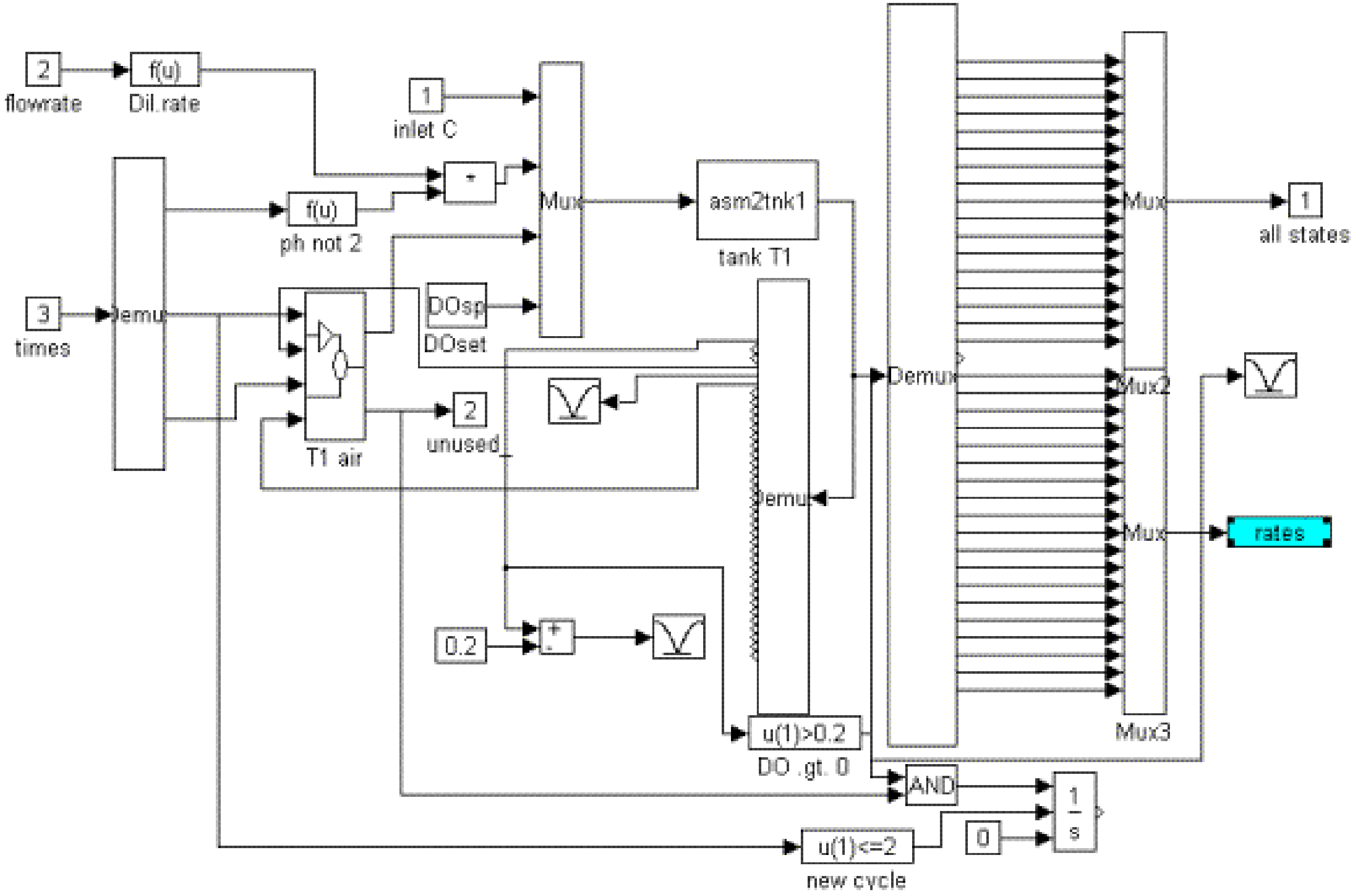
| | |
|---|---|
| **1.Aerobic Hydrolysis** | $K_h \cdot \frac{S_{O2}}{S_{O2}+K_{O2}} \cdot \frac{X_s/X_H}{K_X+X_s/X_H} \cdot X_H$ |
| **2.Anoxic Hydrolysis** | $K_h \cdot \eta_{NO3} \cdot \frac{K_{O2}}{S_{O2}+K_{O2}} \cdot \frac{S_{NO3}}{S_{NO3}+K_{NO3}} \cdot \frac{X_s/X_H}{K_X+X_s/X_H} \cdot X_H$ |
| **3.Anaerobic Hydrolysis** | $K_h \cdot \eta_{fe} \cdot \frac{K_{O2}}{S_{O2}+K_{O2}} \cdot \frac{K_{NO3}}{S_{NO3}+K_{NO3}} \cdot \frac{X_s/X_H}{K_X+X_s/X_H} \cdot X_H$ |
| **4.Aerobic Growth on $S_F$** | $\mu_H \cdot \frac{S_F}{S_F+K_F} \cdot \frac{S_{O2}}{S_{O2}+K_{O2}} \cdot \frac{S_F}{S_F+S_A} \cdot \frac{S_{NH4}}{S_{NH4}+K_{NH4}} \cdot \frac{S_{PO4}}{S_{PO4}+K_P} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot X_H$ |
| **5.Aerobic Growth on $S_A$** | $\mu_H \cdot \frac{S_A}{S_A+K_A} \cdot \frac{S_{O2}}{S_{O2}+K_{O2}} \cdot \frac{S_A}{S_F+S_A} \cdot \frac{S_{NH4}}{S_{NH4}+K_{NH4}} \cdot \frac{S_{PO4}}{S_{PO4}+K_P} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot X_H$ |
| **6.Anoxic Growth on $S_F$ (Denitrification)** | $\mu_H \cdot \eta_{NO3} \cdot \frac{S_F}{S_F+K_F} \cdot \frac{K_{O2}}{S_{O2}+K_{O2}} \cdot \frac{S_F}{S_F+S_A} \cdot \frac{S_{NH4}}{S_{NH4}+K_{NH4}} \cdot \frac{S_{PO4}}{S_{PO4}+K_P} \cdot \frac{S_{NO3}}{S_{NO3}+K_{NO3}} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot X_H$ |
| **7.Anoxic Growth on $S_A$ (Denitrification)** | $\mu_H \cdot \eta_{NO3} \cdot \frac{S_A}{S_A+K_A} \cdot \frac{K_{O2}}{S_{O2}+K_{O2}} \cdot \frac{S_A}{S_F+S_A} \cdot \frac{S_{NH4}}{S_{NH4}+K_{NH4}} \cdot \frac{S_{PO4}}{S_{PO4}+K_P} \cdot \frac{S_{NO3}}{S_{NO3}+K_{NO3}} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot X_H$ |
| **8. Fermentation** | $q_{fe} \cdot \frac{K_{O2}}{S_{O2}+K_{O2}} \cdot \frac{K_{NO3}}{S_{NO3}+K_{NO3}} \cdot \frac{S_F}{S_F+K_{fe}} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot X_H$ |
| **9. Lysis** | $b \cdot X_H$ |

| | |
|---|---|
| **10. Storage of $X_{PHA}$ (phosphorus release)** | $q_{PHA} \cdot \frac{S_A}{S_A + K_A} \cdot \frac{X_{PP}/X_{PAO}}{K_{PP} + X_{PP}/X_{PAO}} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{PAO}$ |
| **11. Storage of $X_{PP}$ (phosphorus uptake)** | $q_{PP} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{PAO}$ |
| **12. Aerobic Growth of $X_{PAO}$ on $X_{PHA}$** | $\mu_{PAO} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO}$ |
| **13. Lysis of $X_{PAO}$** | $b_{PAO} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{PAO}$ |
| **14. Lysis of $X_{PP}$** | $b_{PP} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{PP}$ |
| **15. Lysis of $X_{PHA}$** | $b_{PHA} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{PHA}$ |
| **16. Aerobic Growth of $X_{AUT}$** | $\mu_{AUT} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}} \cdot \frac{S_{ALK}}{S_{ALK} + K_{ALK}} \cdot X_{AUT}$ |
| **17. Lysis of $X_{AUT}$** | $b_{AUT} \cdot X_{AUT}$ |
| **18. Anoxic Storage of $X_{PP}$ (phosphorus uptake)** | $q_{PPNO3} \cdot \frac{S_{NO3}}{S_{NO3} + K_{NO3}} \cdot \frac{K_{O2}}{S_{O2} + K_{O2}} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot X_{PAO}$ |
| **19. Anoxic Growth of $X_{PAO}$ on $X_{PHA}$** | $q_{PAONO3} \cdot \frac{K_{O2}}{S_{O2} + K_{O2}} \cdot \frac{S_{NO3}}{S_{NO3} + K_{NO3}} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4}} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO}$ |

