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Extension of the Benchmark Simulation Model no. 2 with a model for chemical precipitation of phosphorus

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Sofie Bydell

ABSTRACT

Extension of the Benchmark Simulation Model No. 2 with a model for chemical precipitation of phosphorus.

Sofie Bydell

At present, there are more than 2000 wastewater treatments plants (WWTPs) in Sweden. Emissions of nitrogen and phosphorus from these, do contribute to the eutrophication of the Baltic Sea and watercourses on a daily basis. To reduce emissions of phosphorus, the Swedish approach has for the last 50 years been to use chemical precipitation.

Today, software is used to test and evaluate different strategies in WWTPs, this in order to improve the operation and get a holistic view over the process. One model that can be used to achieve a holistic view is the Benchmark Simulation Model No. 2 (BSM2). In order to get a software like BSM2 to best mirror the reality, it is important that the model well describes the actual process. Today, BSM2 does not take the load of phosphorus into account, which, if it was included in the model, would describe the process better.

In this master thesis, the author has investigated the possibility of extending the BSM2 model, to include phosphorus and chemical precipitation. Thereafter the results from simulations in BSM2 were compared with measurements from Henriksdals WWTP in Stockholm.

The results showed that a model, after some simplifications, for phosphorus and chemical precipitation could be included in BSM2. The model uses primary precipitation. Precipitation chemical was added with assistance of a PI controller. Generally the results showed that the model had potential to describe the *total flow of phosphorus* in the WWTP. In measurements from Henriksdal the *average total phosphorus* effluent from primary and secondary sedimentation were 3.97 and 0.43 mg/l, respectively. From a steady state simulation in BSM2 the values were 4.26 and 0.44 mg/l and the *average values* of a dynamic simulation 3.96 and 0.46 mg/l.

Although the average values of total phosphorus matches quite well, it was found difficult to simulate the different *fractions of phosphorus* effluent from the secondary sedimentation. In order to better evaluate the results and how the simplifications of the model affects them, more measurements need to be done and a comparison with the results received from the BSM2 needs to be carried out. Also an adjustment of parameters in BSM2 must be done, this to achieve a better compliance with the given plant.

Keyword: BSM2, phosphate, phosphorus, chemical precipitation, wastewater treatment

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REFERAT

Utvidgning av Benchmark Simulation Modell No. 2 med en modell för kemisk fällning av fosfor

Sofie Bydell

Sverige har idag drygt 2000 reningsverk. Reningsverkens utsläpp av kväve och fosfor bidrar dagligen till övergödning i Östersjön och därtill anslutna vattendrag. För att minska utsläpp av fosfor har i Sverige sedan mitten på 1960-talet kemisk fällning använts.

Idag används programvara för att testa och utvärdera olika strategier i reningsverken, detta med syftet att förbättra driften och få en helhetsbild över processen. En av dessa modeller är Benchmark Simulation Model No. 2 (BSM2). För att simuleringsprogram ska ge en så bra bild som möjligt av verkligheten är det viktigt att de beskriver processen, i detta fall avloppsvattenrening, på ett bra sätt. BSM2 tar i dagsläget inte hänsyn till belastningen av fosfor, om fosfor inkluderades i modellen skulle det beskriva processen bättre.

I detta examensarbete, har författaren undersökt möjligheten att utvidga BSM2, till att inkludera fosfor och kemisk fällning i modellen. Resultaten erhållna från modellen har därefter jämförts med mätdata från Henriksdals reningsverk i Stockholm.

Resultatet visade att en modell för fosfor och kemisk fällning kunde, efter vissa förenklingar, inkluderas i BSM2. I modellen användes förfällning och fällningskemikalier tillsattes med hjälp av en PI regulator. Generellt visade resultaten att modellen hade förmåga att beskriva det *totala flödet av fosfor* i reningsverket. I mätningarna från Henriksdal var *medelvärdet på total fosfor* ut från försedimenteringen 3,97 mg/l och från eftersedimenteringen 0,43 mg/l. Från en steady state simulering i BSM2 blev värdena 4,26 och 0,44 mg/l och *medelvärdena* från en dynamisk simulering 3,96 och 0,46 mg/l.

Även om medelvärdena på totalfosfor stämmer relativt bra överens, fann man det svårt att simulera olika *fraktioner av fosfor* ut från eftersedimenteringen. För att bättre kunna bedöma resultatet och hur förenklingar i modellen påverkar resultatet behöver flera mätningar göras och jämföras med modellens resultat. En justering av parametrar i BSM2 måste även göras, detta för att anpassa modellen till det givna avloppsreningsverket bättre.

Nyckelord: BSM2, fosfat, fosfor, kemisk fällning, reningsverk

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PREFACE

This work is a master thesis of 30 ECTS within the Master of Science program in Environmental and Water Engineering at Uppsala University. The thesis has been carried out for IVL Swedish Environmental Institute as a part of the project “Development and dynamic analysis of operational strategies for enhanced energy efficiency of wastewater treatment systems” with Magnus Rahmberg as supervisor. Subject reviewer was Bengt Carlsson at the Department of Information Technology, the Division of Systems and Control, Uppsala University. Examiner was Fritjof Fagerlund, Department of Earth Sciences, the Division Air, Water and Landscape Sciences, Uppsala University.

I would like to thank my supervisor, Magnus, for listening and answering all my questions and for all the help throughout the thesis. Also thanks to Linda Åmand, for helping me with the controller part. You both made me feel welcome at IVL, thanks for that. Thanks to Bengt Carlsson for giving me advice throughout the work.

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POPULÄRVETENSKAPLIG SAMMANFATTNING

Utvidgning av Benchmark Simulation Modell No. 2 med en modell för kemisk fällning av fosfor Av: *Sofie Bydell*

Utsläpp av kväve och fosfor från avloppsreningsverk bidrar dagligen till övergödningen av Östersjön och därtill anslutna vattendrag. För att minska mängden fosfor, som via reningsverk påverkar övergödningen, används ofta en metod som kallas kemisk fällning. Metoden har använts i Sverige sedan mitten på 1960-talet och kan minska utsläppen av fosfor med upp till 90 %. *Kemisk fällning* innebär att man reducerar fosforkoncentrationen i utgående vatten från avloppsreningsverket med hjälp av att tillsätta ett metallsalt. Metallsaltet är ofta baserat på järn eller aluminium och får fosfor att omvandlas till ett komplex som sedan kan avskiljas och behandlas.

I och med Sveriges åtaganden i BSAP (Baltic Sea Action Plan) och EU:s vattendirektiv kommer framtiden innebära strängare krav på både kväve och fosfor, detta för att minska belastningen på Östersjön. För att klara dessa krav kan processutformningen på avloppsreningsverken behöva förändras.

I dag används olika programvaror och modeller för att testa och utvärdera nya strategier och för att ge en helhetsbild över avloppsreningsverkens miljöpåverkan. En av dessa modeller är Benchmark Simulation Model No. 2 (BSM2). För att simuleringsprogram som BSM2 ska ge en så bra bild som möjligt av verkligheten är det viktigt att de beskriver processen, i detta fall avloppsvattenrening, på ett bra sätt. BSM2 tar i dagsläget inte hänsyn till belastningen av fosfor, vilket är en del av modellen som skulle kunna beskrivas bättre.

Ett försök till att inkludera fosfor och kemisk fällning i BSM2 har under våren utförts. I modellen (BSM2) har fällningsmetoden, förfällning lagts till. *Förfällning* är en fällningsmetod som används i avloppsreningsverk, som namnet antyder sker själva fällningen och doseringen av fällningskemikalier (metallsaltet) tidigt i processen. Vanligen doseras kemikalien redan i inloppet till reningsverket.

För att dosera fällningskemikalier i modellen användes en PI regulator. *En regulator* används för att reglera ett system på ett önskvärt sätt, en *PI regulator* används ofta och består av två element: en proportionerlig del och en integrerande del.

Efter att både fällningsmetod och doseringen av fällningskemikalier lagts till i BSM2, gjordes en bedömning över hur väl fosfor i modellen har samma beteende som fosfor i ett verkligt reningsverk. Detta genom att jämföra resultat från simuleringar i BSM2 med uppmätta värden från Henriksdals reningsverk i Stockholm.

Resultatet visade att modellen för fosfor i BSM2 hade förmåga att generellt kunna beskriva beteendet för det *totala flödet av fosfor* i avloppsreningsverket Henriksdal.

Fosfor i avloppsvatten förekommer i olika fraktioner, både som organiskt bunden fosfor och som löst fosfat. Hur dessa fraktioner av fosfor varierade, visade sig dock svårt att simulera med modellen.

Modellen för fosfor och kemisk fällning i BSM2 är en förenkling av verkligheten och tar bland annat inte hänsyn till hur pH och temperatur påverkar fällningsprocessen. För att bättre kunna analysera modellens resultat och hur dessa förenklingar påverkar, ansågs det därför önskvärt att under en längre tidsperiod samla in mätdata att jämföra mot modellens resultat. Detta skulle antingen kunna stärka modellens trovärdighet eller påvisa var förbättringar skulle behöva göras.

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ABBREVIATIONS AND DEFINITIONS

Aerobic: Aerobic is a process or an organism that need access to oxygen for its survival.

Anaerobic: An anaerobic organism or process does not require oxygen for growth.

Anoxic: Anoxic conditions means just as anaerobic that oxygen is missing. In anoxic conditions however molecules containing oxygen may be present.

Ammonification: the bacterial process that leads to the production of the nitrogen ammonium.

ASM1: Activated Sludge Model no. 1

ASP: Activated Sludge Process

Autotrophic bacteria: Bacteria that are able to capture carbon dioxide from the air to build up the cell structure.

BOD: Biological Oxygen Demand, BOD is the amount of oxygen consumed in the biological degradation of the organic matter in a water sample.

BSM2: Benchmark Simulation Model no. 2

COD: Chemical Oxygen Demand, COD is used to measure the total amount of oxygen-consuming substances in the total chemical breakdown of organic substances in water.

Heterotrophic bacteria: Bacteria that utilize organic carbon to build up the cell structure.

Hydrolysis: Hydrolysis is biological processes that convert large complex molecules to readily biodegradable molecules available for microbial growth.

LCA: Life Cycle Analysis

Metabolism: A term used to describe all chemical reactions involved in maintaining the living state of the cells and the organism.

PI: A controller that is composed of two elements, a proportionate part and an integral part.

Substrate: Source of energy for microorganisms, organic, inorganic or light.

TSS: Total Suspended Solids, the total amount suspended material

WWTP: Waste Water Treatment Plant

Yield: the ratio of amount of substance generated to the amount of substance consumed

SYMBOLS

Symbol	Comment	unit
alk	Alkalinity	
b_{AT}	Autotrophic decay rate	1/day
b_{HT}	Heterotrophic decay rate	1/day
C_{sludge}	Chemical sludge	mg/l
e	Control error	
F_P	Formed precipitate	mg/l
f_p	Fraction of biomass yielding particulate products	
$f_{sx,k}$	Structural factor defining the fraction of particulate matter of each fraction	
f_x	Ratio of particulate COD from total COD (mean value)	
f_k	Effluent concentration factor	
f_{corr}	Correction factor for removal efficiency (tuning parameter)	
f_{corr2}	Correction factor for removal efficiency (tuning parameter)	
f_{corr3}	Correction factor for removal efficiency (tuning parameter)	
$\eta_{COD}(t)$	COD removal efficiency (total)	%
$\eta_{COD,P}(t)$	COD removal efficiency (particulate)	%
η_g	Correction factors for anoxic growth of heterotrophic bacteria	
η_h	Correction factors for anoxic hydrolysis	
i_{XB}	Mass N/mass COD in biomass	g N/g COD in biomass
i_{XP}	Mass N/mass COD in products from biomass	g N/g COD in inert material
i_{XBP}	Mass P/mass COD in biomass	mass P/mass COD in biomass
i_{XEP}	Mass P/mass COD in inert material	mass P/mass COD in inert material

K	Gain (control parameter)	
k_{aT}	Ammonification rate	m^3/(g COD day)
K_{precip}	Constant for formed precipitate for every gram phosphorus removed	g precipitate/g P
$K_{chemical}$	Constant for chemical required for every gram phosphorus removed	g chemical/g P
K_S	Half saturation constant for heterotrophs	g COD/m^3
$K_{O,H}$	Half saturation constant for oxygen heterotrophs	g O_2/m^3
K_{NO}	Half saturation constant for nitrate for denitrifying heterotrophs	g NO_3-N/m^3
$K_{O,A}$	Half saturation constant for oxygen for autotrophs	g O_2/m^3
K_{NH}	Half saturation constant for ammonia for autotrophs	g NH_3-N/m^3
K_X	Half saturation constant for hydrolysis of slowly biodegradable substrate	g slowly biodeg. COD/(g cell COD)
k_{hT}	Maximum specific hydrolysis rate	g slowly biodeg. COD/(g cell COD day)
k_{pp}	Constant used for phosphate in the biological process	m^3/(g COD day)
K_{PO4}	Half saturation constant for phosphate	mg P/l
λ	Lambda, in the lambda method	
p	User selection in the lambda method	
$P_{part_{bio}}$	Assumed biodegradable part of particulate phosphorus	
$\rho_{1,as}$	Aerobic growth of heterotrophic biomass	mg/(day·l)
$\rho_{2,as}$	Anoxic growth of heterotrophic bacteria	mg/(day·l)
$\rho_{3,as}$	Aerobic growth of autotrophic	mg/(day·l)

	bacteria	
$\rho_{4,as}$	Decay of heterotrophic bacteria	mg/(day·l)
$\rho_{5,as}$	Decay of autotrophic bacteria	mg/(day·l)
$\rho_{6,as}$	Ammonification of soluble organic nitrogen	mg/(day·l)
$\rho_{7,as}$	Hydrolysis of entrapped organics	mg/(day·l)
$\rho_{8,as}$	Hydrolysis of entrapped organic nitrogen	mg/(day·l)
$\rho_{9,as}$	Hydrolysis process of particulate phosphorus	mg/(day·l)
Q_i	flow rate	m^3/day
Q_{po}	Primary effluent flow	m^3/day
Q_{pu}	Primary sludge flow	m^3/day
Q_{pi}	Influent flow	m^3/day
q_f	Precipitation chemical	mg/l
r	Set-point (controller)	
$r_{S_{ND}}$	Conversion rate for S_{ND}	mg/(day·l)
$r_{X_{ND}}$	Conversion rate for X_{ND}	mg/(day·l)
S	Concentration of growth limiting substrate	mg/l
S_I	Soluble non-biodegradable material	mg COD/l
S_{ND}	Soluble biodegradable organic nitrogen	mg N/l
S_{NO}	Nitrification of ammonia to nitrogen	mg N/l
S_O	Dissolved oxygen concentration	mg -COD/l
S_S	Readily biodegradable substrate	mg COD/l
S_{PO4}	Soluble phosphate	mg P/l
S_{NH}	Ammonia nitrogen	mg N/l
TSS	Total suspended solids	mg/l
T	Temperature	°C

t	Time	day
t_h	Hydraulic retention time	day
T_i	Integral time (control parameter)	
T_t	Anti-windup (control parameter)	
μ	Specific growth rate	1/day
μ_{max}	Maximum specific growth rate	1/day
μ_{AT}	Autotrophic maximum specific growth rate	1/day
μ_{HT}	Heterotrophic maximum specific growth rate	1/day
u	Control signal	
ν_{kj}	Stoichiometric parameter	
X_S	Slowly biodegradable substrate	mg COD/l
X_{ND}	Particulate biodegradable organic nitrogen	mg N/l
$X_{B,A}$	Autotrophic biomass	mg COD/l
$X_{B,H}$	Heterotrophic biomass	mg COD/l
X_I	Particulate non-biodegradable material	mg COD/l
X_P	Inert particulate products from biomass decay	mg COD/l
X_{PP}	Particulate phosphorus	mg P/l
y	Output (controller)	
Z_{po}	Effluent concentration from primary clarifier	mg/l
Z_{pu}	Sludge concentration from primary clarifier	mg/l
$Z_{pc,k}$	Concentration in mixing tank (primary clarifier)	mg/l
$Z_{pi,k}$	Influent concentration to primary sedimentation	mg/l

1. INTRODUCTION

Emissions of nitrogen and phosphorus from wastewater treatment plants (WWTPs), contribute to the eutrophication of the Baltic Sea and watercourses on a daily basis. In order to reduce phosphorus effluent from wastewater metal salt, mainly iron or aluminum salts, are commonly used (Svenskt Vatten, 2010). The salt form low solubility compounds with phosphorus which can be separated by sedimentation (Svenskt Vatten, 2010). Chemical precipitation of phosphorus is according to Svenskt Vatten (2010) capable of reducing incoming phosphorus with up to 90 %.