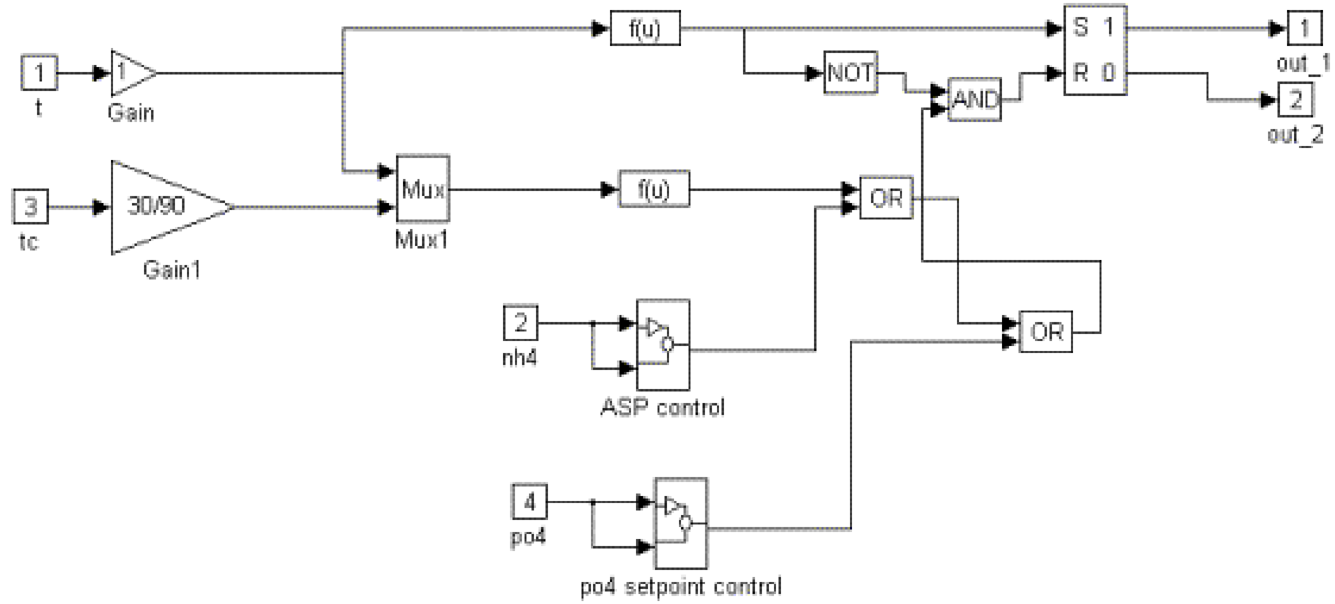
# Simulink Program

# Appendix C: Simulink Model of the Pilot Plant



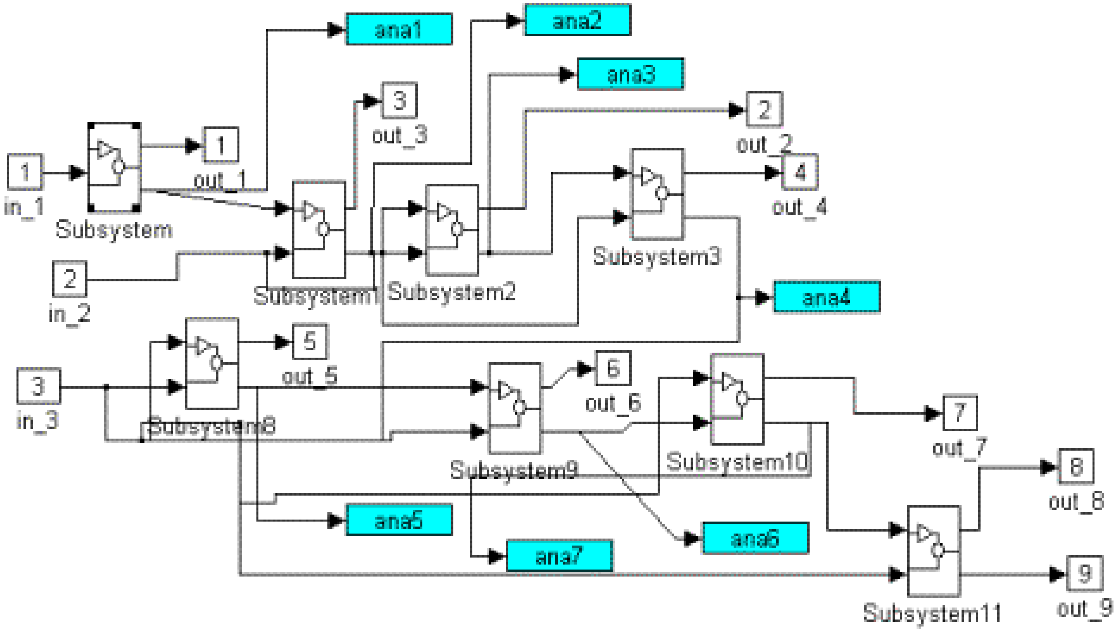

2
flowrate
f(u)
Dil.rate
1
inlet C
+
f(u)
ph not 2
Mux
asm2tnk1
tank T1
1
all states
3
times
Demux
T1 air
DOsp
DOset
2
unused
Demux
Demux
Mux
Mux2
Mux
rates
Mux3
0.2
+
-
u(1)>0.2
DO .gt. 0
AND
1
s
0
u(1)<=2
new cycle

tank T1

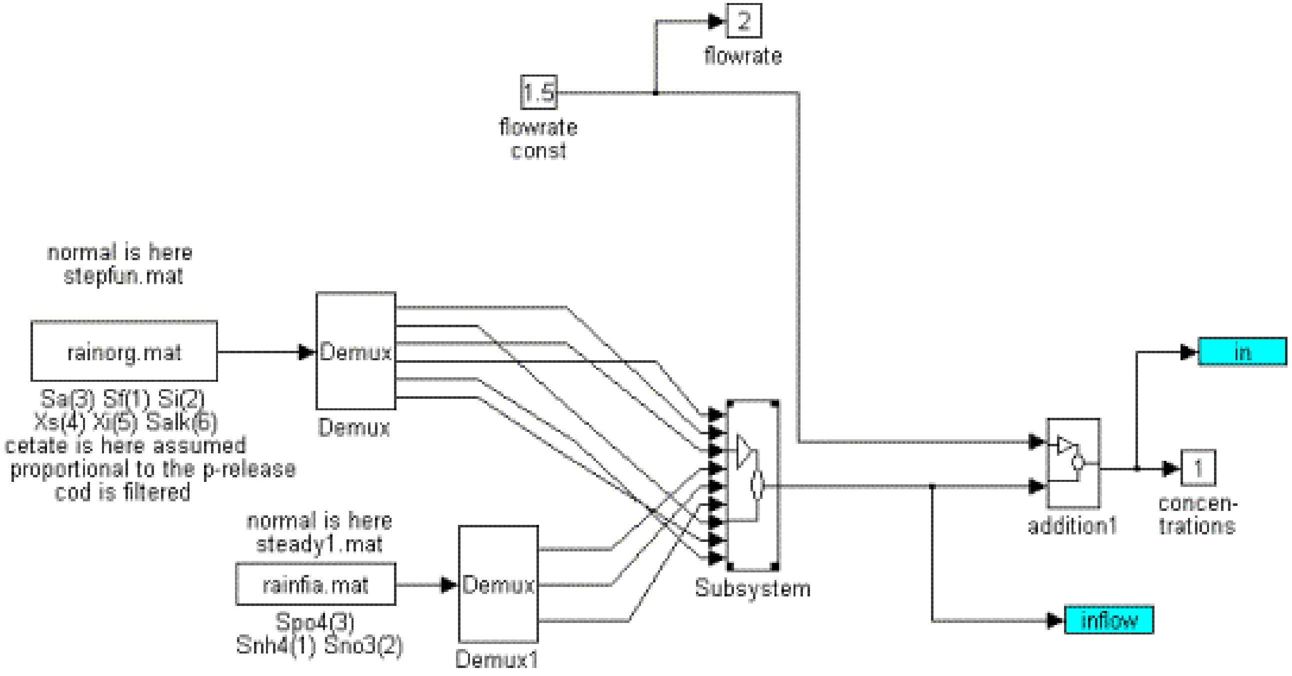

1
t
1
Gain
3
tc
30/90
Gain1
Mux
Mux1
f(u)
f(u)
NOT
AND
S 1
R 0
1
out_1
2
out_2
OR
OR
2
nh4
ASP control
4
po4
po4 setpoint control

T1 air

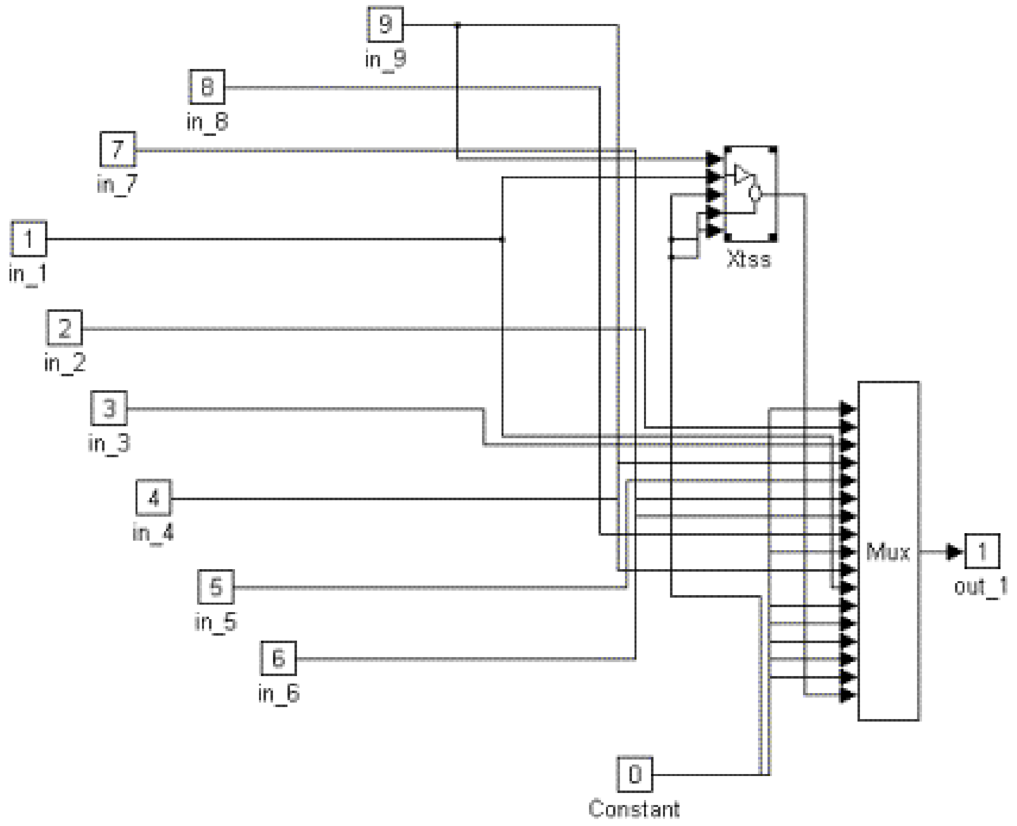
# Appendix C: Simulink Model of the Pilot Plant



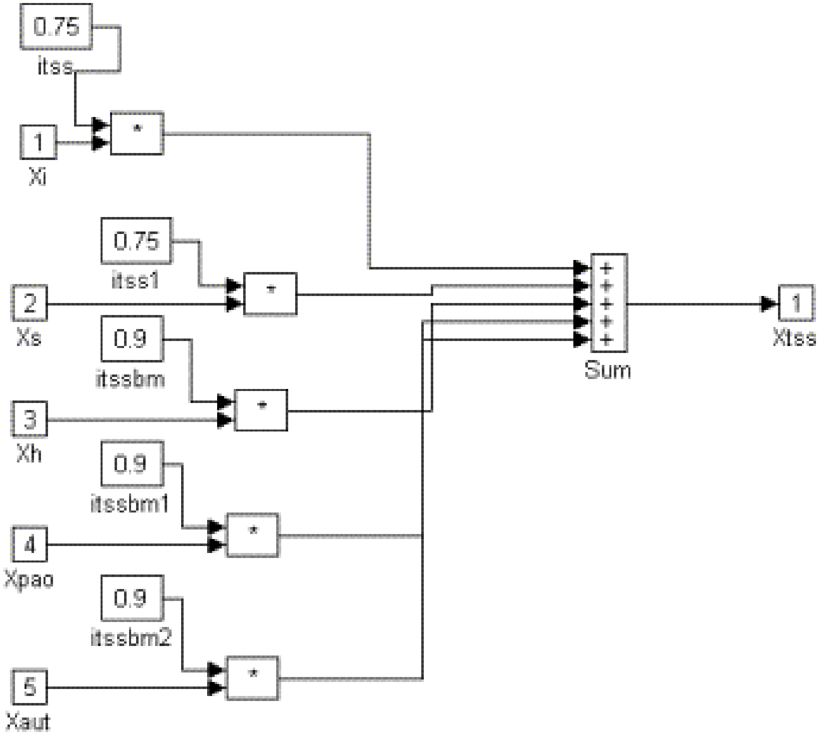
Anaerobic column as 8 CSTR


2
flowrate
1.5
flowrate const
normal is here stepfun.mat
rainorg.mat
Sa(3) Sf(1) Si(2)
Xs(4) Xi(5) Salk(6)
cetate is here assumed proportional to the p-release
cod is filtered
Demux
Demux
normal is here steady1.mat
rainfia.mat
Spo4(3)
Snh4(1) Sno3(2)
Demux
Demux1
Subsystem
addition1
in
1
concen-trations
inflow

inputs1

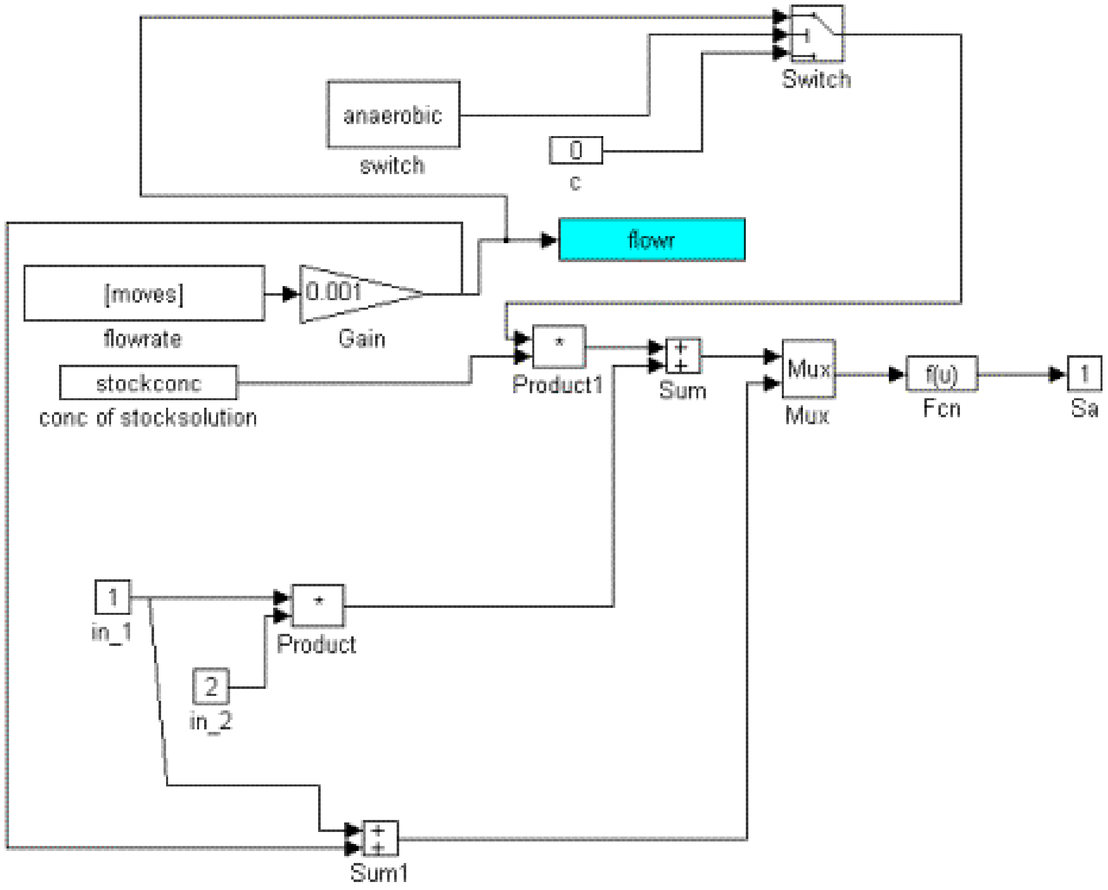

9
in_9
8
in_8
7
in_7
1
in_1
2
in_2
3
in_3
4
in_4
5
in_5
6
in_6
Xtss
Mux
1
out_1
0
Constant

Subsystem

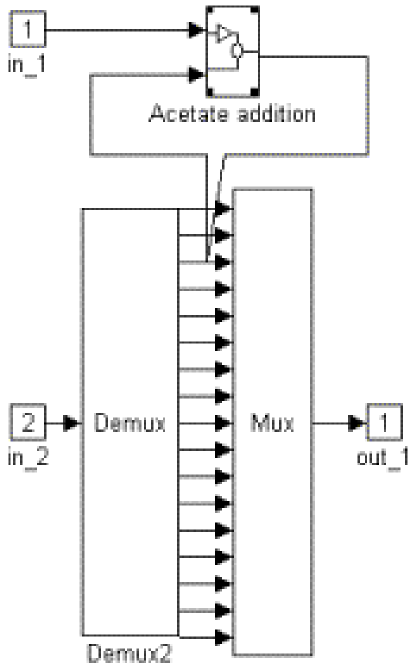

0.75
itss
1
Xi
*
0.75
itss1
2
Xs
*
0.9
itssbm
3
Xh
*
0.9
itssbm1
4
Xpao
*
0.9
itssbm2
5
Xaut
*
+
+
+
+
+
Sum
1
Xtss