A model named Benchmark Simulation Model no 2 (BSM2), is currently used by IVL Swedish Environmental Institute to provide a holistic view of WWTPs environmental impact and perform life-cycle analysis (LCA). To perform a good LCA a requirement is that the process, in this case wastewater treatment, is well described in the model. Today, BSM2 does not take the load of phosphorus into account, which, if it was included in the model, would describe the process better.

1.1 OVERALL AIM

The overall aim of this master thesis is to describe the process of wastewater treatment in BSM2 better, in order to in future enabling a more complete LCA.

The specific objectives of this master thesis is to:

- Develop the existing process model BSM2 for wastewater treatment; in particular, developing a module for precipitation of phosphorus that is compatible with the current model.
- Further the objective includes choosing a precipitation method and chemical to be included in the precipitation module.

1.2 WORK FLOW

The thesis is performed in the following steps:

- Literature study
- Development of model
- Analysis of results
- Report writing

The literature study will focus on literature about the existing BSM2, and articles about phosphorus in wastewater. A great deal of work will be placed on understanding the existing model structure and developing a "module" for precipitation of phosphorus.

The simulated results of the model are then compared to empirical data measured from a real WWTP. Data for the analysis was provided by IVL Swedish environmental institute and represent measurements from Henriksdals WWTP in Stockholm.

1.3 LIMITATIONS

- The model for chemical precipitation will not be affected by temperature and pH changes which the process in reality is. This in order to keep the complexity of the model within the timeframe of the thesis.
- BSM2 is a complex model and includes a large number of variables that varies between different WWTP, a calibration to adjust BSM2 to Henriksdals WWTP is not included.
- Water treatment in generally produces a lot of sludge, which usually is fed to an anaerobic digestion process. How phosphorus is affected in this process is not included in the thesis.

2. THEORY

This theory section introduces some basic knowledge of wastewater treatment, with focus on chemical treatment. It also gives an introduction to Benchmark Simulation Model no 2 (BSM2) and finally introduces how automatic control can be used for dosing of precipitation chemicals.

2.1 WASTEWATER TREATMENT IN SWEDEN

The wastewater influent to wastewater treatment plants (WWTPs) is treated in several steps before fed back to the recipient. The Process of WWT in Sweden in general includes mechanical, chemical and biological treatment (Figure 1).

Figure 1 *The process of wastewater treatment including mechanical, chemical and biological treatment. Formed sludge from each step is past to sludge treatment, usually an anaerobic digestion process.*

2.2 MECHANICAL TREATMENT

Mechanical treatment (Figure 2) separates larger objects and particles using grids and sand traps (Svenskt Vatten, 2010). The wastewater is then passed to primary sedimentation and suspended solids are removed by gravity, formed primary sludge is passed to sludge treatment (Svenskt Vatten, 2010).

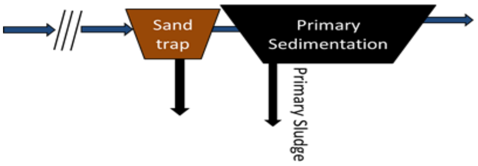


Figure 2 *Mechanical treatment, with grids, sand trap and primary sedimentation.*

2.3 BIOLOGICAL TREATMENT

A common method for biological treatment is the activated sludge process (ASP), ASP typically consists of an aeration basin followed by sedimentation and can be modified to reduce both nitrogen (N) and phosphorus (P) (Svenskt Vatten, 2010).

2.3.1 Biological nitrogen reduction

Biological nitrogen removal is based on the processes that naturally occur in the environment. Nitrogen in wastewater is usually in the form of ammonium. Special bacteria called nitrifying bacteria is able to convert ammonium to nitrate, this process is called nitrification and require an aerobic environment (Carlsson and Hallin, 2010). Other bacteria are then capable of converting nitrate to nitrogen gas, this process is called denitrification and require an anoxic environment (Carlsson and Hallin, 2010). The nitrogen gas then exit to the atmosphere and sedimentation separates formed biological sludge. One difficulty in the technical application of nitrifying and denitrifying bacteria is that they require different environment to survive and reproduce.

Two various process configurations of biological nitrogen reduction is after- and primary denitrification (Carlsson and Hallin, 2010). In both wastewater passes through alternating anoxic and aerobic zones, to promote nitrifying and denitrifying bacteria (Figure 3).

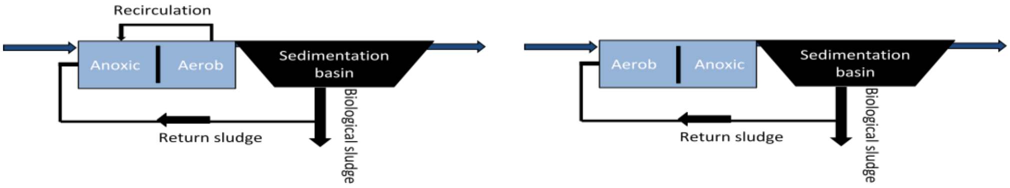


Figure 3 *Biological treatment with ASP, aeration tank followed by sedimentation.*
Left picture: ASP with primary denitrification. As denitrification takes place before nitrification, nitrate-rich water is recycled back from the aerobic zones where denitrification occurs. The sedimentation basin separates formed biological sludge. Right picture: ASP with after denitrification.

2.3.2 Biological phosphorus reduction

In biological phosphorus removal, the fact that certain bacteria are able to take up phosphate to a larger extent is utilized. The microorganisms are "stressed" to take up phosphorus by alternately be in the anaerobic and aerobic environments, and thus phosphate ends up in the biological sludge which can be removed by sedimentation (Carlsson and Hallin, 2010).

2.3.3 The specific growth rate

In general, biological processes involve growth and decay of bacteria. The bacteria use substrate for growth and when the food source is limiting the cells starts to decay. An often used parameter is the specific growth rate (μ), the specific growth rate depends on the substrate concentration and can be described by a Monod function, an empiric relation often used is (1) (Carlsson, 2010a).

$$\mu = \mu_{max} \frac{S}{K_S + S} \tag{1}$$

where

μ_{max} is maximum specific growth rate [1/day]

S is concentration of growth limiting substrate [mg/l]

K_s is half saturation constant [mg/l]

2.4 CHEMICAL TREATMENT

The main reason for using chemical treatment in WWT is to reduce phosphorus in effluent water, but also BOD (biological oxygen demand), bacteria and metals are reduced (Svenskt Vatten, 2010).

2.4.1 Phosphorus in wastewater

Phosphorus is divided into three major categories (Svenskt Vatten, 2010):

- Orthophosphates
- Polyphosphates
- Organically bound phosphorus

Organic phosphorus is mainly bound in solids and removed with primary sludge while polyphosphate and orthophosphate mostly are present in dissolved form and reduced by chemical precipitation (Svenskt Vatten, 2010). Orthophosphate can be present either as $H_2PO_4^-$, H_3PO_4, HPO_4^{2-} or PO_4^{3-} and the division between those are dependent on the pH-value (Svenskt Vatten, 2010).

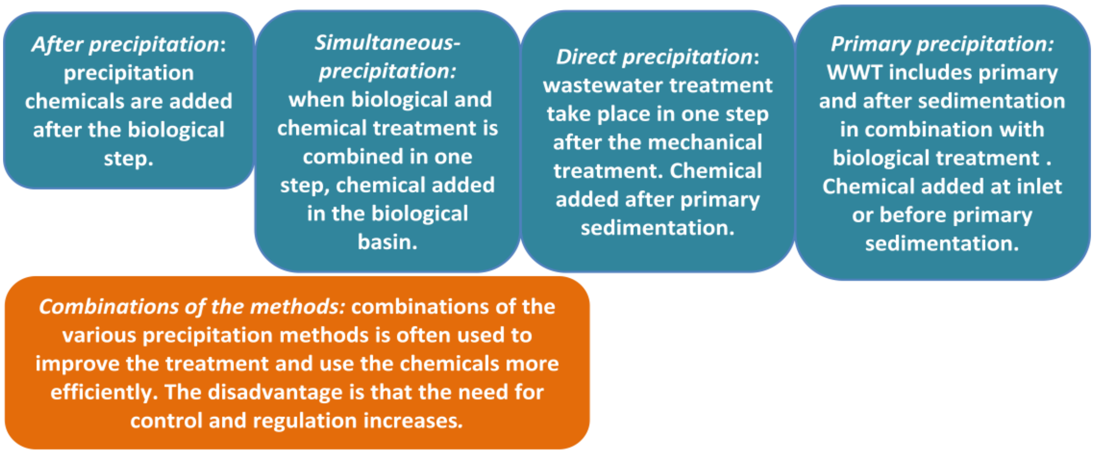
2.4.2 Chemical precipitation of phosphorus

The mechanisms of chemical precipitation is that dissolved inorganic phosphorus in wastewater by means of metal salt is converted to low solubility metal phosphate (Svenskt Vatten, 2010). Colloidal particles in natural water are charged (Kemira, 2013). Most of them have a negative net charge and therefore repel each other and remain atomized in the liquid, chemical precipitation and flocculation instead get the particles to attract each other and then settle (Kemira, 2013). The solubility of the newly formed precipitate varies strongly with pH and dissolves both for low and high pH-values (Svenskt Vatten, 2010). Precipitation with metal salts also forms hydroxides, and thereby reduces the hydroxide concentration which reduces pH (Kemira, 2013).

As precipitated phosphate and hydroxide settle they also, by adsorption, capture particulate materials which otherwise would not settle (Carlsson and Hallin, 2010). Therefore the process does also improve the separation of solid particles in wastewater (Carlsson and Hallin, 2010).

2.4.3 Precipitation method

Depending on where the precipitation chemical is added different precipitation methods is used. The four main types are: direct-, primary-, simultaneous- and after-precipitation (Svenskt Vatten, 2010) (Figure 4).



***After precipitation*:** **precipitation chemicals are added after the biological step.**

Simultaneous-precipitation: **when biological and chemical treatment is combined in one step, chemical added in the biological basin.**

***Direct precipitation*:** **wastewater treatment take place in one step after the mechanical treatment. Chemical added after primary sedimentation.**

Primary precipitation: **WWT includes primary and after sedimentation in combination with biological treatment . Chemical added at inlet or before primary sedimentation.**

Combinations of the methods: **combinations of the various precipitation methods is often used to improve the treatment and use the chemicals more efficiently. The disadvantage is that the need for control and regulation increases.**

Figure 4 *Short introduction of the precipitation methods: after, simultaneous, direct and primary precipitation.*

2.4.4 Precipitation chemical

Commonly used precipitation chemicals according to Svenskt Vatten (2010) are:

- Trivalent iron (Fe^{3+})
- Aluminum (Al^{3+})

Trivalent iron salts

Precipitation chemicals based on trivalent iron can be combined with sulfate or chloride but also consist of a mixture of these (Svenskt Vatten, 2010). The sulfate and chloride ions do not take part in the precipitation reaction (Svenskt Vatten, 2010). The exact chemical reaction is not known, but Jeppsson et.al (2005) suggests:

$$3\,Fe^{3+} + 2\,PO_4^{3-} + 3\,H_2O \rightarrow (FeOH)_3(PO_4)_2 + 3\,H^+ \qquad (2)$$

$$Fe^{3+} + 3\,H_2O \rightarrow Fe(OH)_3 + 3H^+ \qquad (3)$$

Iron salts gives precipitation of phosphate at pH around 4-8 (Svenskt Vatten, 2010). Iron not only react with phosphate, but also with particles and the water itself. To precipitate phosphorus it is required 1.5 mole trivalent iron per mole phosphorus and 0.5 mole precipitate is then formed (if (3) assumed negligible) (Jeppsson et.al, 2005).

Aluminum salts

Precipitation chemicals based on aluminum can be combined with sulfate or chloride but also consist of a mixture of these (Svenskt Vatten, 2010). The sulfate and chloride ion does not take part in the precipitation reaction, and the reaction is comparable to that of trivalent iron (Svenskt Vatten, 2010):

$$3\,Al^{3+} + 2\,PO_4^{3-} + 3\,H_2O \rightarrow (AlOH)_3(PO_4)_2 + 3\,H^+ \qquad (4)$$

$$3\,Al^{3+} + 3\,H_2O \rightarrow Al(OH)_3 + 3H^+ \qquad (5)$$

Aluminum salts work best at pH around 5.7–6.5 (Svenskt Vatten, 2010). Just as for trivalent iron 1.5 mole aluminum per mole phosphorus is required, and 0.5 mole of precipitate is then formed (if (5) assumed negligible).

Selection of precipitation chemical

Some important factors in the selection of precipitation chemical is according to Svenskt Vatten (2010):

- Chemical costs (lower for iron than aluminum)
- The character of influent wastewater (variations in flow, phosphorus, pH etc.)
- Phosphorus reduction requirements
- Precipitation method
- Chemical sludge formed

2.4.5 Precipitation chemical and formed precipitate

The concentration of precipitation chemical required to achieve a certain phosphorus reduction without overdosing is hard to predict. Jeppsson et. al. (2005) suggests that added precipitation chemical and formed precipitate, for every gram phosphorus removed, can be estimated based on the incoming and outgoing phosphate concentration in the precipitation "step":

$$q_f = K_{chemical} \cdot \left(S_{PO4}^{in} - S_{PO4}^{out}\right) \tag{6}$$

$$F_P = K_{precip} \cdot \left(S_{PO4}^{in} - S_{PO4}^{out}\right) \tag{7}$$

where

q_f is precipitation chemical [mg/l]

S_{PO4}^{out} is effluent concentration phosphate [mg/l]

S_{PO4}^{in} is influent concentration phosphate [mg/l]

$K_{chemical}$ constant for chemical required for every gram phosphorus removed [g chemical/g P]

K_{precip} constant for formed precipitate for every gram phosphorus removed [g precipitate/g P]

F_P is formed precipitate [mg/l]

2.5 BENCHMARK SIMULATION MODEL NO. 2 (BSM2)

BSM2 is a simulation environment that defines a WWTP, from influent wastewater to effluent water. BSM2 is developed by IWA Task Group on Benchmarking of Control Strategies for WWTP:s and includes primary sedimentation, biological treatment (a five compartment activated sludge reactor with primary denitrification), secondary sedimentation thickening and dewatering of sludge and anaerobic digestion (Figure 5) (Alex et al., 2008). The idea behind BSM2 is that the user should be able to test and evaluate different control strategies.