Xtss

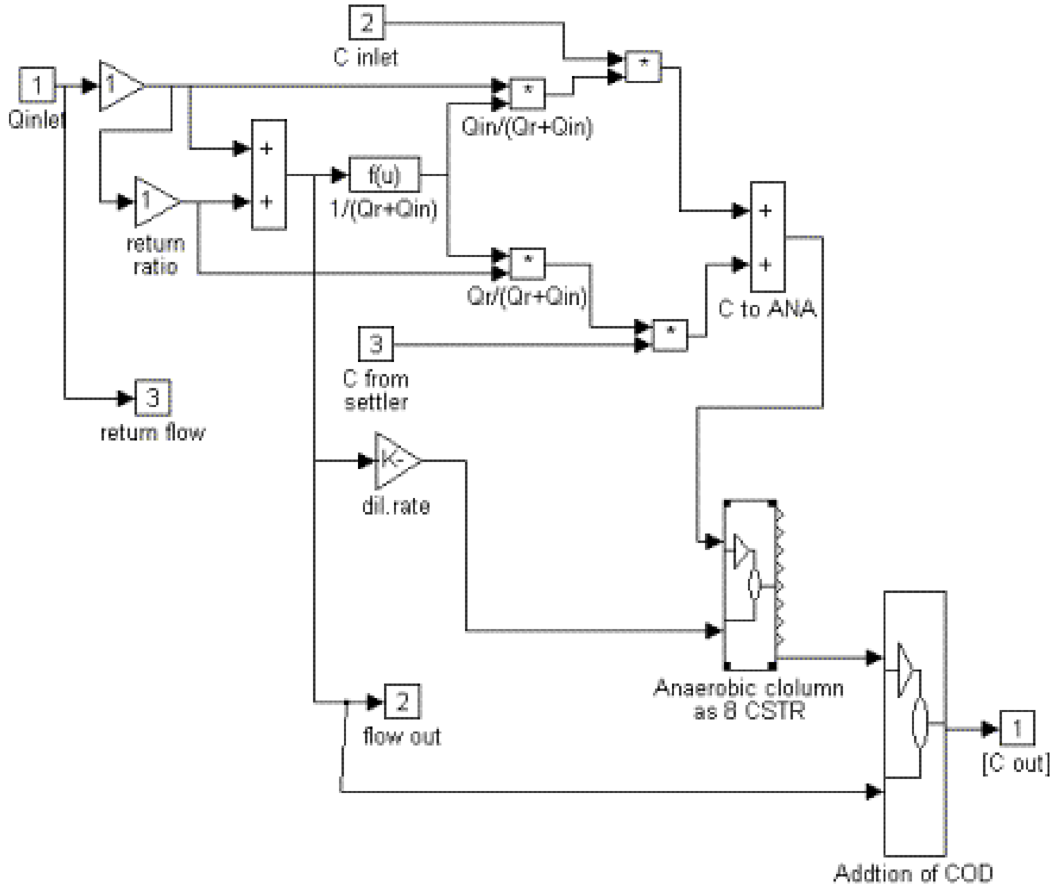
# Appendix C: Simulink Model of the Pilot Plant



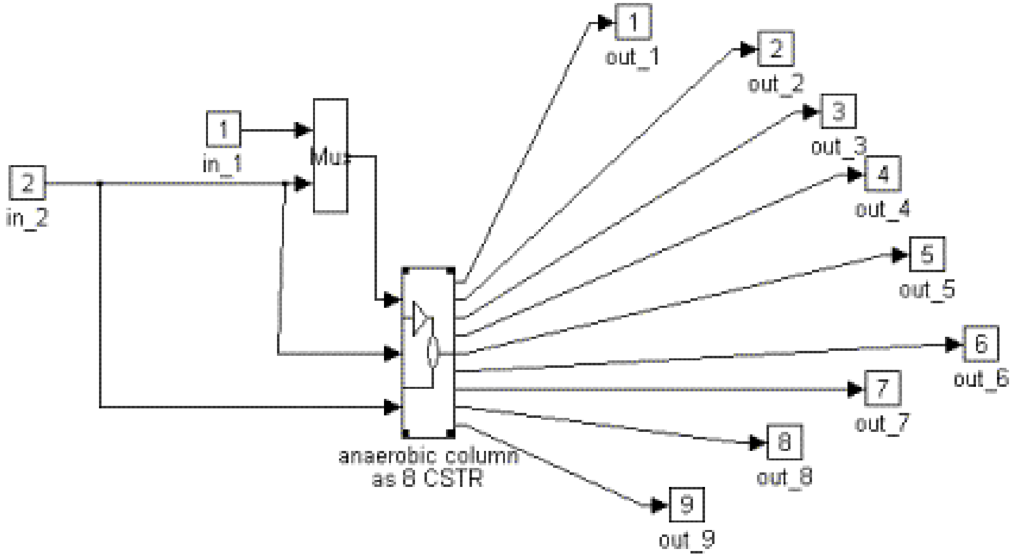
Acetate addition



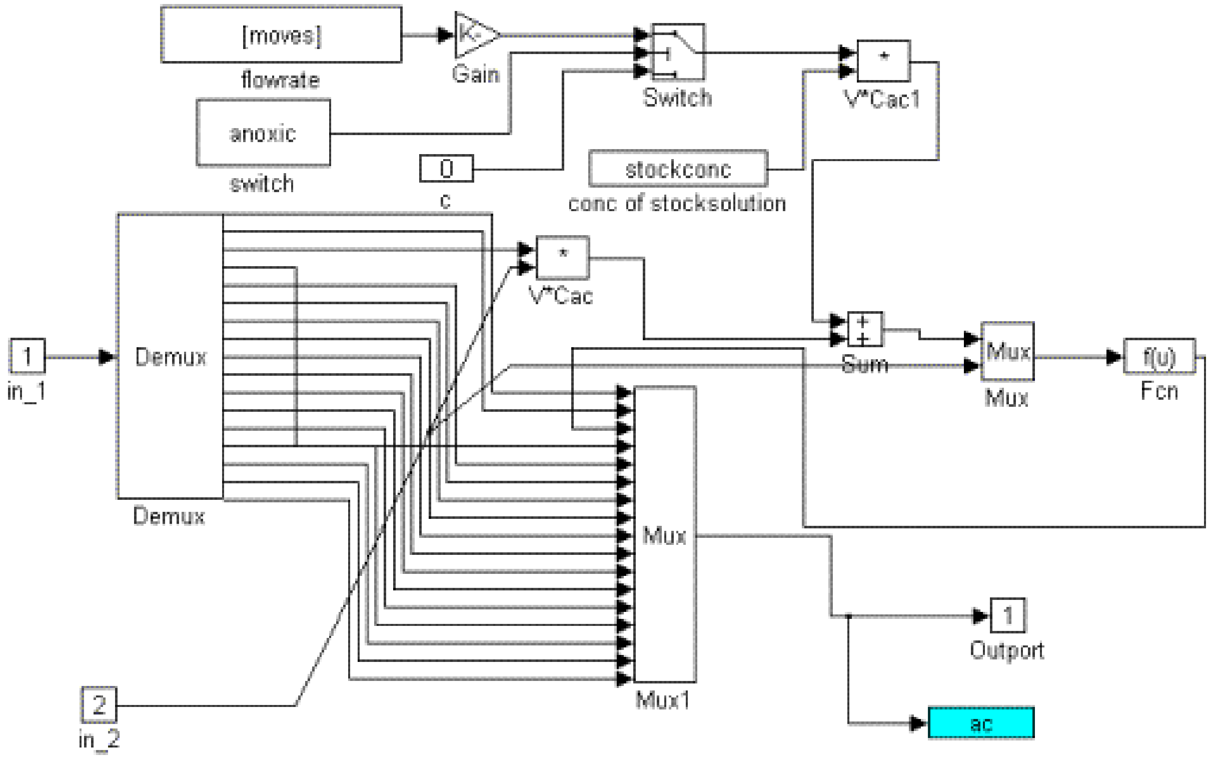
addition1


2
C inlet
1
Qinlet
1
*
*
Qin/(Qr+Qin)
+
+
f(u)
1/(Qr+Qin)
1
return ratio
*
Qr/(Qr+Qin)
+
+
C to ANA
*
3
C from settler
3
return flow
-K-
dil.rate
Anaerobic clolumn as 8 CSTR
2
flow out
1
[C out]
Addtion of COD

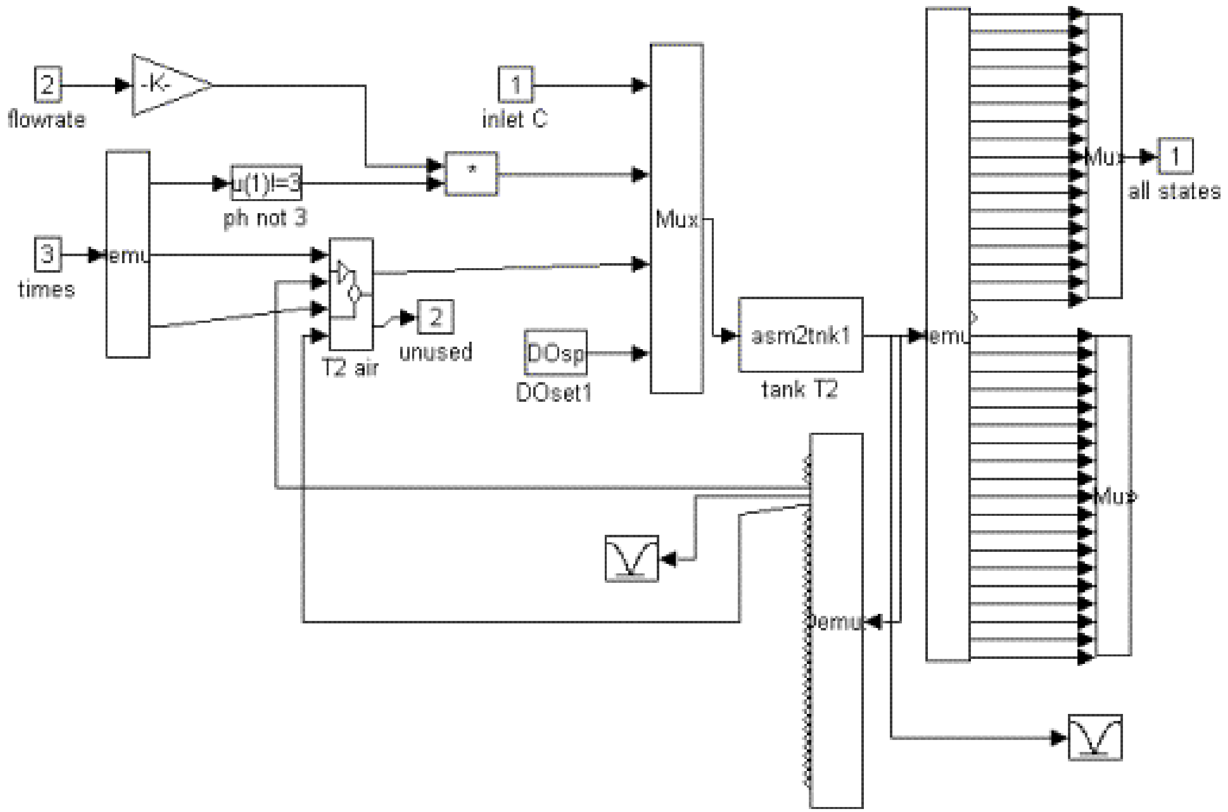
ANAsubsys



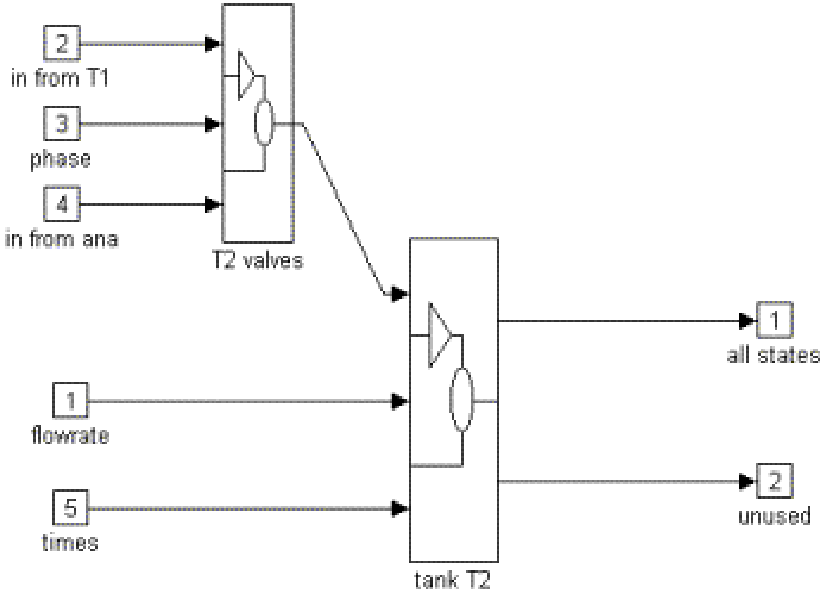
Anaerobic column as 8CSTR



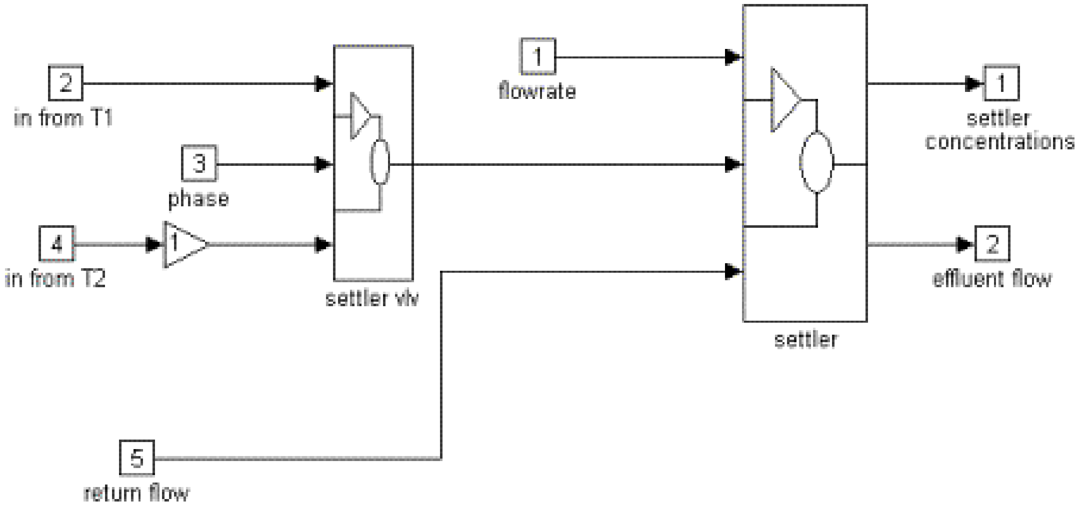
Addition of COD


2
flowrate
-K-
1
inlet C
*
u(1)!=3
ph not 3
3
times
Demu
T2 air
2
unused
Mux
DOsp
DOset1
asm2tnk1
tank T2
Demu
Demu
Mux
1
all states
Mux

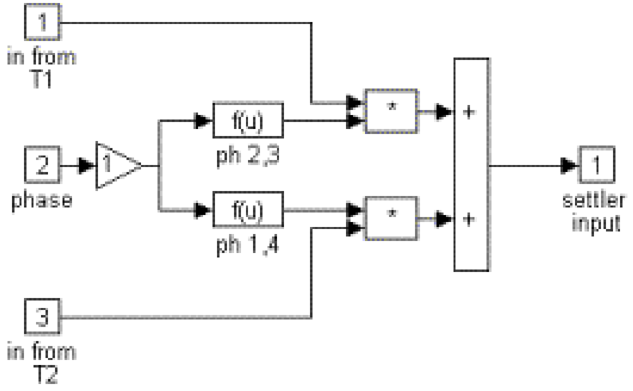
tank T2


2
in from T1
3
phase
4
in from ana
T2 valves
1
flowrate
5
times
tank T2
1
all states
2
unused