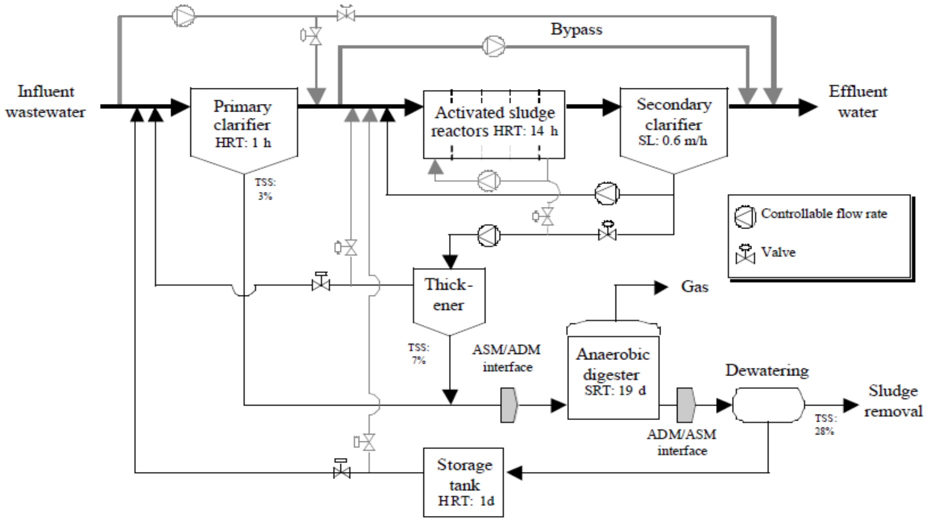


Figure 5 *General overview of Benchmark Simulation Model no. 2 (BSM2) (Alex et al., 2008).*

2.5.1 Description of BSM2

BSM2 is a Simulink (Figure 6) and Matlab based program that is built up of variables and equations formed into models describing the various processes of a WWTP. In this report, only the parts relevant to the thesis will be described. For a complete description of all models in BSM2 see the report Benchmark Simulation Model no. 2 (Alex et al., 2008).

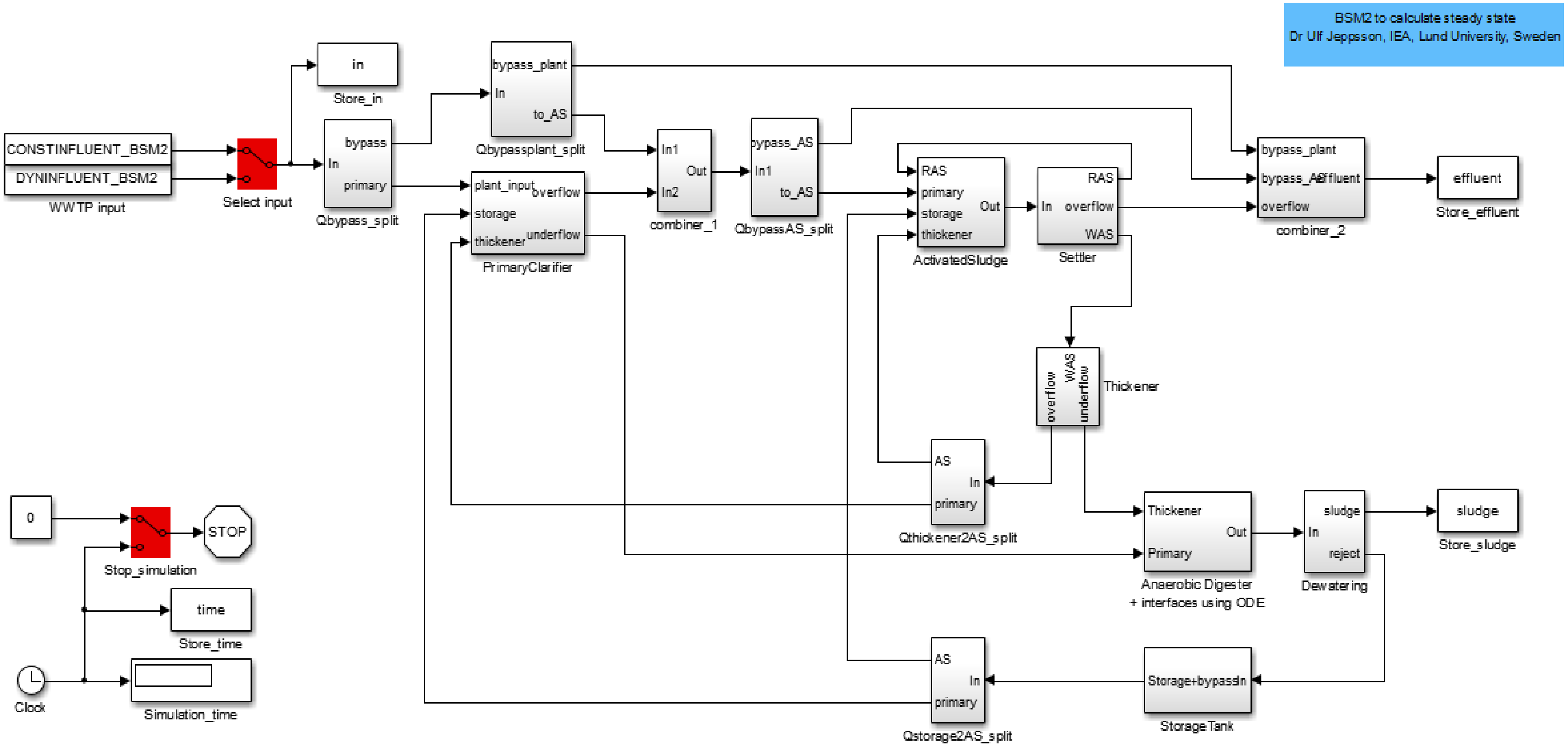

BSM2 to calculate steady state
Dr Ulf Jeppsson, IEA, Lund University, Sweden

Figure 6 *General overview of the Simulink model for BSM2. In upper left corner influent data is added and passed to primary sedimentation further to the activated sludge process and secondary sedimentation and then to effluent in upper right corner. The bottom right corner represents the anaerobic digester process and sludge disposal.*

2.5.2 File description

BSM2 is a combination of Simulink models, C-files, initialization files and influent data. The files used in this thesis are shortly presented in the four categories: Simulink models, C-files, initializations files and influent data.

- Simulink models
  - *BSM2_ss.mdl:* Simulates the WWTP in steady state using constant input data.
  - *BSM2_ol.mdl:* Simulates the WWTP in open loop using dynamic input data.
- C-files
  - *asm1_bsm2.c:* file containing the biological treatment model.
  - *primclar_bsm2.c:* file containing the primary sedimentation model.
- Initializations files
  - All parameters and variables are defined in initialization files. The files have names associated with the model they influence for example *asm1init_bsm2.m* or *primclarinit_bsm2.m*.
- Influent data
  - *constinfluent_bsm2.mat:* a constant value influent file, which represents the average vales for one full year of dynamic data.
  - *dyninfluent_bsm2.mat:* full dynamic influent data file for 609 days.

2.5.3 Input data

To understand the different components in the input files it is essential to know the differences between slowly biodegradable substrate, readily biodegradable substrate, biomass and inert material. The relation between the components is that slowly biodegradable substrate is by the hydrolysis process broken down to readily biodegradable substrate, this is in turn used by organisms to “build up” new biomass (Carlsson, 2010b). Biomass decay due to substrate shortage and produces both inert and slowly biodegradable substrate (Figure 7) (Carlsson, 2010b).

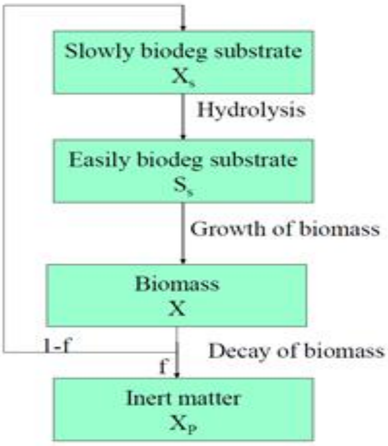
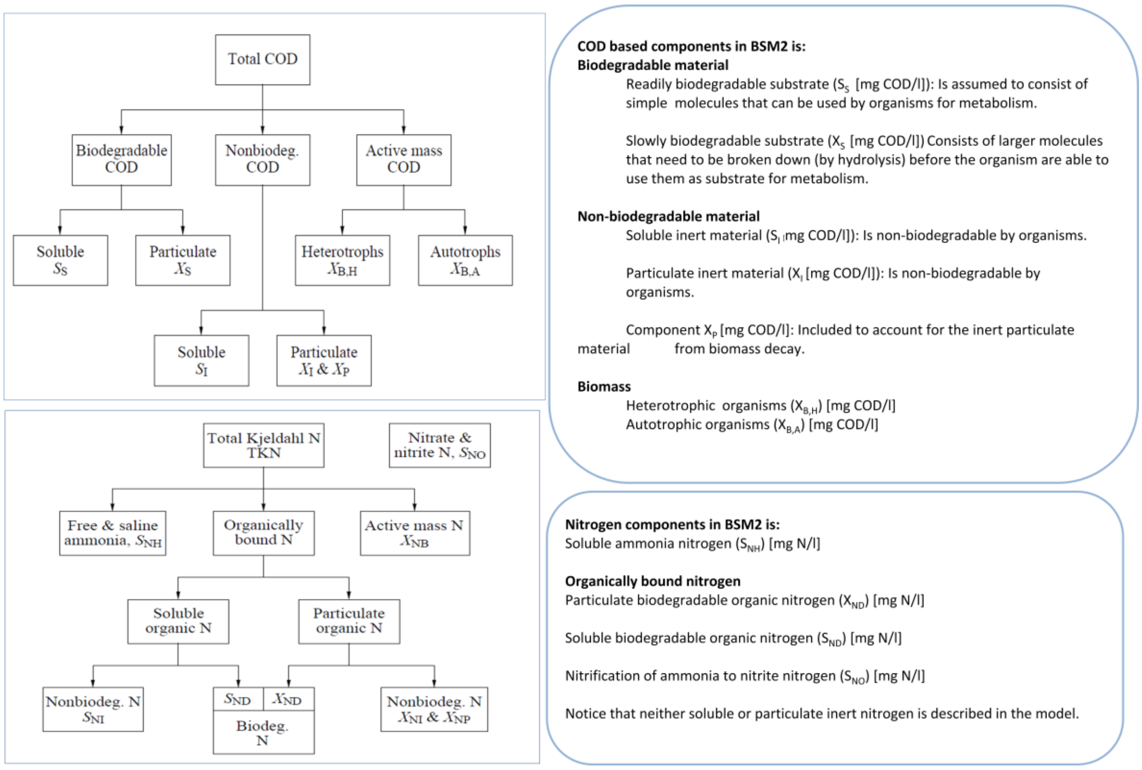


Figure 7 *The relation between slowly biodegradable substrate, readily biodegradable substrate, biomass and inert material (Carlsson, 2010b). Notice that when biomass decays, one part forms inert material and the other part slowly biodegradable substrate.*

Input data - BSM2

Input data to BSM2 consists of three different categories: COD (chemical oxygen demand) based components, nitrogen based components (Figure 8) and other (Jeppsson, 1996). The other components are: time (t) [day], temperature (T) [°C], alkalinity (alk), flow rate (Q_i) [m^3/day], dissolved oxygen concentration (So) [mg -COD/l], total suspended solids (TSS) [mg/l] and five "dummy" states which can be used for further extension of the model (Alex et al. 2008).



COD based components in BSM2 is:
Biodegradable material

Readily biodegradable substrate (S_S [mg COD/l]): Is assumed to consist of simple molecules that can be used by organisms for metabolism.

Slowly biodegradable substrate (X_S [mg COD/l]) Consists of larger molecules that need to be broken down (by hydrolysis) before the organism are able to use them as substrate for metabolism.

Non-biodegradable material

Soluble inert material (S_I mg COD/l]): Is non-biodegradable by organisms.

Particulate inert material (X_I [mg COD/l]): Is non-biodegradable by organisms.

Component X_P [mg COD/l]: Included to account for the inert particulate material from biomass decay.

Biomass

Heterotrophic organisms ($X_{B,H}$) [mg COD/l]
Autotrophic organisms ($X_{B,A}$) [mg COD/l]

Nitrogen components in BSM2 is:
Soluble ammonia nitrogen (S_{NH}) [mg N/l]

Organically bound nitrogen
Particulate biodegradable organic nitrogen (X_{ND}) [mg N/l]

Soluble biodegradable organic nitrogen (S_{ND}) [mg N/l]

Nitrification of ammonia to nitrite nitrogen (S_{NO}) [mg N/l]

Notice that neither soluble or particulate inert nitrogen is described in the model.

Figure 8 *COD and nitrogen based components in BSM2 (Jeppsson, 1996). Notice that some components is not explained in the figure, these are not a part of the BSM2 model used in this thesis.*

2.5.4 Primary sedimentation in BSM2

Primary sedimentation in BSM2 is based on a model developed by Otterpohl and Freuds (1992) and can be described by a completely mixed tank that separates influent flow (Q_{pi} [m^3/day]) to primary effluent (Q_{po} [m^3/day]) and primary sludge flow (Q_{pu} [m^3/day]) (Figure 9) (Alex et al. 2008). The effluent concentration (Z_{po} [mg/l]) and sludge concentration (Z_{pu} [mg/l]) is calculated according to (8) and (9) (Alex et al. 2008).

The most important parameter for this thesis is the tuning parameter f_{corr}, which can be modified to increase or decrease effluent concentration (Z_{po} [mg/l]) and concentration formed sludge (Z_{pu} [mg/l]) from primary sedimentation. In order to get a more detailed description of the parameters it is referred to report Benchmark Simulation Model no. 2 (Alex et al., 2008).

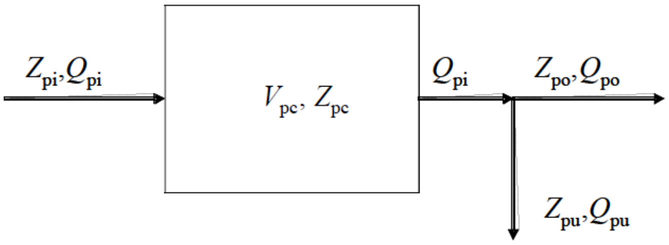


Figure 9 *General overview of primary sedimentation in BSM2, (Alex et al. 2008).*

$$Z_{po,k}(t) = f_k \cdot Z_{pi,k}(t) \tag{8}$$

$$Z_{pu,k}(t) = ((1 - f_k)\ \frac{Q_{pi}(t)}{Q_{pu}(t)} + f_k)Z_{pc,k}(t) \tag{9}$$

where

$Z_{pc,k}$ is concentration in mixing tank [mg/l]

$Z_{pi,k}$ is influent concentration to primary sedimentation [mg/l]

f_k is effluent concentration factor [-] calculated,

$$f_k = 1 - \frac{\eta_{COD,P}}{100} \cdot f_{sx,k} = 1 - \frac{\left(\frac{\eta_{COD}}{f_x}\right)}{100} \cdot f_{sx,k} \tag{10}$$

f_x is the ratio of particulate COD from total COD (mean value)

$f_{sx,k}$ is a structural factor defining the fraction of particulate matter of each fraction [-] (0 for all soluble fraction, 1 for particulate fractions except X_S)

$\eta_{COD,P}(t)$ is the COD removal efficiency (particulate) [%]

$\eta_{COD}(t)$ is the COD removal efficiency (total) [%] calculated,

$$\eta_{COD}(t) = f_{corr}(2.88 \cdot f_x - 0.118) \cdot \left(1.45 + 6.15 \cdot Ln(t_h(t) \cdot 24 \cdot 60)\right) \tag{11}$$

f_{corr} is a correction factor for removal efficiency (tuning parameter) [-]

$t_h(t)$ is the hydraulic retention time [d]

2.5.5 The active sludge process in BSM2

A model named ASM1 describes the biological treatment in BSM2. The model uses eight basic processes (12-19) to describe the complexity of the biologic behavior (Henze et. al., 2000). The growth rates in these processes are described by Monod kinetics (Henze et. al., 2000). The microorganisms are assumed to die at a certain rate and partly result in slowly biodegradable substrate and partly in non-biodegradable substrate and added to X_P (Henze et. al., 2000).