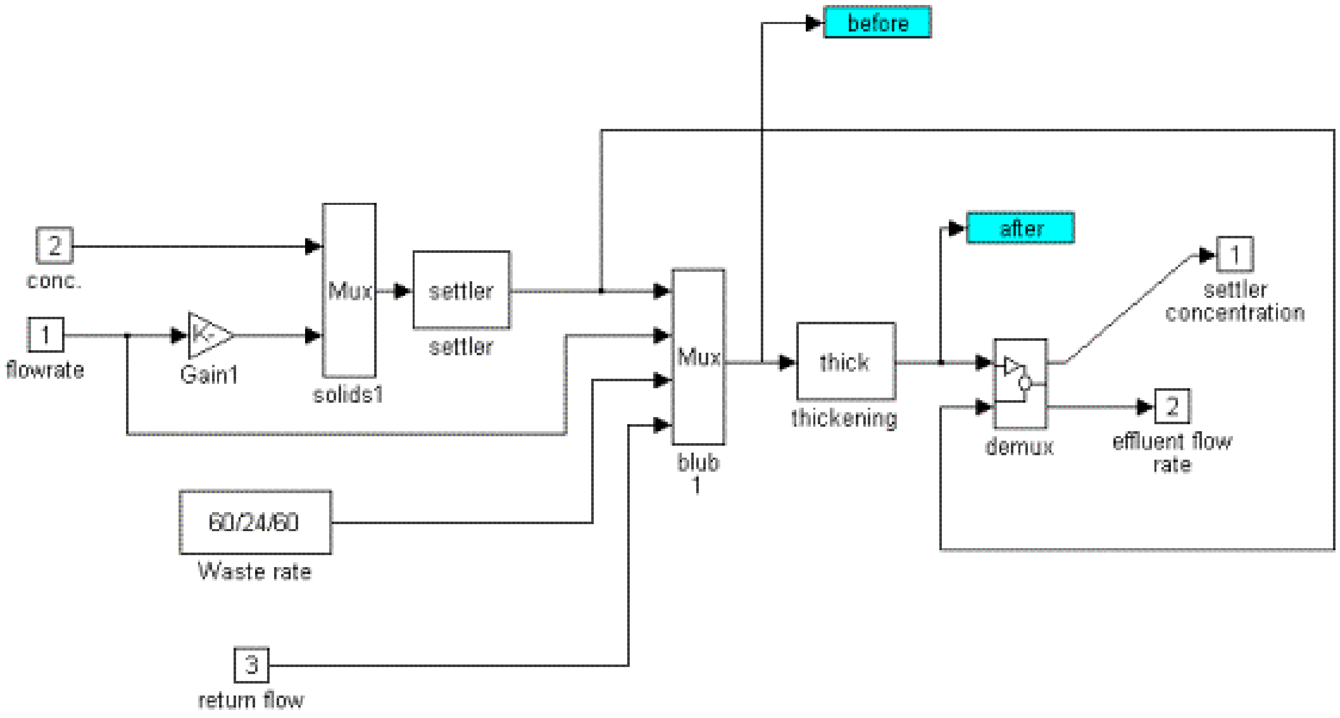
T2 subsys1



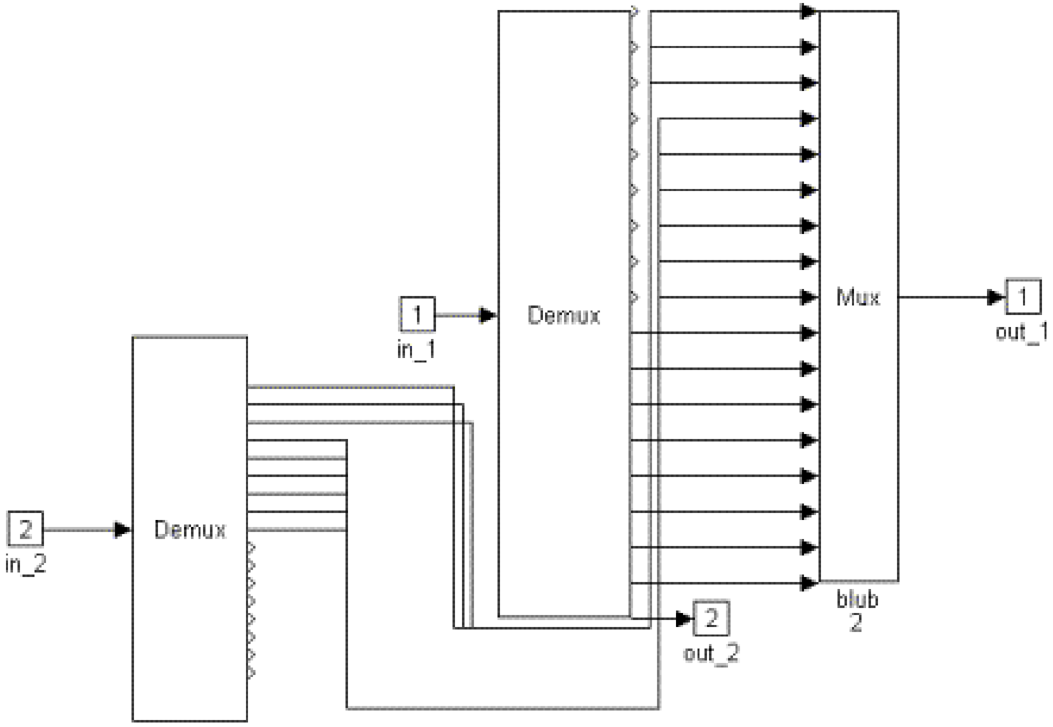
Settler subsys


1
in from
T1
2
phase
1
f(u)
ph 2,3
f(u)
ph 1,4
*
*
+
+
1
settler
input
3
in from
T2

Settler vlv


before
2
conc.
Mux
settler
settler
1
flowrate
K-
Gain1
solids1
Mux
blub
1
thick
thickening
after
1
settler
concentration
demux
2
effluent flow
rate
60/24/60
Waste rate
3
return flow