1. Aerobic growth of heterotrophic biomass, $\rho_{1,as}$ [mg/(day·l)], is given by:

$$\rho_{1,as} = \mu_{HT}\left(\frac{S_s}{K_s+S_s}\right)\left(\frac{S_O}{K_{O,H}+S_O}\right)X_{B,H} \tag{12}$$

2. Anoxic growth of heterotrophic bacteria, $\rho_{2,as}$ [mg/(day·l)], is given by:

$$\rho_{2,as} = \mu_{HT}\left(\frac{S_s}{K_s+S_s}\right)\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_g X_{B,H} \tag{13}$$

3. Aerobic growth of autotrophic bacteria, $\rho_{3,as}$ [mg/(day·l)], is given by:

$$\rho_{3,as} = \mu_{AT}\left(\frac{S_{NH}}{K_{NH}+S_{NH}}\right)\left(\frac{S_O}{K_{O,A}+S_O}\right)X_{B,A} \tag{14}$$

4. Decay of heterotrophic bacteria, $\rho_{4,as}$ [mg/(day·l)], is given by:

$$\rho_4 = b_{HT}X_{B,H} \tag{15}$$

5. Decay of autotrophic bacteria, $\rho_{5,as}$ [mg/(day·l)], is given by:

$$\rho_5 = b_{AT}X_{B,A} \tag{16}$$

6. Ammonification of soluble organic nitrogen, $\rho_{6,as}$ [mg/(day·l)], is given by:

$$\rho_6 = k_{aT}S_{ND}X_{B,H} \tag{17}$$

7. Hydrolysis of entrapped organics, $\rho_{7,as}$ [mg/(day·l)], is given by:

$$\rho_{7,as} = k_{hT}\cdot\frac{\frac{x_S}{X_{B,H}}}{K_x+\frac{x_S}{X_{B,H}}}\left[\left(\frac{S_O}{K_{O,H}+S_O}\right)+\left(\frac{K_{O,H}}{K_{O,H}+S_O}\right)\left(\frac{S_{NO}}{K_{NO}+S_{NO}}\right)\eta_h\right]X_{B,H} \tag{18}$$

8. Hydrolysis of entrapped organic nitrogen, $\rho_{8,as}$ [mg/(day·l)], is given by:

$$\rho_{8,as} = \rho_{7,as}\left(\frac{X_{ND}}{X_S}\right) \tag{19}$$

where

the symbols S_S, S_O, S_{NO}, $X_{B,H}$, S_{NH}, $X_{B,A}$, S_{ND}, X_S and X_{ND} are referred to (Figure 8)

b_{HT} is heterotrophic decay rate [1/day]

b_{AT} is autotrophic decay rate [1/day]

k_{hT} is maximum specific hydrolysis rate [g slowly biodeg. COD/g cell COD day]

k_{aT} is ammonification rate [m^3/(g COD day)]

η_g correction factors for anoxic growth of heterotrophic bacteria [-]

η_h is correction factors for anoxic hydrolysis [-]

μ_{HT} is heterotrophic maximum specific growth rate [1/day]

μ_{AT} is autotrophic maximum specific growth rate [1/day]

K_S is the half saturation constant for heterotrophs [g COD/m^3]

$K_{O,H}$ is the half saturation constant for oxygen heterotrophs [g COD/m^3]

K_{NO} is nitrate half saturation constant for denitrifying heterotrophs [g NO$_3$-N/m^3]

$K_{O,A}$ is oxygen half saturation constant for autotrophs [g O$_2$/m^3]

K_{NH} ammonia for autotrophs [g NH$_3$-N/m^3]

K_X and for hydrolysis of slowly biodegradable substrate [g slowly biodeg. COD/(g cell COD·day)]

The eight basic processes are then combined with stoichiometric coefficients according to (20) (Alex et al. 2008). This gives conversions rates (r_k) for the 13 components: S_I, S_S, X_I, X_S, $X_{B,H}$, $X_{B,A}$, X_P, S_O, S_{NO}, S_{NH}, S_{ND}, X_{ND} and S_{ALK} (the symbols are explained above in Figure 8) (Alex et al. 2008). Conversion rates for S_{ND} and X_{ND} is given in (21) and (22), the other is referred to Appendix A.

$$r_k = \sum_j \nu_{kj} \rho_{j,as} \tag{20}$$

$$r_{S_{ND}} = -\rho_{6,as} + \rho_{8,as} \tag{21}$$

$$r_{X_{ND}} = \left(i_{XB} - f_p i_{XP}\right)\rho_{4,as} + \left(i_{XB} - f_p i_{XP}\right)\rho_{5,as} - \rho_{8,as} \tag{22}$$

where

$r_{S_{ND}}$ is the conversion rate for S_{ND} [mg/(day·l)]

$r_{X_{ND}}$ is the conversion rate for X_{ND} [mg/(day·l)]

$\rho_{j,as}$ is the process j [mg/(day·l)]

ν_{kj} stoichiometric parameter

f_p fraction of biomass yielding particulate products [-]

i_{XB} is the mass N/mass COD in biomass [g N/g COD in biomass]

i_{XP} mass N/mass COD in products from biomass [g N/g COD in inert material]

2.5.6 The secondary sedimentation in BSM2

The secondary sedimentation in BSM2 allow the microorganisms and other solids to settle after the biological treatment. This sludge is partly fed back into the inlet of the primary sedimentation and partly to the anaerobic digestion process (Figure 5). The settler model using the Takács et. al. (1991) double exponential settling function, and is modeled as a 10-layers, non-reactive model and not temperature depended (Alex et al. 2008). For a more detailed description of the sedimentation model see (Takásc et. al., 1991) or (Alex et al. 2008).

2.6 AUTOMATIC CONTROL TO DOSE PRECIPITATION CHEMICAL

Dosing sufficient amount, but not overdosing, precipitation chemical to precipitate phosphate is difficult and it is usual that WWTP:s are overdosing the precipitation chemical. Overdosing of precipitation chemical leads to negative effects both for the environment and the economy, and it is therefore desirable to optimize the process. Two different control strategies that Carlsson and Hallin (2010) discusses are:

- Flow-proportional control
- Feedback control

In order to get a flow-proportional control strategy to work well, incoming phosphorus concentration to the chemical treatment must be relatively constant, which rarely is a correct assumption (Carlsson and Hallin, 2010). Allowing dosage of precipitation chemical to be controlled by a feedback of effluent phosphate, from flocculation basins or primary sedimentation, is therefore an alternative (Carlsson and Hallin, 2010).

2.6.1 PI controller

A proportional controller is usually not enough to eliminate a disturbance, therefore often a proportional integrating (PI) controller is used (Carlsson and Hallin, 2010). The controllers task is to, despite of the influence of disturbances, keep the output (y) close to the set point (r). The control signal to a PI controller is according to Carlsson and Hallin (2010):

$$u(t) = K(e(t) + \frac{1}{T_i}\int_0^t e(\tau)d\tau) \tag{23}$$

where

e is the control error, the control error describes the difference between the set-point (r) and the value the system actually keeps (y)

K is the gain (control parameter)

T_i is the integral time (control parameter)

u is the control signal

To verify the controller a step response experiment is often used, thus the set point (r) is changed from one level to another and the response in the output (y) is studied (Carlsson and Hallin, 2010). If the output adjusts to the new set point in a reasonable time it is assumed that also disturbances in the process quickly can be controlled.

2.6.2 The Lambda method

One method to set the control parameters (K and T_i) is the lambda method. The method is outlined in Carlsson and Hallin (2010) described in four steps (1-4 below).

1. Use a step response for the control signal and note the amplitude for the step (Δu).

2. Measure the step response in the output, and decide how much the output has increased (Δy). Note possible dead time (L) and the time (T) it takes for the output signal to reach 63% of the final value (Figure 10). Then calculate the gain,

$$K_S = \frac{\Delta y}{\Delta u} \tag{24}$$

3. Chose lambda (λ) according to,

$$\lambda = p \cdot T \tag{25}$$

   where p is a user selection, a larger p gives a slower but "safer" control. Typically p is chosen between 2 and 3.

4. Given the values on T and K_s the control parameters is calculated according to,

$$\left.\begin{aligned} K &= \frac{T}{K_S(\lambda+L)} \\ T_i &= T \end{aligned}\right\} \tag{26}$$

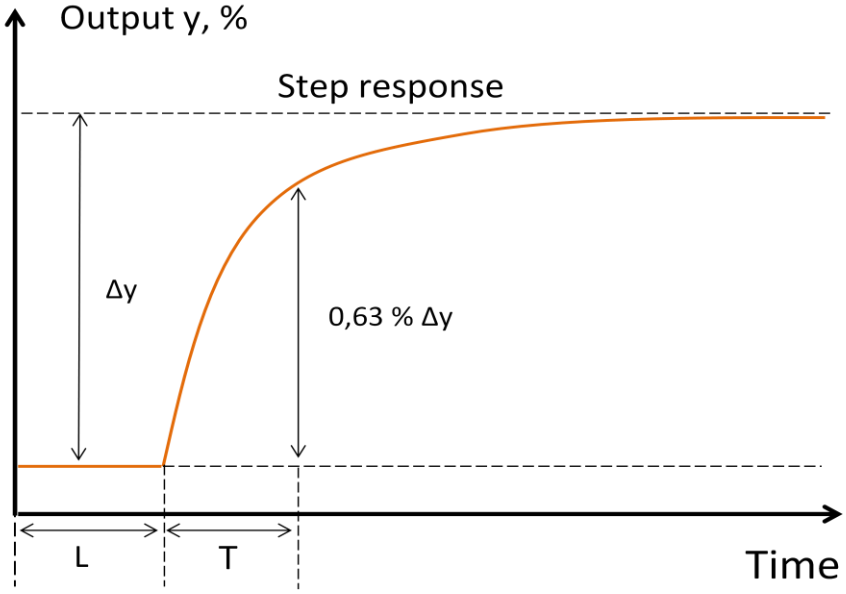


Figure 10 *Step response that shows the variables for the lambda method.*

3. METHOD

After some simplifications assumptions phosphorus and chemical precipitation were included in BSM2. The method used can shortly be described:

- Precipitation method
- Precipitation chemical
- Input data (include phosphorus)
- Control strategy
- Precipitation module
- Primary sedimentation (include phosphorus)
- Activated sludge process (include phosphorus)

All the steps (above) are described in the different sections below.

3.1 PRECIPITATION METHOD

As BSM2 includes both primary and secondary sedimentation combined with biological treatment, primary precipitation was chosen to be included in BSM2.

To include primary precipitation a precipitation module was placed directly before primary sedimentation in the Simulink model (Figure 11).

3.2 PRECIPITATION CHEMICAL

The precipitation chemicals included were:

- Trivalent iron: Iron chloride ($FeCl_3$) and iron sulfate ($AlSO_4^{2-}$)
- Aluminum: Aluminum chloride ($AlCl_3$) and aluminum sulfate ($AlSO_4^{2-}$)

According to the theory (section 2.4.4) 1.5 mole metal per mole phosphorus reduced was required. This means that 1.3 gram aluminum and 2.7 gram iron were required, per gram phosphorus reduced (this was accomplished by mass calculations). The values for both the metals (Fe and Al) and the metal salts are found in (Table 1), mass calculations in Appendix B. The constants were then used in the precipitation module (section 3.5).

In the thesis the precipitation metal iron (Table 1) was used for evaluating the model.

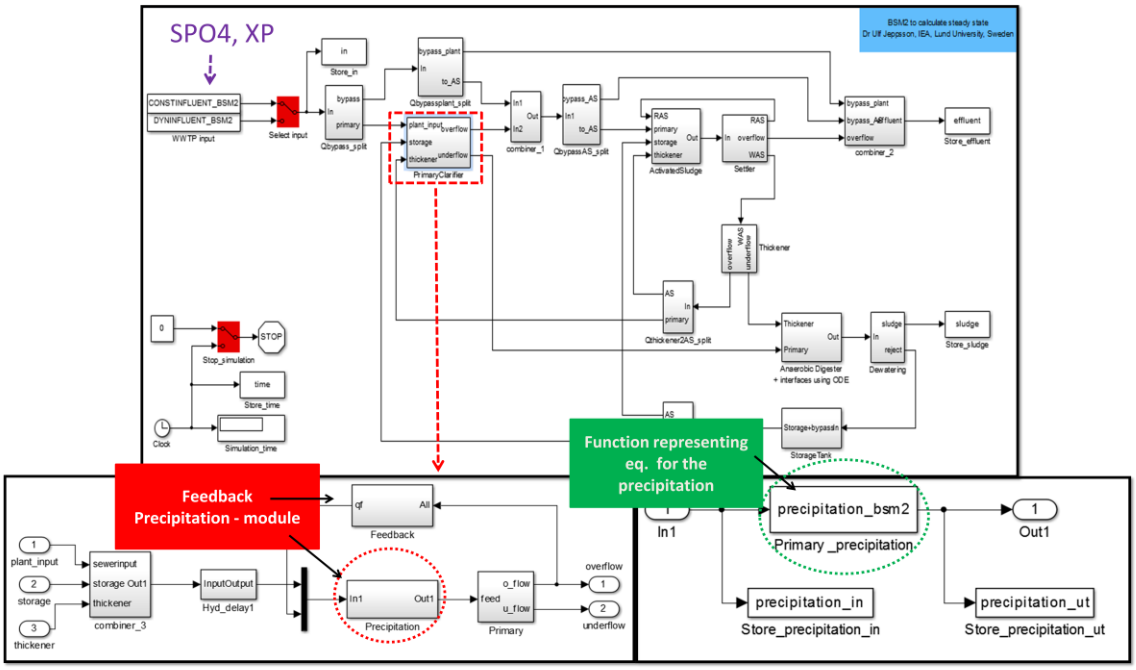


Figure 11 *Primary sedimentation is the red rectangle in upper picture. The precipitation module, red circle in lower left corner, is placed right before the sub-system for primary sedimentation. The sub-system for the precipitation module is shown in the lower right corner, green circle. Notice the sub-system Feedback in bottom left picture where the controller later was built up.*

Table 1 *Precipitation chemical required for each gram (g) phosphorus (P) reduced ($K_{chemical}$) and precipitate formed for each gram phosphorus reduced (K_{precip}).*

Precipitation chemical	K_{precip}	$K_{chemical}$
Precipitation metal		
Iron (Fe) [g Fe/g P]	6.6	2.7
Aluminum (Al) [g Al/g P]	5.2	1.3
Metal salt		
Iron(III)chloride ($FeCl_3$) [g $FeCl_3$/g P]	6.6	7.9
Iron(III)sulfate ($Fe_2(SO_4)_3$) [g $Fe_2(SO_4)_3$/g P]	6.6	19.4
Iron(II)sulfate ($Fe(SO_4)$) [g $Fe(SO_4)$/g P]	5.8	7.4
Aluminum chloride ($AlCl_3$) [g $AlCl_3$/g P]	5.2	6.5
Aluminum sulfate ($Al_2(SO_4)_3$) g $Al_2(SO_4)_3$/g P]	5.2	16.4

3.3 PHOSPHORUS IN INFLUENT DATA

Phosphorus was in the precipitation model chosen to be represented by two fractions, and for simplicity chosen to be independent of pH. The two chosen fractions were:

- Dissolved phosphate (S_{PO4})
- Particulate phosphorus (X_{PP})

As provided data from Henriksdals WWTP were measurements of total phosphorus and phosphate concentration, the variable S_{PO4} is assumed to represent all soluble fractions of phosphate and X_{PP} to represent the total sum of particulate phosphorus ($X_{PP} = TOT\text{-}P - S_{PO4}$). Of the five “dummy” variables available in BSM2 for further extension, one and five have been chosen to represent S_{PO4} respective X_{PP}.

For steady-state simulations the file for constant input (*constinfluens_bsm2.mat*) was updated to include averages of S_{PO4} and X_{PP}. Data represent averages from measurements of incoming water to Henriksdals WWTP. The value were set to 2.82 and 7.85 mg/l for S_{PO4} respective X_{PP}. Measured data are shown in Appendix C.

For open-loop simulations the file for dynamic input (*dyninfluent_bsm2.mat*) was updated to include values from measurements of incoming water to Henriksdals WWTP. As the data only measured every half hour for five days, and the dynamic input format in BSM2 required 609 days (15 min samples) the data first was interpolated between values and then repeated. Measured data are shown in Appendix C.

3.4 CONTROL STRATEGY

A feedback of effluent phosphate from primary sedimentation was chosen as control strategy. This was done to control added precipitation chemical and keep the effluent phosphorus level close to the set point (r) (Figure 12). As set point an average value of effluent phosphate from primary sedimentation was used, based on data from Henriksdals WWTP. Measured data are shown in Appendix C and the value were rounded and set to 0.40 mg/l.

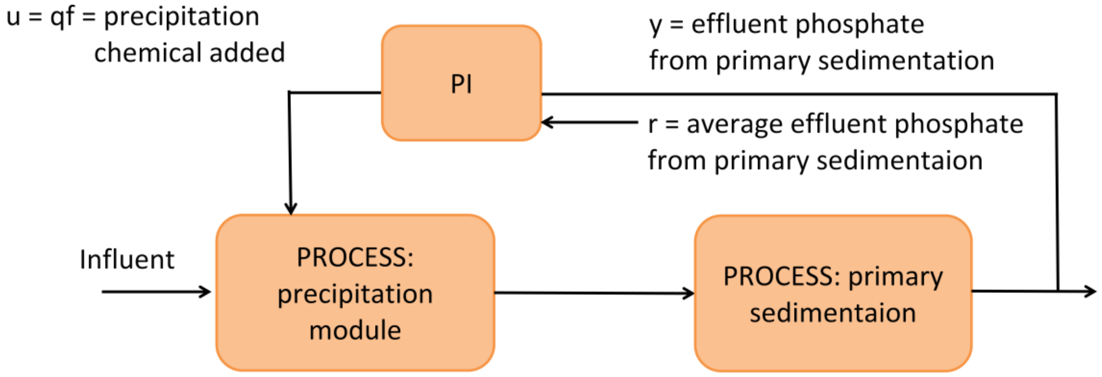


Figure 12 *General overview of the feedback control strategy.*

3.4.1 PI controller in Simulink

Dosage of precipitation chemical was controlled with the help of a PI controller. The controller was built up in Simulink (Figure 13) and uses eq. (23) as control signal. Tuning a PI controller can be tricky, one must choose control parameters that gives a reasonable fast system but not too sensitive to noise. The controller was tuned with the lambda method (section 2.6.2) and the control parameters were calculated according to eq. (26). Different control parameters were tested in the model, with p in eq. (25) set to 1, 2 and 3 (Table 2).

***Table 2** Control parameters for the PI controller.*

Control parameter	p = 1	p = 2	p = 3
T_i	0.01	0.01	0.01
K	-2.80	-1.40	-0.93

3.4.2 Saturation limits and anti-windup

To prevent that the control signal saturates, and the integral part of the controller continues to grow (Carlsson and Hallin, 2010), restrictions on the control signal were included. Saturation limits represents the minimum and maximum concentrations of precipitation chemical allowed to dose and were in the model chosen according to (Table 3).

***Table 3** Saturation parameters for the PI controller.*

Chemical	Min	Max	Comment
Iron (Fe^{3+})	0	30	Normally 10-15 mg Fe/l wastewater is required, when primary precipitation is used (Svenskt Vatten, 2010).
Aluminum (Al^{3+})	0	30	Normally 10-12 mg Al/l wastewater is required, when primary precipitation is used (Svenskt Vatten, 2010).

Anti-windup was included in the controller, in order to prevent the integrator controller part from growing large and cause overshoot. An important property of anti-windup compensation is that it leaves the loop unaffected as long as saturation does not occur (Åström and Rundqwist, 1989). Anti-windup in the model is thereby only used if the saturation limits of dosed precipitation chemical are reached. Saturation limits (Table 3) were in the model chosen to have a quite wide range, which the control signal is expected to work within and anti-windup thereby not used. Anti-windup had one control parameter, T_t, this could according to Åström and Rundqwist (1989) be calculated as:

$$T_t = 0.8 \cdot T_i \tag{27}$$

and was in the model set to 0.008.

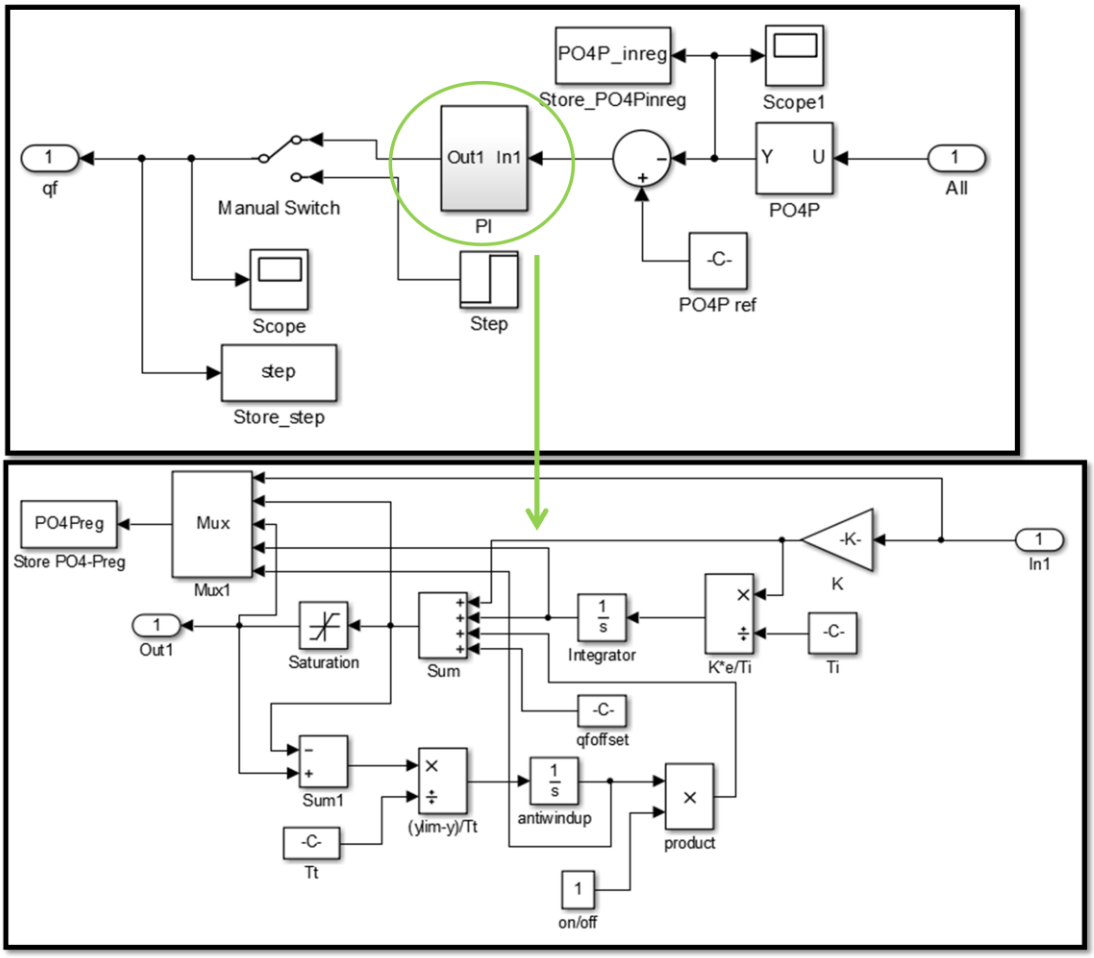


Figure 13 *General overview of the PI controller in Simulink. Top picture: The sub-system for the Feedback in (Figure 11). Set-point is PO4P_ref and the feedback variable is referred to as PO4P. Bottom picture: The actual controller, the control parameters are K and* T_i*. The parameter* T_t *is the control parameter for the anti-windup. Also notice the saturation function which is used to set a minimum and maximum to the dosage of the precipitation chemical. The constant on/off is set to one which means that anti-windup is activated in the controller.*

3.5 PRECIPITATION MODULE

The behavior of the precipitation module is presented in the following three steps.

1. *Calculate effluent phosphate due to added precipitation chemical:* Effluent phosphate in the precipitation module was calculated based on eq. (6). As the output from the PI-controller is added precipitation chemical (q_f) the effluent phosphate (S_{PO4}^{out}) was calculated according to

$$S_{PO4}^{out} = S_{PO4}^{in} - \frac{q_f}{K_{chemical}} \tag{28}$$

$K_{chemical}$ is required precipitation chemical to reduce one gram phosphorus (Table 1)

The reduction in phosphate could then simply be calculated by subtracting the effluent phosphate from influent.

2. *Calculate formed precipitate:* Formed precipitate (F_P) was calculated according to eq. (7),

$$F_P = K_{precip} \cdot (S_{PO4}^{in} - S_{PO4}^{ut})$$

K_{precip} is the formed precipitate from one gram phosphorus reduced (Table 1)

3. *Distribute the fractions in effluent from the precipitation module in a way compatible with BSM2:* The fractions from the precipitation module were distributed according to (Table 4).

Table 4 *Distribution of effluent fractions involved in the chemical precipitation process.*

Fraction	Effluent	Comment
S_{PO4}^{out}	Eq. (28)	
$X_{PP,Tot}^{out}$	$X_{PP,Tot}^{out} = X_{PP}^{in} + \left(S_{PO4}^{in} - S_{PO4}^{ut}\right)$	Removed phosphate is assumed to form particulate phosphorus and settle.
$Chemical\ Sludge$	$C_{sludge} = K_{precip} \cdot (S_{PO4}^{in} - S_{PO4}^{ut}) + q_f$	Formed precipitate and added precipitation chemical were assumed to form chemical sludge and then in the primary sedimentation settle ideally.

As pointed out in the theory section microorganisms in the biological treatment use substrate for growth, one essential nutrient is phosphorus (Svenskt Vatten, 2010). When using primary precipitation it is thereby desirable not to precipitate all phosphorus before the biological step. As the set point (r) in the PI controller was set to the average effluent value from primary sedimentation, and the ASP at Henriksdals WWTP performed well during the measuring period (Rahmberg, 2013), this was in the model assumed to be enough phosphorus for the microorganisms.

3.5.1 The function precipitation_bsm2.c

The equations and variables the precipitation module uses to calculate effluent phosphate (S_{PO4}), formed precipitate and particulate phosphorus (X_{PP}) is defined in the function *precipitation_bsm2.c* and the initialization file *precipitaioninit_bsm2.m*. The codes for these two are given in Appendix D.

3.6 PRIMARY SEDIMENTATION IN BSM2

S_{PO4} and X_{PP} were included in primary sedimentation and affected by same equation as the other soluble and particulate variables in BSM2. Influent S_{PO4} and X_{PP} will thereby be divided between effluent and formed sludge concentration. To include the factor that particulate material settles better when a precipitation chemical was added (Carlsson and Hallin, 2010) the parameter f_{corr} was changed to the higher value 0.70 (default value 0.65). This leads to that a larger part of particulate material forms primary sludge and a minor part follows the flow to the ASP. Also a "new" variable, f_{corr2}, was added, this to be able to adjust effluent particulate phosphorus from the primary sedimentation, without affecting other particulate material. The f_{corr2} variable thereby only affects X_{PP} and was set to 0.85.

Formed precipitate and added precipitation chemical were in the precipitation module assumed to form chemical sludge and to settle ideally. To fulfill this also f_{corr3} was added and set to one. f_{corr3} only affects formed chemical sludge.

3.7 THE ACTIVATED SLUDGE MODEL IN BSM2

To include phosphorus in the biological process it was assumed that none of the influent phosphorus, soluble or particulate, is non-biodegradable (inert) material. But, that all is biodegradable, and available for microbial growth. Then a Monod function for phosphate,

$$\left(\frac{S_{PO4}}{K_{PO4}+S_{PO4}}\right) \tag{29}$$

was used and allowed to affect the processes 1,2 and 3 in BSM2:

- Aerobic growth of heterotrophic biomass
- Anoxic growth of heterotrophic bacteria
- Aerobic growth of autotrophic bacteria

The half-saturation constant for phosphate (K_{PO4}) was set to 0.05 [mg P/l] (Jeppsson et. el. 2005).

Therefore, the biodegradable phosphorus was assumed to consist of both readily and slowly biodegradable material. To take into account that complex molecules are broken down, a hydrolysis process for phosphorus was included. A hydrolysis process for the particulate phosphorus could according to Jeppsson et. al. (2005) look like (30) and this was also used in the model.

$$\rho_{9,as} = \rho_{7,as} \cdot \left(\frac{P_{part_{bio}}}{X_S}\right) \tag{30}$$

where
$\rho_{9,as}$ is the hydrolysis process
$\rho_{7,as}$ is the hydrolysis of entrapped organic in ASM1
$P_{part_{bio}}$ is assumed to be the biodegradable part calculated,

$$P_{part_{bio}} = \frac{(X_{PP} \cdot X_S)}{(X_S+X_{B,H}+X_{B,A})+(X_I+X_P)} \tag{31}$$

The expression,

$$\rho_{9,as} = \rho_{7,as} \cdot \left(\frac{X_{PP}}{X_S}\right) \tag{32}$$

was also tested as hydrolysis process.