settler



demux

# $C^{++}$ Program

```
#define S_FUNCTION_NAME asm2tnk1

/* the name entered above is the name of the program */

/* next lines needed for matlab useage of C++ file  */

#include <stdio.h>
#ifdef MATLAB_MEX_FILE
#include "mex.h"
#endif
#include "simstruc.h"
/* include "mex.h" to use Matlab's own memory allocation routines */


/* written by Ulrich Krühne
 *
 *
 *
 * model includes 17 states, reactions 0-16 from the ASM2
 * and reactions 17 and 18 as described in the IAWQ report
 *
 * terminology: see ASM2
 *
 */

/* Input: u is a vector of the 17 inlet concentrations followed by the
 * dilution rate followed by a flag variable to say whether the
 * tank is aerated or not followed by the DO setpoint value.
 * Output: the 17 states plus the oxygen flag.
 *
 *
 * This version includes oxygen dynamics. The dynamics are turned on
 * if the difference between the setpoint (inputted) and the current DO value
 * (state value) is greater than a minimum (delDO). If DO is to decrease or if
 * airflg is 0 then klaval is set to 0, otherwise to the value kla which is
 * inputted as a parameter value.
 *
 *
 * After compilation, the program can be called from the Matlab command
 * line level as follows:
 *
 *    [sys,X0]=asm2tnk1([],[],[],0,[],[])
 *     will return size information in
 *     varialbe sys, and initial values in variable X0. The []'s are place
 *     holders for the other input arguments, which are not needed in this
 *     case.
 *
 *    sys=asm2tnk1(t,x,u,1,PAR,X0)
 *     will return the derivatives in sys. t is
 *     time, x are states, u are the inputs, PAR are the parameters, and
 *     X0 are initial values of states. In the program coding below, u is
 *     a vector containing 20 elements: The first 17 are the concentrations
 *     of the 17 states in the input stream to the tank. The 18th is the
 *     dilution rate, and the 19th is a flag to say whether the tank is
 *     aerated or not.Number 20 is providing the Do-Setpoint.
 *       PAR has 50 elements which are the model parameters
 *     (see list below).
 *
 *    [t,x,y]=rk45('asm2tnk1',[t0 tfinal],X0,OPTPARS,inputvec,PAR,[])
 *     will use rk45 to integrate the program model on the matlab command
 *     level. OPTPARS is the vector or parameters requested by rk45, for
 *     example [1e-4,1e-5,0.1]. inputvec is a matrix of input values, where
 *     the first column or row is reserved for time. In this case, therefore,
 *     inputvec needs to be 20 by n. rk45 does interpolation to find the
```

```
 *     inputs from inputvec for each time step. PAR is as above. The
 *     last argument [] is a place holder for the initial values. It must be
 *     there because the argument is expected, but rk45 substitutes the X0
 *     found in the argument prior to OPTPARS.
 *
 * terminology: see ASM2
 *
 */


/* following lines define how many input arguments are expected, and
   in what order they are found.  */

#define PAR     ssGetArg(S, 0)
#define X0      ssGetArg(S, 1)

/* the following lines are to obtain the model parameters from the input
   PAR, and to define the accronyms used later. */




#define   fsi      (mxGetPr(PAR)[0])
#define   fxi      (mxGetPr(PAR)[1])
#define   Yh       (mxGetPr(PAR)[2])
#define   Ypao     (mxGetPr(PAR)[3])
#define   Ypo4     (mxGetPr(PAR)[4])
#define   Ypha     (mxGetPr(PAR)[5])
#define   Yaut     (mxGetPr(PAR)[6])
#define   Kh       (mxGetPr(PAR)[7])
#define   nynoy    (mxGetPr(PAR)[8])
#define   nyfe     (mxGetPr(PAR)[9])
#define   Ko2hy    (mxGetPr(PAR)[10])
#define   Knohy    (mxGetPr(PAR)[11])
#define   Kxhy     (mxGetPr(PAR)[12])
#define   myhe     (mxGetPr(PAR)[13])
#define   qfhe     (mxGetPr(PAR)[14])
#define   nynoe    (mxGetPr(PAR)[15])
#define   bhe      (mxGetPr(PAR)[16])
#define   Ko2he    (mxGetPr(PAR)[17])
#define   Kfhe     (mxGetPr(PAR)[18])
#define   Kfehe    (mxGetPr(PAR)[19])
#define   Kahe     (mxGetPr(PAR)[20])
#define   Knohe    (mxGetPr(PAR)[21])
#define   Knhhe    (mxGetPr(PAR)[22])
#define   Kphe     (mxGetPr(PAR)[23])
#define   Kalke    (mxGetPr(PAR)[24])
#define   qpha     (mxGetPr(PAR)[25])
#define   qpp      (mxGetPr(PAR)[26])
#define   mypao    (mxGetPr(PAR)[27])
#define   bpao     (mxGetPr(PAR)[28])
#define   bpp      (mxGetPr(PAR)[29])
#define   bpha     (mxGetPr(PAR)[30])
#define   Ko2p     (mxGetPr(PAR)[31])
#define   Kap      (mxGetPr(PAR)[32])
#define   Knhp     (mxGetPr(PAR)[33])
#define   Kpsto    (mxGetPr(PAR)[34])
#define   Kpgro    (mxGetPr(PAR)[35])
#define   Kalkp    (mxGetPr(PAR)[36])
#define   Kpp      (mxGetPr(PAR)[37])
#define   Kmax     (mxGetPr(PAR)[38])
#define   Kipp     (mxGetPr(PAR)[39])
#define   Kpha     (mxGetPr(PAR)[40])
#define   myaut    (mxGetPr(PAR)[41])
```

```
#define   baut      (mxGetPr(PAR)[42])
#define   Ko2au     (mxGetPr(PAR)[43])
#define   Knhau     (mxGetPr(PAR)[44])
#define   Kalka     (mxGetPr(PAR)[45])
#define   Kpaut     (mxGetPr(PAR)[46])
#define   qppno3    (mxGetPr(PAR)[47])
#define   qpao      (mxGetPr(PAR)[48])
#define   Ya        (mxGetPr(PAR)[49])


   /*
    * get the states from the state vector
    */

#define  Som    ( x[0]  )   /* dynamic oxygen */
#define  Sf     ( x[1]  )   /* (mgCOD/l) */
#define  Sa     ( x[2]  )   /* fermentable organics (mgCOD/l) */
#define  Snh    ( x[3]  )   /* Ammonium (mgN/l) */
#define  Sno    ( x[4]  )   /* Nitrate (mgN/l) */
#define  Spo4   ( x[5]  )   /* inorganic phosphorus (mgP/l) */
#define  Si     ( x[6]  )   /* soluble inerts */
#define  Salk   ( x[7]  )   /* alkalinity */
#define  Sn2    ( x[8]  )   /* nitrogen gas */
#define  Xi     ( x[9]  )   /* insoluble inerts */
#define  Xs     ( x[10] )   /* slowly biodegradable organics (mgCOD/l) */
#define  Xh     ( x[11] )   /* heterotrophic biomass (mgCOD/l) */
#define  Xpao   ( x[12] )   /* phosphate accumulating biomass (mgCOD/l) */
#define  Xpp    ( x[13] )   /* stored poly-p in Xpao (mgP/l) */
#define  Xpha   ( x[14] )   /* stored organics in Xpao (mgCOD/l) */
#define  Xaut   ( x[15] )   /* Nitrifying biomass (mgCOD/l) */
#define  Xtss   ( x[16] )   /* Total suspended solids (mgCOD/l) */

/*  The accronyms D and airflg are defined below */

#define  D      ( u[17] )  /* tank dilution rate */
#define  airflg ( u[18] )  /* aeration flag      */
#define  SoSet  ( u[19] )  /* DO setpoint        */


#define  insi    ( 0.01 )   /* N content of inert soluble COD */
#define  insf    ( 0.03 )   /* N content of soluble substrate */
#define  inxi    ( 0.03 )   /* N content of inert particulate COD */
#define  inxs    ( 0.04 )   /* N content of particulate substrate */
#define  inbm    ( 0.07 )   /* N content of biomass XH,XPAO,XAUT */
#define  ipsi    ( 0.00 )   /* P content of inert soluble COD */
#define  ipsf    ( 0.01 )   /* P content of soluble substrate */
#define  ipxi    ( 0.01 )   /* P content of inert particulate COD */
#define  ipxs    ( 0.01 )   /* P content of particulate substrate */
#define  ipbm    ( 0.02 )   /* P content of biomass XH,XPAO,XAUT */
#define  itssxi  ( 0.75 )   /*TSS to XI ratio*/
#define  itssxs  ( 0.75 )   /*TSS to XS ratio*/
#define  itssbm  ( 0.90 )   /*TSS to biomass ratio for XH,XPAO,XAUT*/



#define  P1      ( -ipsf*(1-fsi)-ipsi*fsi+ipxs )
#define  P2      ( ipbm-(1-fxi)*ipxs-fxi*ipxi )
#define  N1      ( -insf*(1-fsi)-insi*fsi+inxs )
#define  N2      ( inbm-(1-fxi)*inxs-fxi*inxi )
#define  A1      ( (N1/14.0)-(1.5*P1/31.0) )
#define  A7      ( (N2/14.0)-(1.5*P2/31.0) )
#define  T1      ( fxi*itssxi+(1.0-fxi)*itssxs-itssbm )

/* #define    hlf1      (  myhe * (Snh/(Snh+Knhhe)) * (Spo4/(Spo4+Kphe)) * Xh ) */
```

```
#define    SwHY_air  (  (Som/(Som+Ko2hy))           )
#define    SwHY_par  (  ((Xs/Xh)/((Xs/Xh)+Kxhy)) )
#define    SwHY_no   (  (Sno/(Sno+Knohy))        )
#define    SwH_air   (  (Som/(Som+Ko2he))          )
#define    SwA_air   (  (Som/(Som+Ko2au))          )
#define    SwP_air   (  (Som/(Som+Ko2he))            )
#define    SwP_alk   (  (Salk/(Salk+Kalkp))      )

#define delDO1  (0.3)       /* value of how close to setpoint DO should approach */
#define delDO2  (0.2)       /* value of how close to setpoint DO should approach */
#define delDO3  (0.001)     /* value of how close to approach 0 */


   /*
    * saturation functions
    */




#define N_STATES 17
#define N_RATES  19

/*
 * ---------------------------------------------------------------------------
 */

static void mdlInitializeSizes(S)
    SimStruct *S;
{
    ssSetNumContStates    (S, N_STATES); /* number of continuous states */
    ssSetNumDiscStates    (S, 0);      /* number of discrete states */
    ssSetNumInputs        (S, 20);      /* number of inputs */
    ssSetNumOutputs       (S, N_STATES+1+N_RATES); /* number of outputs */
    ssSetDirectFeedThrough(S, 0);      /* direct feedthrough flag */
    ssSetNumSampleTimes   (S, 1);      /* number of sample times */
    ssSetNumInputArgs     (S, 2);      /* number of input arguments */