3.7.1 Conversion rates

Conversion rates (r_k) for S_{PO4} and X_{PP} were then added to the model. It is important to remember that this is not a proper solution of how phosphorus behaves in the biological process, but only a solution to keep the model simple in order to simulate the total phosphorus effluent from the ASP. Two different methods were tested:

1. Based on conversion rates (r_k) for to soluble (S_{ND}) and particulate biodegradable nitrogen (X_{ND})used in ASM1, which gave

$$r_{S_{PO4}} = -\rho_{10,as} + \rho_{9,as} \tag{33}$$

$$\rho_{10} = k_{pp} S_{PO4} X_{B,H} \tag{34}$$

$$r_{X_{PP}} = \left(i_{XBP} - f_p i_{XEP}\right)\rho_{4,as} + \left(i_{XBP} - f_p i_{XEP}\right)\rho_{5,as} - \rho_{9,as} \tag{35}$$

where

ρ is the process (see section 2.5.5)

S_{PO4} is influent S_{PO4}

k_{pp} is a constant used for phosphate in the biological process, in the model set to same value as k_{aT} (Appendix E)

i_{XBP} is mass P/mass COD in biomass [mass P/mass COD in biomass]

f_p is the fraction of biomass that ends up as inert material [-]

i_{XEP} is mass P/mass COD in inert material [mass P/mass COD in inert material]

2. Based on equations from the report The URWARE Wastewater Treatment Plant Models (Jeppsson et. al., 2005):

$$r_{PO4} = -i_{XBP}\left(\rho_{1,as} + \rho_{2,as} + \rho_{3,as}\right) + \rho_{9,as} \tag{36}$$

$$r_{X_{PP}} = \left(i_{XBP} - f_p i_{XEP}\right)\rho_{4,as} + \left(i_{XBP} - f_p i_{XEP}\right)\rho_{5,as} - \rho_{9,as} \tag{37}$$

Method one was later chosen. This as it gave more realistic results for the fractions S_{PO4} and X_{PP} effluent from the biological treatment, for the given input data from Henriksdals WWTP. For the parameters i_{XBP}, i_{XEP} and f_p Jeppsson et. al. (2005) suggests the values 0.02, 0.01 and 0.08.

The parameters in ASM1 vary in different WWTP and they largely affect the behavior of the biological process. A thesis to calibrate ASM1 to Henriksdals WWTP was in 2005 done at IVL. The values in the thesis (from 2005) that differ from the default values in ASM1 were in this thesis used to adjust the parameters in ASM1. The thesis (from 2005) also pointed out that some of the parameters in the secondary sedimentation were changed. The parameters and final values can be seen in Appendix E.

3.7.2 Mass balance in ASM1

To check if the mass balance in ASM1 was met the total in- and outgoing phosphorus from one of the five reactors in ASM1 were examined. The principal used to check the mass-balance for phosphorus was:

$$P_{TOT} = S_{PO4} + X_{PP} + i_{XBP}\left(X_{B,H} + X_{B,A}\right) + i_{XEP} \cdot X_P \tag{38}$$

3.8 OTHER CHANGES IN BSM2

Other changes and assumptions, for this thesis, in BSM2 are briefly described below.

- The actual models in BSM2 are all written in C-code and thereby must be compiled before used in Matlab. The models use Simulink's C-mex principles and S-function capability and BSM2 includes an overall mex-file, *mexall_bsm2.m*, which unpacks "*mexes*" all functions files. In this *precipitation_bsm2.c* was included.
- All initialization files in BSM2 are called from a main initialization script *init_bsm2.m*. In this script the initialization routine *precipitationinit_bsm2.m* was added.
- All initializing files are assigned initialize values for the fractions of phosphorus, the initial values were received from an open-loop simulation with constant influent data.
- Secondary sedimentation after the ASP is not changed (except for the values in Appendix E), and thereby S_{PO4} and X_{PP} are here assumed to settle as other soluble and particulate material in BSM2.
- S_{PO4} and X_{PP} that settle in primary and secondary sedimentation will be fed to the anaerobic digestion process. As anaerobic digestion not is a part in the thesis the fraction of phosphorus is just allowed to pass through the process.
- In order to not get chemical sludge fed back to primary sedimentation, the return flow of this component was set to zero in the interface to the anaerobic digestion process.

4. RESULTS

The results are divided into two sections, these are: steady state and dynamic/open loop simulations. In all results presented, trivalent iron was used as precipitation chemical and unless otherwise stated the parameters used were the ones in Table 1, 2, 3, 1-E and section 3.6 and 3.7.

Notice that in all results (except for section 4.1.4) the total phosphorus is the sum of the fractions soluble and particulate phosphorus (S_{PO4} respective X_{PP}). Also notice that when the TSS concentration in a simulation in BSM2 exceeds 10 mg/l the effluent total particulate phosphorus should result in a concentration of 0.1-0.2 mg/l particulate phosphor (Jeppsson, 2013). As the total phosphorus in the results is the sum of the fractions soluble and particulate phosphorus (S_{PO4} respective X_{PP}) the particulate fraction phosphorus due to the TSS in the wastewater is in this thesis not taken into consideration.

4.1 STEADY STATE SIMULATION

4.1.1 Precipitation

A steady state simulation with control parameters for p=2 (Table 2) showed that the controller dosed precipitation chemical, 6.39 mg/l, and that the effluent phosphate (S_{PO4}) from primary sedimentation was then reduced to the set-point, 0.40 mg/l. The precipitated phosphate, 2.37 mg/l, was added to the particulate phosphorus (X_{PP}) (Table 5). Note also the formed chemical sludge effluent from the precipitation, this fraction was in the primary sedimentation assumed to settle ideally.

4.1.2 Primary sedimentation

In primary sedimentation the particulate material was reduced, partly due to the parameters f_{corr} and f_{corr2}. Particulate phosphorus was in the steady state simulation reduced to 3.86 mg/l. The high concentration primary sludge produced from particulate material is due to that underflow from the primary sedimentation is much lower (than effluent and influent flow), while the particles accumulate (settling).

To demonstrate the effects of f_{corr} and f_{corr2}, a simulation with the parameter f_{corr} changed from 0.70 to 0.65 and f_{corr2} from 0.85 to 0.65 was run. As expected the settling ability for particulate material was reduced and less sludge formed, compare (Table 5 and 6).

4.1.3 Biological treatment and secondary sedimentation

After the biological process and secondary sedimentation S_{PO4} and X_{PP} were reduced to 0.23 and 0.21 mg/l, respectively. And the total effluent phosphorus (TOT-P) from the secondary sedimentation was thereby 0.44 mg/l (Table 5). The reduction is in theory due to that the microorganisms use substrate (phosphorus) for metabolism.

Table 5 *Results from the Steady state simulation.* f_{corr} *set to 0.70 and* f_{corr2} *set to 0.85.*

	S_{PO4} [mg/l]	X_{PP} [mg/l]	TOT-P [mg/l]	q_f [mg/l]	F_P [mg/l]	C_{sludge} [mg/l]
Influent	2.82	7.85	10.7	-	-	-
Precipitation influent	2.77	7.90	10.7	6.39	-	-
Precipitation effluent	0.40	10.3	10.7	-	15.6	22.0
Primary effluent	0.40	3.86	4.26	-	-	-
Primary underflow	0.40	919	919	-	-	2312
Secondary effluent	0.23	0.21	0.44	-	-	-
Secondary underflow	0.23	144	144	-	-	-

Table 6 *Steady state simulation with parameters* f_{corr} *and* f_{corr2} *set to 0.65.*

	S_{PO4} [mg/l]	X_{PP} [mg/l]	TOT-P [mg/l]
Primary effluent	0.40	5.36	5.76
Primary underflow	0.40	705	705

4.1.4 Mass balance calculation

The mass balance was calculated in reactor four in ASM1, based on the last point in a steady-state simulation. The difference in in-and outgoing total phosphorus was 0.05 mg P/l (Table 7), which was considered as a acceptable small difference. That the mass balance calculation does not quit fit is probably due to the numerical approximations made in BSM2.

Table 7 *The mass balance calculation for reactor four in ASM1.*

	Influent reactor 4 [mg P/l]	Effluent reactor 4 [mg P/l]	Difference [mg P/l]
Acc. to eq. (38)	151.26	151.21	0.05

4.2 OPEN LOOP/DYNAMIC SIMULATION

The results for S_{PO4}, X_{PP} and total phosphorus (TOT-P) in the dynamic simulation is presented separately in the sections 4.3.2, 4.3.3 and 4.3.4. In section 4.3.5 the underflow from primary and secondary sedimentation are shown and section 4.3.6 shows the results from both the steady state and dynamic simulation with the hydrolysis process according to eq. (32). Finally a short summary is presented. First the results from the PI controller are presented.

4.2.1 Control of effluent phosphate

A dynamic simulation with control parameters for p=2 (Table 2), showed that the effluent S_{PO4} varied between about 0.10-0.80 mg/l, and fluctuated around the set-point 0.40 mg/l (Figure 14). Added precipitation chemical (q_f) in the simulation varied between approximately 5-10 mg/l.

If p was selected lower (p=1) the fluctuations in q_f increased while the variation in effluent phosphate decreased and vice versa if p was selected higher (p=3) (Figure 15). Control parameters for p=2 were thereafter chosen.

A simulation with a step as set-point, from 0.80 to 0.40 mg/l, showed that the controller was able to keep the effluent phosphate close to the set-point quite well (Figure 16).

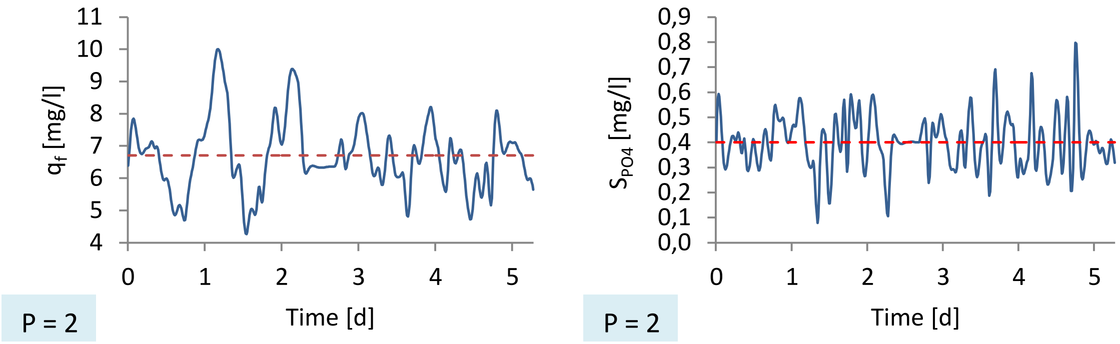


Figure 14 *Left picture: Dosed precipitation chemical to control the effluent phosphate from primary sedimentation. Right picture: Effluent phosphate from primary sedimentation. The red line represent the average value of* q_f *respective* S_{PO4}.

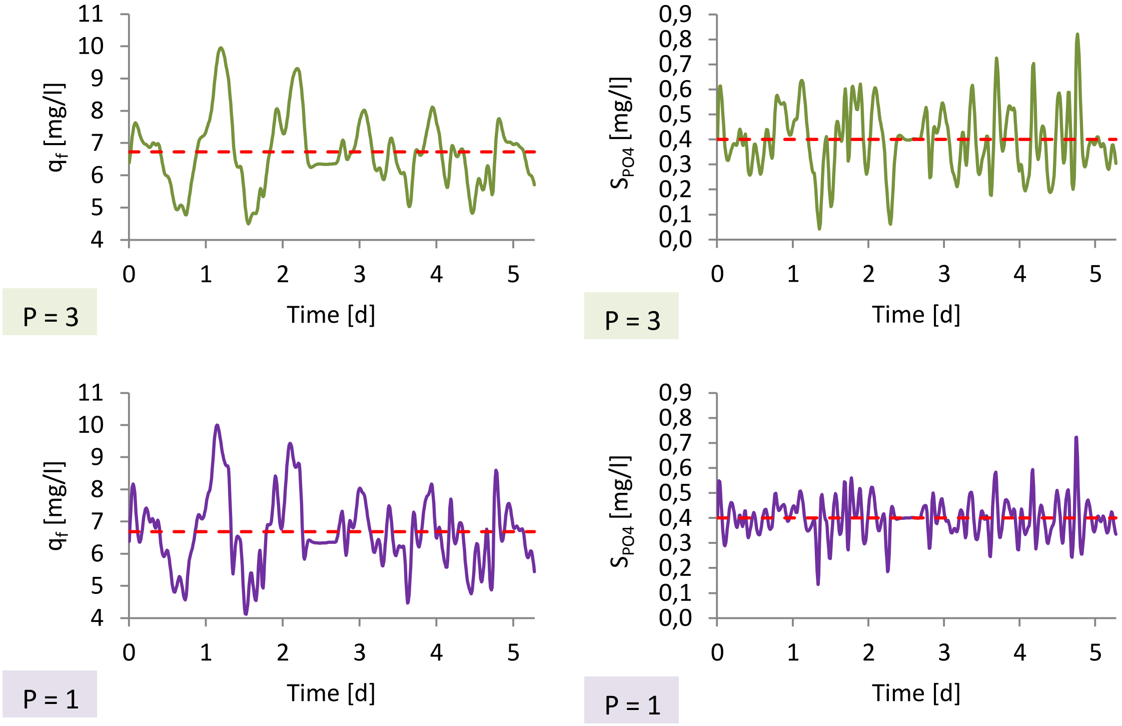


Figure 15 *Left picture: Dosed precipitation chemical in order to control the effluent phosphate from primary sedimentation. Right picture: Effluent phosphate from primary sedimentation. The red line represent the average value of* q_f *respective* S_{PO4}.

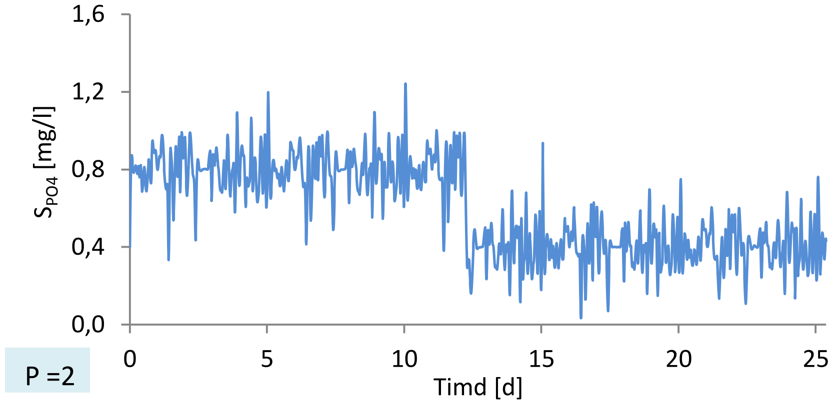


Figure 16 *Simulation with a step as set-point from 0.8 to 0.4 mg/l. The step was taken at 12.5 d.*

4.2.2 Dynamic simulation - phosphate (S_{PO4})

Influent phosphate to BSM2 varied in-between approximately 1.48 and 4.10 mg/l (Figure 17). The dynamic simulation showed that the controller dosed precipitation chemical in the range between about 5-10 mg/l and that the effluent phosphate (S_{PO4}) from primary sedimentation was then reduced from approximately 2.82 mg/l (average influent value of S_{PO4}) to the set-point 0.40 mg/l (Figure 17). In the biological process and secondary sedimentation, S_{PO4} was reduced additionally (Figure 17). Dosed precipitation chemical (q_f) and formed precipitate (F_P) effluent from the precipitation can be seen in (Figure 18).

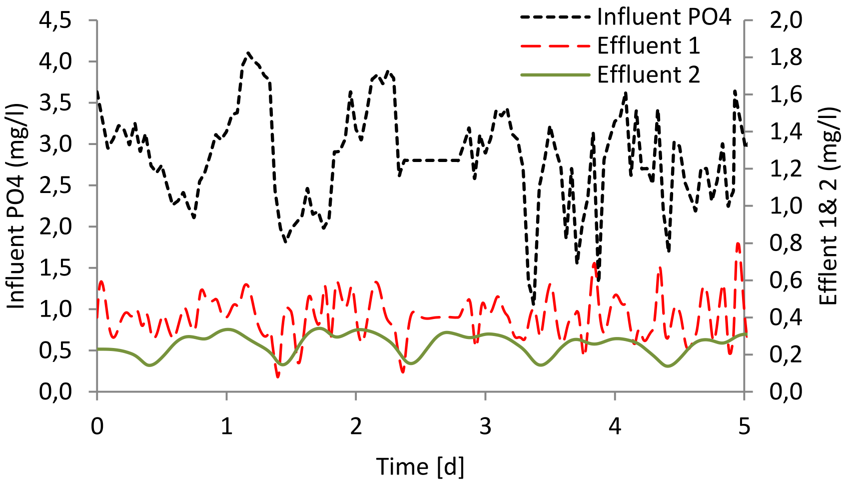


Figure 17 *S_{PO4} in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

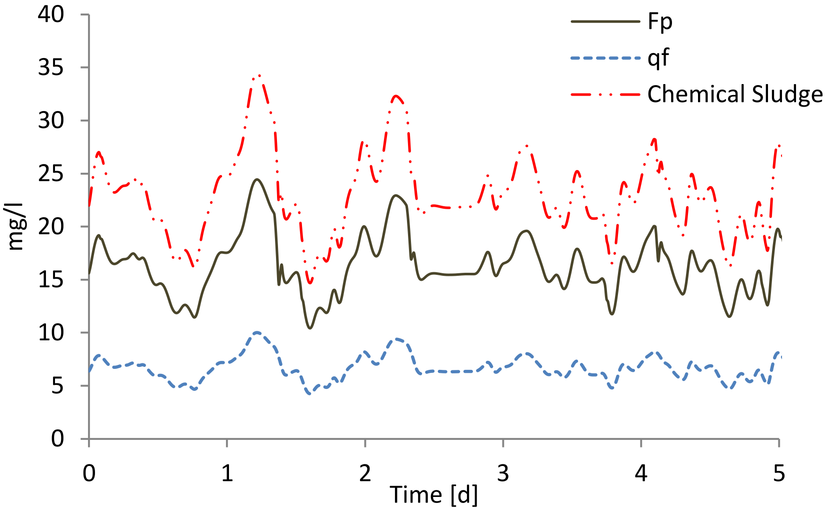


Figure 18 *Dosed precipitation chemical (q_f) and effluent precipitate (F_P) from the precipitation module. The red line, chemical sludge, represents in the model the sum of these two fractions.*

4.2.3 Dynamic simulation - particulate phosphorus (X_{PP})

Influent particulate phosphorus varied in-between approximately 2 and 22 mg/l. The primary sedimentation then reduces X_{PP} and the result can be seen in the effluent 1 graph in (Figure 19). In the biological process and secondary sedimentation X_{PP} was reduced further (Figure 19).

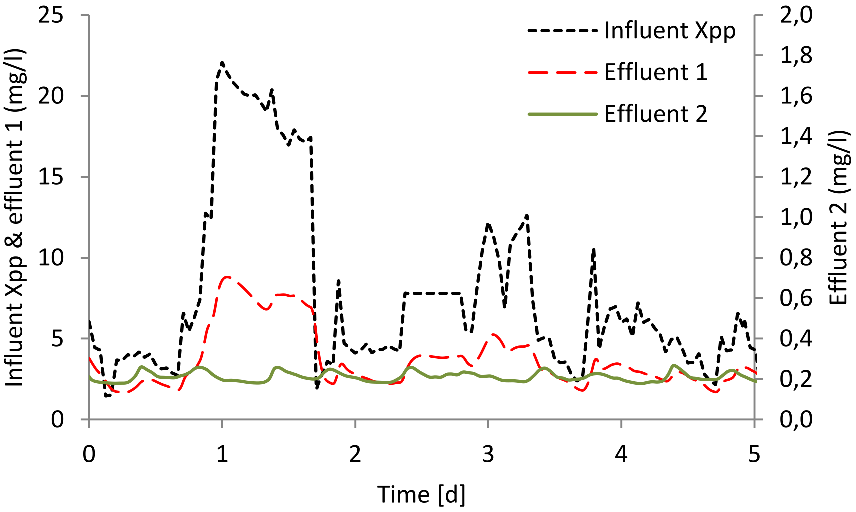


Figure 19 *X_{PP} in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

4.2.4 Dynamic simulation - total phosphorus

A graph to describe,

- TOT-P influent
- TOT-P effluent from primary sedimentation (effluent 1)
- TOT-P effluent from the settler (effluent 2)

is provided in (Figure 20).

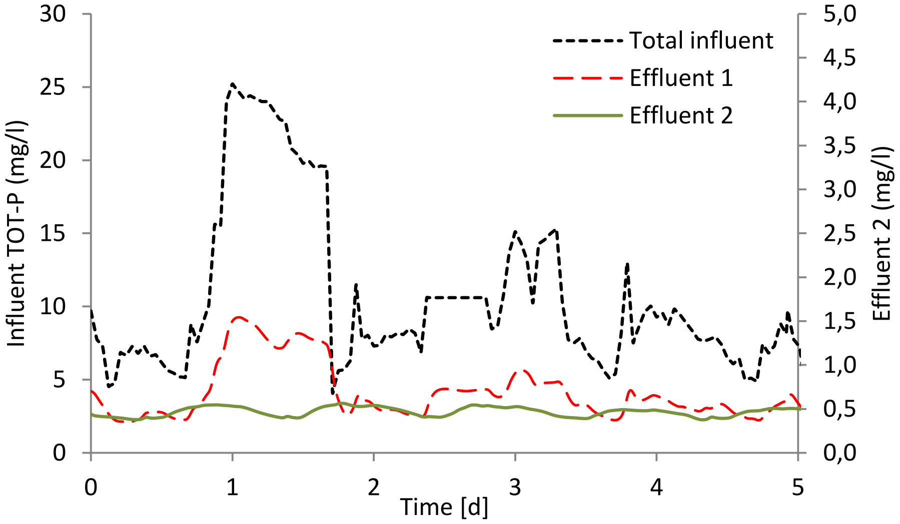


Figure 20 *Total phosphorus in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

4.2.5 Dynamic simulation - formed sludge (underflow)

Formed sludge from primary and secondary sedimentation (primary sludge and biological sludge), can be seen in (Figure 21), chemical sludge from primary sedimentation in (Figure 22).

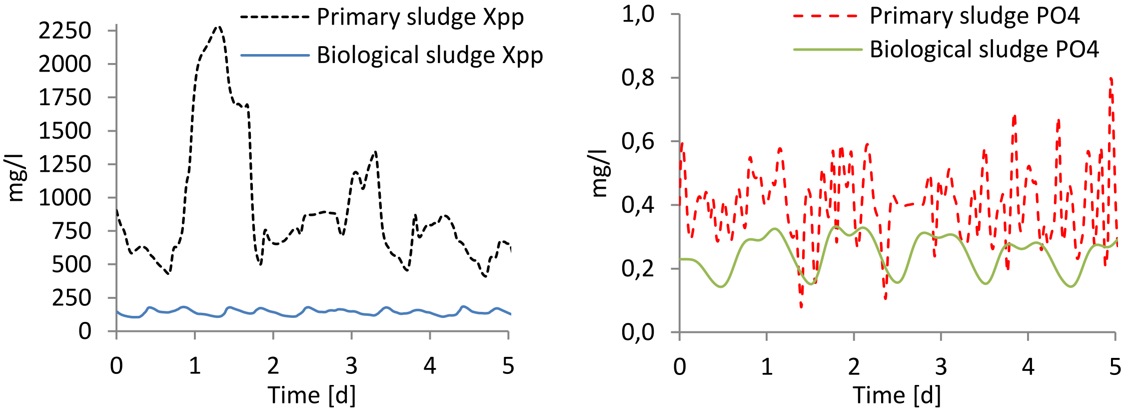


Figure 21 *Underflow (formed sludge) from primary and secondary sedimentation in the dynamic simulation in BSM2.*

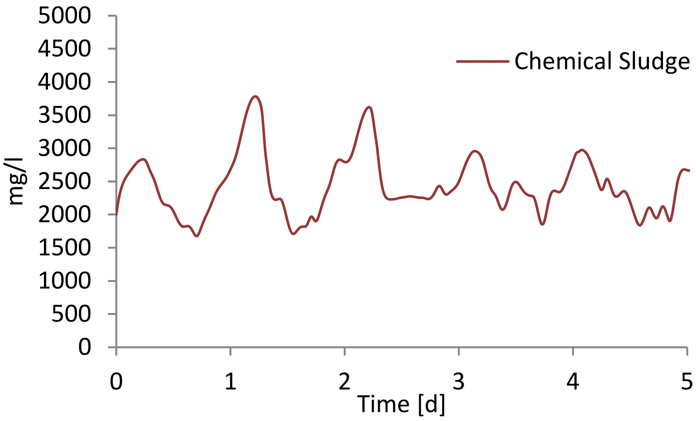


Figure 22 *Chemical sludge formed from precipitate and precipitation chemical added.*

4.2.6 Dynamic and steady state simulation - the hydrolysis process

The simulation with the hydrolysis process according to eq. (32) showed essentially the same results as seen above. The exceptions were that effluent phosphate from secondary sedimentation was in the steady state simulation increased from 0.23 to 0.37 mg/l and that the effluent particulate fraction was approximately zero (Table 8). The dynamic simulation for phosphate, particulate phosphorus and total phosphorus showed the same behavior (Figure 23, 24 and 25).

Table 8 *Results from the steady state simulation.*

	S_{PO4} [mg/l]	**X_{PP} [mg/l]**	**Total P [mg/l]**	**q_f [mg/l]**	**F_P [mg/l]**	**C_{sludge} [mg/l]**
Influent	2.82	7.85	10.7			
Precipitation influent	2.77	7.81	10.6	6.40		
Precipitation effluent	0.40	10.2	10.6		15.6	22.0
Primary effluent	0.40	3.83	4.23			
Primary underflow	0.40	912	912			2312
Secondary effluent	0.37	0.00031	0.37			
Secondary underflow	0.37	0.21	0.58			

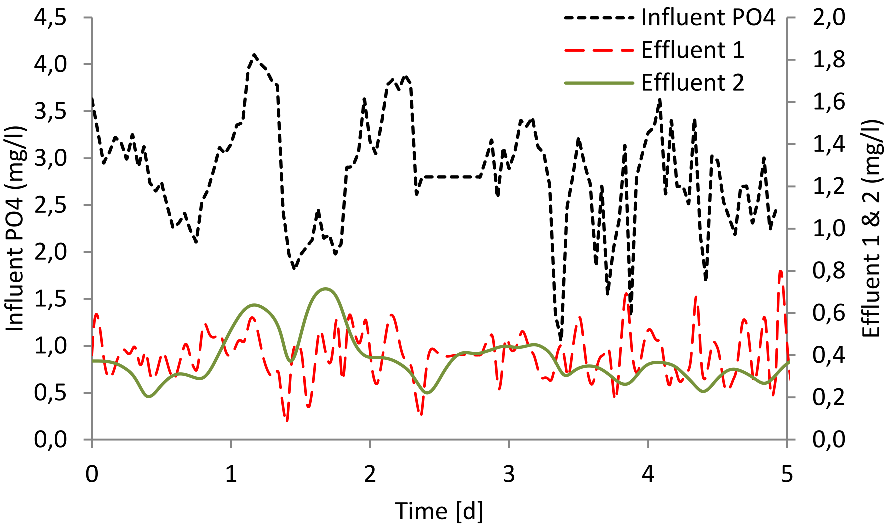


Figure 23 *S_{PO4} in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

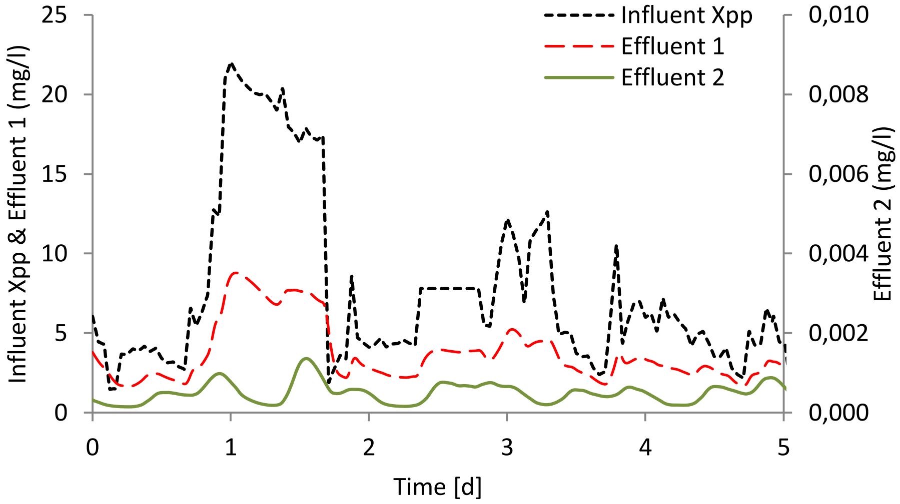


Figure 24 *X_{PP} in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

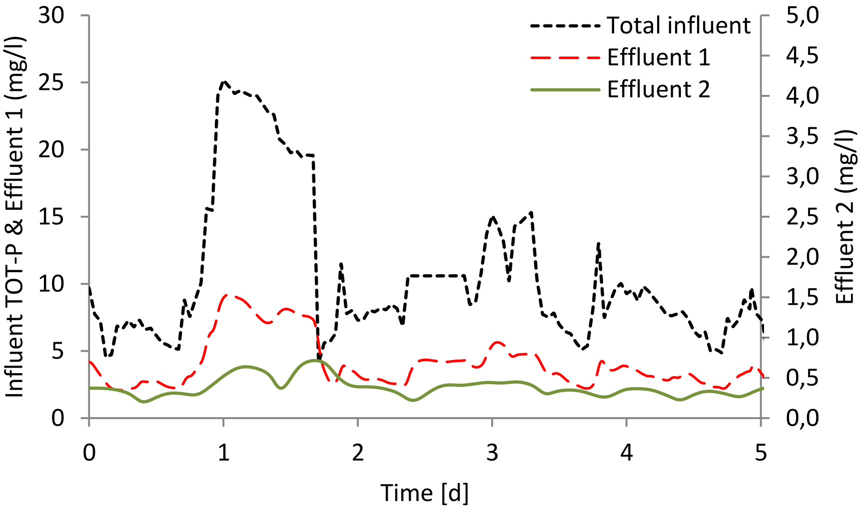


Figure 25 *Total phosphorus in the dynamic simulation. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

4.3 SHORT SUMMARY

A summary with average values from the measurements in Henriksdals WWTP, with the values from the steady state simulation and average values from the open loop/dynamic simulation are presented in (Table 9). To separate the two cases with different hydrolysis processes the one with eq. (31) is referred to as (1) and the one with eq. (32) as (2).

Also a comparison between the measured data and the dynamic/open loop (1) simulation is provided (Figure 26 and 27).