    ssSetNumRWork         (S, N_RATES);  /* number of real work vector elements */
    ssSetNumIWork         (S, 0);      /* number of integer work vector elements */
    ssSetNumPWork         (S, 0);      /* number of pointer work vector elements */
}


static void mdlInitializeSampleTimes(S)
    SimStruct *S;
{
    ssSetSampleTimeEvent(S, 0, 0.0);
    ssSetOffsetTimeEvent(S, 0, 0.0);
}


static void mdlInitializeConditions(x0, S)
    double *x0;
    SimStruct *S;
{
    int i, nstates;

    /*
     * if the initial condition parameter is not an empty matrix,
     * then use it to set up the initial conditions, otherwise,
     * set the intial conditions to all 0.0
     */

    nstates = ssGetNumContStates(S);
```

```
    if (mxGetM(X0) != 0) {
      double *pr;

      pr = mxGetPr(X0);
      for (i = 0; i < nstates; i++)
          *x0++ = *pr++;
    } else {
/* "default" initial values are inserted below */
              x0[0] = 0.0;     /* Som     */
              x0[1] = 6.044;   /* Sf      */
              x0[2] = 0;       /* Sa      */
              x0[3] = 0.0;     /* Snh4    */
              x0[4] = 0.0;     /* Sno3    */
              x0[5] = 0;       /* Spo4    */
              x0[6] = 41.0;    /* Si      */
              x0[7] = 7.70;    /* Salk    */
              x0[8] = 4.71;    /* Sn2     */
              x0[9] = 1024.0;  /* Xi      */
              x0[10] = 320.0;  /* Xs      */
              x0[11] = 697.5;  /* Xh      */
              x0[12] = 463.8;  /* Xpao    */
              x0[13] = 115;    /* Xpp     */
              x0[14] = 95.6;   /* Xpha    */
              x0[15]= 14.33;    /* Xaut    */
              x0[16] = 4700;   /* Xtss    */
    }
}



static void mdlOutputs(y, x, u, S, tid)
    double *y, *x, *u;
    SimStruct *S;
    int tid;
{
    double *rate = ssGetRWork(S);
    int i;

    for (i=0; i<N_STATES; i++)
      y[i] = x[i];                   /* output = continuous states*/
    y[N_STATES] = airflg;            /* oxygen from the input vector */
    for (i=0; i<N_RATES; i++)
      y[i+N_STATES+1] = rate[i];
}


/*
 * mdlUpdate - perform action at major integration time step
 *
 * This function is called once for every major integration time step.
 * Discrete states are typically updated here, but this function is useful
 * for performing any tasks that should only take place once per integration
 * step.
 */

static void mdlUpdate(x, u, S, tid)
    double *x;
    double *u;
    SimStruct *S;
    int tid;
{
    int i;
```

```
    for (i=0; i<N_STATES; i++)
    {
      if (x[i] < 0.0) x[i] = 0;
       if (airflg == 1)
    { x[0] = SoSet;
    }
    }
}

static void mdlDerivatives(dx, x, u, S, tid)
    double *dx, *x, *u;
    SimStruct *S;
    int tid;
{

   /*
    * calculate the rates of reaction; according to ASM2 and KS thesis
    */

    double *rate = ssGetRWork(S);
    static double   hlf1;
    static double   fsnhhe;
    static double   fsnhp;
    static double   fsnhau;




    if (airflg == 1)
      { Som = SoSet;
      } else
      { if (Som > 0.0)
           { Som = Som;
           } else
           { Som = 0.0;
           }
      }


    if ( Knhhe < 0.0001 )
    { fsnhhe = 1.0;
    } else
    { fsnhhe = (Snh/(Snh+Knhhe));
    }
    if ( Knhp < 0.0001 )
    { fsnhp = 1.0;
    } else
    { fsnhp = (Snh/(Snh+Knhp));
    }
    if ( Knhau < 0.0001 )
    { fsnhau = 1.0;
    } else
    { fsnhau = (Snh/(Snh+Knhau));
    }
    hlf1  =     myhe * fsnhhe * (Spo4/(Spo4+Kphe)) * Xh ;

    rate[0]  =  Kh * SwHY_air * SwHY_par * Xh;
    rate[1]  =  Kh * nynoy * (1.0-SwHY_air) * SwHY_no * SwHY_par * Xh;
    rate[2]  =  Kh * nyfe * (1.0-SwHY_air) * (1.0-SwHY_no) * SwHY_par * Xh;
    rate[3]  =  hlf1 * SwH_air * (Sf/(Sf+Kfhe)) * (Sf/(Sf+Sa))
                * (Salk/(Salk+Kalke));
    rate[4]  =  hlf1 * SwH_air * (Sa/(Sa+Kahe)) * (Sa/(Sa+Sf))* (Salk/(Salk+Kalke));
    rate[5]  =  hlf1 * nynoe * (1.0-SwH_air) * (Sf/(Sf+Kfhe)) *
```

```
                (Sf/(Sf+Sa)) * (Sno/(Sno+Knohe))* (Salk/(Salk+Kalke));
    rate[6]  =  hlf1 * nynoe * (1.0-SwH_air) * (Sa/(Sa+Kahe)) *
                (Sa/(Sa+Sf)) * (Sno/(Sno+Knohe))*(Salk/(Salk+Kalke));
    rate[7]  =  qfhe * (1.0-SwH_air) * (1.0-(Sno/(Sno+Knohe))) *
                (Sf/(Sf+Kfehe)) * (Salk/(Salk+Kalke)) * Xh;
    rate[8]  =  bhe * Xh;
    rate[9] =   qpha*(1- (Sno/(Sno+Knohe)))* (1 - SwH_air) * (Sa/(Sa+Kap)) *
((Xpp/Xpao)/((Xpp/Xpao)+Kpp)) * SwP_alk*Xpao;
    rate[10] =  qpp * SwP_air * (Spo4/(Spo4+Kpsto))
                * ((Xpha/Xpao)/((Xpha/Xpao)+Kpha))
                * ((Kmax-(Xpp/Xpao))/((Kmax-(Xpp/Xpao))+Kipp)) * SwP_alk *Xpao;
    rate[11] =  mypao * SwP_air * fsnhp * SwP_alk
                * (Spo4/(Spo4+Kpgro)) * ((Xpha/Xpao)/((Xpha/Xpao)+Kpha)) * SwP_alk* Xpao;
    rate[12] =  bpao * Xpao * SwP_alk;
    rate[13] =  bpp * Xpp * SwP_alk;
    rate[14] =  bpha * Xpha * SwP_alk;
    rate[15] =  myaut * SwA_air * fsnhau * (Spo4/(Spo4+Kpaut)) *
                (Salk/(Salk+Kalka)) * Xaut;
    rate[16] =  baut * Xaut;

    rate[17] =  qppno3 * (Sno/(Sno+Knohe)) * (1 - SwH_air) * (Spo4/(Spo4+Kpsto))
                * ((Xpha/Xpao)/((Xpha/Xpao)+Kpha))
                * ((Kmax-(Xpp/Xpao))/((Kmax-(Xpp/Xpao))+Kipp))* SwP_alk*Xpao;
    rate[18] =  qpao * (Sno/(Sno+Knohe)) * (1 - SwH_air) * fsnhp * SwP_alk
                * (Spo4/(Spo4+Kphe)) *  ((Xpha/Xpao)/((Xpha/Xpao)+Kpha)) * Xpao;

   /*
    *
    * mass balances
    *
    */

    /* if current value of DO is not near DO setpoint, dynamics are activated */
/* transport term for DO is deleted, so that only the rise or fall due to
   reactions in the tank will be considered.                          */


    if (airflg == 1)

      { dx[0] = 0.0;
      } else
      { if (Som > delDO3 )
        { dx[0] = (1-1/Yh)*rate[3]+(1-1/Yh)*rate[4]-Ypha*rate[10]+(1-1/Yh)*rate[11]+
            ((Yaut-4.57)/Yaut)*rate[15];
        } else
        { dx[0] = 0.0;
        }
      }


   dx[1] = D*(u[1]-Sf)+ (1.0-fsi)*( rate[0]+ rate[1]+ rate[2]) + (-1.0/Yh)*(rate[3]+
rate[5]) - rate[7];

    dx[2] = D*(u[2]-Sa)+ (-1.0/Yh)*(rate[4]+ rate[6]) + rate[7] + rate[14] - rate[9];

    dx[3] = D*(u[3]-Snh)+ N1*(rate[0]+rate[1]+rate[2]) + ((insf/Yh)-
inbm)*(rate[3]+rate[5])
            - inbm*(rate[4]+rate[6]+rate[11]) + insf*rate[7] + N2*(rate[8]+ rate[12]+
rate[16])
            - (inbm+(1.0/Yaut))*rate[15];

    dx[4] =  D*(u[4]-Sno)+ (-(1.0-Yh)/(2.86*Yh))*(rate[5]+ rate[6]+ rate[17])
            +(1.0/Yaut)*rate[15]+ (-Ypha/2.86)*rate[18];
```

```
    dx[5] = D*(u[5]-Spo4)+ P1*(rate[0]+rate[1]+rate[2]) + ((ipsf/Yh)-
ipbm)*(rate[3]+rate[5])
             - ipbm*(rate[4]+rate[6]+rate[11]+rate[15]+rate[18])
             + ipsf*rate[7] + P2*(rate[8]+rate[16]) + Ypo4*rate[9]
             + rate[13]-rate[10]-rate[17] + (ipbm-fxi*ipxi-(1-fxi)*ipxs)*rate[12];

    dx[6] =  D*(u[6]-Si)+ fsi*(rate[0]+rate[1]+rate[2]);

    dx[7] =  D*(u[7]-Salk)+ A1*(rate[0]+rate[1]+rate[2])
             + ((-1.5*((ipsf/Yh)-ipbm)/31.0)+(((insf/Yh)-inbm)/14.0))*rate[3]
             + ((1.0/(64*Yh))-(inbm/14.0)+(1.5*ipbm/31.0))*rate[4]
             + ((-1.5*((ipsf/Yh)-ipbm)/31.0)+(((insf/Yh)-inbm)/14.0) +
               ((1.0-Yh)/(14.0*2.86*Yh)))*(rate[5]+rate[6])
             + ((-1.0/64.0)+(insf/14.0)-(1.5*ipsf/31.0))*rate[7]
             + A7*(rate[8]+rate[16]) + ((1.0/64)-(1.5*Ypo4/31.0))*rate[9]
             + 1.5/31.0*rate[10] + ((-inbm/14.0)+(1.5*ipbm/31.0))*rate[11]
             + ((N2/14.0)-(1.5*(ipbm-fxi*ipxi+(1-fxi)*ipxs)/31.0))*rate[12]
             - 1.5/31*rate[13] - 1.0/64*rate[14]
             + (((-inbm-(1.0/Yaut))/14.0)-(1.0/(14*Yaut))+(1.5*ipbm/31.0))*rate[15];

    dx[8] = D*(u[8]-Sn2)+ (1-Yh)/(2.86*Yh)*(rate[5]+rate[6])
             + (1-Yh)/(2.86*Yh)*(rate[17])+(Ypha/2.86)*rate[18];

    dx[9]  = D*(u[9]-Xi)+ fxi*(rate[8]+rate[12]+rate[16]);

    dx[10] = D*(u[10]-Xs)-(rate[0]+rate[1]+rate[2]) + (1.0-
fxi)*(rate[8]+rate[12]+rate[16]);

    dx[11] = D*(u[11]-Xh)+ rate[3]+rate[4]+rate[5]+rate[6]-rate[8];

    dx[12] = D*(u[12]-Xpao)+ rate[11]+rate[18]-rate[12];

    dx[13] = D*(u[13]-Xpp)- Ypo4*rate[9] + rate[10] - rate[13]+ rate[17] ;

    dx[14] = D*(u[14]-Xpha)+ rate[9] - Ypha*(rate[10]+rate[17])
             - (1.0/Ya)*rate[18] - (1.0/Ypao)*rate[11] - rate[14];

    dx[15] = D*(u[15]-Xaut)+ rate[15]-rate[16];

    dx[16] = D*(u[16]-Xtss) - itssxs*(rate[0]+rate[1]+rate[2])
             + itssbm*(rate[3]+rate[4]+rate[5]+rate[6]+rate[15])
             + T1*(rate[8]+rate[12]+rate[16]) + (-3.23*Ypo4+0.6)*rate[9]
             + (3.23-(0.6*Ypha))*(rate[10]+rate[17]) + (itssbm-
(0.6/Ypao))*(rate[11]+rate[18])
             - 3.23*rate[13] - 0.60*rate[14];



 }


static void mdlTerminate(S)
    SimStruct *S;
{
}

#ifdef  MATLAB_MEX_FILE    /* Is this file being compiled as a MEX-file? */
#include "simulink.c"      /* MEX-file interface mechanism */
#else
#include "cg_sfun.h"       /* Code generation registration function */
#endif
```