Table 9 *Average values of measured data from Henriksdals WWTP together with steady state results and average values from the open loop/dynamic simulation. Remember that in the method the set-point were set to 0.40.*

	Average data:	Steady state:		Average open loop/dynamic:	
Effluent primary sedimentation:					
TOT-P [mg/l]	3.97	4.26 (1)	4.23 (2)	3.96 (1)	3.95 (2)
S_{PO4} [mg/l]	0.37	0.40 (1)	0.40 (2)	0.40 (1)	0.40 (2)
X_{PP} [mg/l]	3.61	3.86 (1)	3.83 (2)	3.56 (1)	3.55 (2)
Effluent secondary sedimentation:					
TOT-P [mg/l]	0.43	0.44 (1)	0.37 (2)	0.46 (1)	0.38 (2)
S_{PO4} [mg/l]	0.36	0.23 (1)	0.37 (2)	0.25 (1)	0.38 (2)
X_{PP} [mg/l]	0.08	0.21 (1)	0.0003 (2)	0.21 (1)	0.0005 (2)

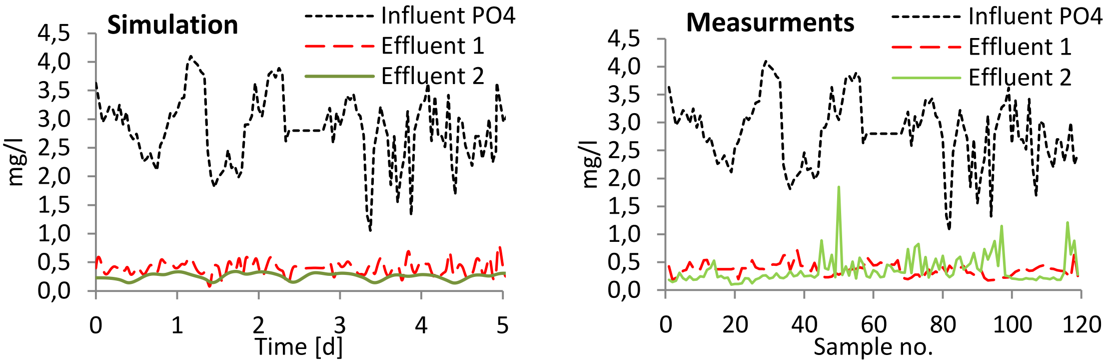


Figure 26 *Phosphate in the dynamic simulation and measurements from Henriksdals WWTP. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

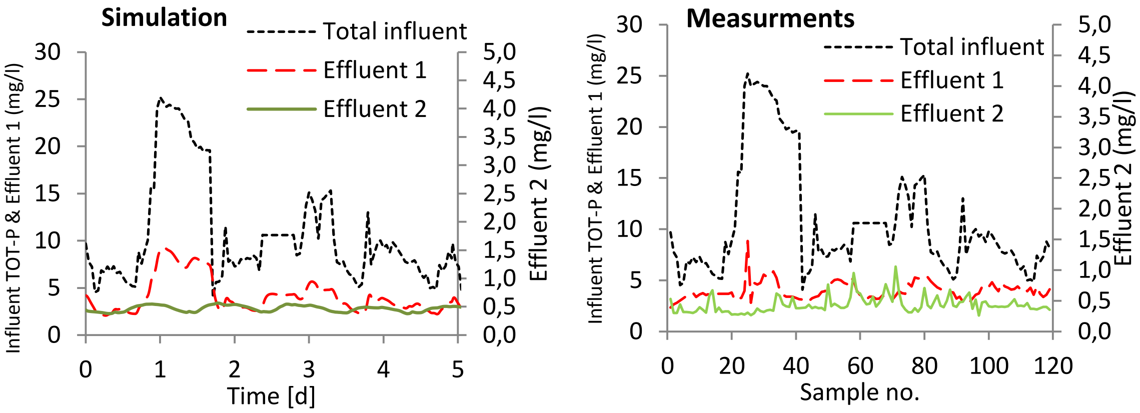


Figure 27 *Total phosphorus in the dynamic simulation and measurements from Henriksdals WWTP. The effluent from primary sedimentation is referred to as effluent 1 and from the secondary sedimentation as effluent 2.*

5. DISCUSSION

5.1 GENERAL

A model, to include phosphorus and chemical precipitation, was added to BSM2. Phosphorus was in the model assumed to consist of two fractions, soluble phosphate (S_{PO4}) and particulate phosphorus (X_{PP}). This is of course a simplification of reality but the choice was motivated by the fact that provided data, from Henriksdals WWTP, were measurements of total phosphorus and phosphate concentration. This made the choice most reasonable in order to be able to compare the simulations with the measurements.

The simplification that chemical precipitation was assumed to be independent of pH and temperature will most likely affect the ability to describe reality. It is difficult to say to which extent this affects the results, but a factor to keep in mind when evaluating the model.

In influent to the biological process (ASM1) phosphorus was, in the model, assumed to be biodegradable and available for microbial growth. In reality some phosphorus can be present as inert material, and thereby this could affect the results of the model. However the part inert phosphorus influent to the biological step is not believed to be large.

The fact that the anaerobic digestion process is not taken into account in the thesis is worth mentioning. Anaerobic digestion is a complex process and affects the model by the return flow to primary sedimentation. This could affect the results of the simulations due to that higher (or lower) concentration of phosphorus is fed back to primary sedimentation. Perhaps the effluent phosphate concentration from primary sedimentation would not be affected to much as more (or lower) precipitation chemical would be dosed to keep the effluent close to the set-point. However f_{corr2} might need to be adjusted to fit a possible higher (or lower) influent of particulate phosphorus. The actual anaerobic digestion process will of course also be affected if primary sludge including precipitation chemical and phosphorus should be digested.

5.2 MODEL RESULTS

By comparing average values from the measurements with the steady state simulation and average from the open loop/dynamic simulation, it is noted that they generally match quite well for both S_{PO4} and X_{PP} in effluent from primary sedimentation (Table 9). Total phosphorus (TOT-P) in effluent from the secondary sedimentation also generally were simulated in quite good agreement to data from Henriksdals WWTP, however, it should be noted that the separate fractions (S_{PO4} and X_{PP}) do not match very well (Table 9). The dynamic simulation showed the same behavior (Figure 26 and 27). Here it can be noted that effluent phosphate and total phosphorus in the measurements showed more variation (peaks) than the simulated. This could be due to that the model is not able to predict reality, but some of the sharp peaks in the measured concentrations can also be a result of something that happened at the plant during the measurement period.

In case (2), the steady state and average values from the dynamic simulation for S_{PO4} in the effluent from the secondary sedimentation showed results more alike the measured ones (Table 9). The particulate fraction is approximately zero, and that renders the total effluent a bit to low compared to the average from the measurements. If desirable, it would certainly possible, by using the parameters in the biological process and secondary sedimentation, to adjust the phosphate concentration in the effluent to some extent. And thus the total phosphorus concentration would also match better.

The fact that it was difficult to simulate the various fractions of phosphorus effluent from the secondary sedimentation well may be explained by several reasons. One explanation is uncertainty in the parameter choices in ASM1. It is however likely that several new components would need to be added to the ASM1 model in order to represent phosphorus in a more accurate way, thus giving better results. Phosphorus in the biological process is to a large extent a simplified solution, only with the purpose to simulate the total effluent phosphorus from the secondary sedimentation.

An assumption that affects X_{PP} in the model is that precipitated phosphate form particulate and thereby the effluent X_{PP} from the precipitation module is higher than the influent (Table 5). As the idea with chemical precipitation is to form low solubility material from soluble, which is able to settle (Svenskt Vatten, 2010), this felt like a good solution even though it is a simplification of what happens in reality.

5.2.1 The PI controller

Effluent phosphate from primary sedimentation was controlled by the PI controller, added to dose the precipitation chemical. How to choose control parameters is tricky. To choose faster control parameters, that are able to keep a lower variance in the output signal (effluent phosphate), is of course in general desirable. However the differences between p=1, 2 and 3 were in the model found small (Figure 14 and 15), and due to that emission requirements on WWTPs not are instantaneous and the fact that a slower controlling (higher p) is both more robust and more noise sensitive the choice of p=2 were found acceptable.

The controller in the model generally dosed lower concentration precipitation chemical then the literature stated. Svenskt Vatten (2010) suggested that a required dosage when trivalent iron was used lied between 10-15 mg Fe/l, while the controller dosed about 5-10 mg Fe/l (in average about 7 mg Fe/l) (Figure 18). At Henriksdals WWTP they dose between 11-20 mg Fe/l (Stockholm Vatten, 2013). The difference between the literature, Henriksdals WWTP and the model can depend on that the model is not taking all mechanisms in the precipitation process such as pH changes or hydroxide precipitation into consideration. For example, if much hydroxide precipitate is formed in theory a certain amount iron will be used to precipitate hydroxide instead of phosphate. Although this would require some extra doses of iron, it is however unlikely that there would be need for much more. A more believable reason to explain the different values is the fact that WWTPs in general overdose the precipitation chemical to control (lower) the pH value in the wastewater. The literature value can also be based on WWTPs that use a flow-proportional control law to add precipitation chemical. This control law often leads to overdosing as influent flow and phosphate concentration in general fluctuate over day, but not necessarily in the same way (Carlsson and Hallin, 2010).

Henriksdals WWTP today uses a time controlled dosage, one dosage on day and one at night (Rahmberg, 2013), this is based on the fact that influent load is regular and can also lead to overdosing the precipitation chemical.

5.3 MEASUREMENTS

As always when working with measured data it is important to remember the measurement uncertainty. To try the model on a specific plant during a longer period and also measuring added precipitation chemical would partly make the uncertainty better and partly make it easier to evaluate how well phosphorus behave in the model.

6. CONCLUSION

After some simplifications it was possible to include phosphorus and chemical precipitation in BSM2. It was found that,

- generally the model for phosphorus had potential to describe the behavior of total phosphorus in the WWTP.
- it was difficult to simulate the separate fractions S_{PO4} and X_{PP} in the effluent from the secondary sedimentation. The main reason for this was thought to be that, to describe phosphorus in ASM1 in a better way several new components would need to be added.
- to better be able to evaluate the results, and how the simplifications of the model affects the results, more measurements need to be performed and compared with the results from BSM2.
- a correction of parameters in BSM2 must be performed in order to adjust the model to the given plant.
- using a PI controller to dose precipitation chemical proved to be a good method. The controller in general dosed lower concentration precipitation chemical than the literature stated. The main reasons for this were thought to be the fact that WWTPs in general overdose added precipitation chemical, or that the literature value is based on WWTPs that use a flow-proportional or time based control law.

Finally I would like to state two things important to remember when working with models:

1. A modeling task is never complete, there is always more work to do.
2. That it is "just a model" a simplification of reality in order to simulate the future or changes in the process behavior.

7. FURTHER WORK

A model can always be improved and represent reality a little better, often the limits are set by the purpose of the model.

If assumed that the limitations of this thesis still apply and that the purpose of the model is to simulate the *total flow of phosphorus*, one thing to study would be the chemical sludge formed in the precipitation module, since chemical precipitation can significantly contribute to the sludge production of a plant, and thereby is important in an LCA analysis. At the moment, the amount of formed chemical sludge depends on theoretical calculations and it would be interesting to see how well those matches reality. If they do not match well, maybe a correction factor (or similar) could be used in the model.

If the purpose instead is to simulate the *fractions* S_{PO4} *and* X_{PP}, a closer look should be taken on phosphorus in ASM1. How can the processes and conversions rates better describe phosphorus? Which components would be added to describe phosphorus better?

Finally it would be interesting trying to also include simultaneous precipitation since several plants today use this method.

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8.1 PERSONAL COMMUNICATION

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APPENDIX A - PROCESS AND CONVERSIONS RATES IN ASM1

The eight basic processes in the activated sludge model (ASM1) (Alex et al., 2008):

- $j = 1$: Aerobic growth of heterotrophs

$$\rho_{1,\mathrm{as}} = \mu_{\mathrm{HT}}\left(\frac{S_{\mathrm{S}}}{K_{\mathrm{S}} + S_{\mathrm{S}}}\right)\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right)X_{\mathrm{B,H}}$$

with:

$$\mu_{\mathrm{HT}} = \mu_{\mathrm{H}} \cdot \exp\left(\left(Ln\left(\frac{\mu_{\mathrm{H}}}{3}\right)\Big/5\right)\cdot\left(T_{as} - 15\right)\right)$$

- $j = 2$: Anoxic growth of heterotrophs

$$\rho_{2,\mathrm{as}} = \mu_{\mathrm{HT}}\left(\frac{S_{\mathrm{S}}}{K_{\mathrm{S}} + S_{\mathrm{S}}}\right)\left(\frac{K_{\mathrm{O,H}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right)\left(\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}} + S_{\mathrm{NO}}}\right)\eta_{\mathrm{g}} X_{\mathrm{B,H}}$$

- $j = 3$: Aerobic growth of autotrophs

$$\rho_{3,\mathrm{as}} = \mu_{\mathrm{AT}}\left(\frac{S_{\mathrm{NH}}}{K_{\mathrm{NH}} + S_{\mathrm{NH}}}\right)\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,A}} + S_{\mathrm{O}}}\right)X_{\mathrm{B,A}}$$

with:

$$\mu_{\mathrm{AT}} = \mu_{\mathrm{A}} \cdot \exp\left(\left(Ln\left(\frac{\mu_{\mathrm{A}}}{0.3}\right)\Big/5\right)\cdot\left(T_{as} - 15\right)\right)$$

- $j = 4$: Decay of heterotrophs

$$\rho_{4,\mathrm{as}} = b_{\mathrm{HT}} X_{\mathrm{B,H}}$$

with:

$$b_{\mathrm{HT}} = b_{\mathrm{H}} \cdot \exp\left(\left(Ln\left(\frac{b_{\mathrm{H}}}{0.2}\right)\Big/5\right)\cdot\left(T_{\mathrm{as}} - 15\right)\right)$$

- $j = 5$: Decay of autotrophs

$$\rho_{5,\mathrm{as}} = b_{\mathrm{AT}} X_{\mathrm{B,A}}$$

with $b_{\mathrm{AT}} = b_{\mathrm{A}} \cdot \exp\left(\left(Ln\left(\frac{b_{\mathrm{A}}}{0.03}\right)\Big/5\right)\cdot\left(T_{\mathrm{as}} - 15\right)\right)$

- $j = 6$: Ammonification of soluble organic nitrogen

$$\rho_{6,\mathrm{as}} = k_{\mathrm{aT}} S_{\mathrm{ND}} X_{\mathrm{B,H}}$$

with $k_{\mathrm{aT}} = k_{\mathrm{a}} \cdot \exp\left(\left(Ln\left(\frac{k_{\mathrm{a}}}{0.04}\right)\Big/5\right)\cdot\left(T_{\mathrm{as}} - 15\right)\right)$

- $j = 7$: Hydrolysis of entrapped organics

$$\rho_{7,\mathrm{as}} = k_{\mathrm{hT}}\frac{X_{\mathrm{S}}/X_{\mathrm{B,H}}}{K_{\mathrm{X}} + \left(X_{\mathrm{S}}/X_{\mathrm{B,H}}\right)}\left[\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right) + \eta_{\mathrm{h}}\left(\frac{K_{\mathrm{O,H}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right)\left(\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}} + S_{\mathrm{NO}}}\right)\right]X_{\mathrm{B,H}}$$

with $k_{\mathrm{hT}} = k_{\mathrm{h}} \cdot \exp\left(\left(Ln\left(\frac{k_{\mathrm{h}}}{2.5}\right)\Big/5\right)\cdot\left(T_{\mathrm{as}} - 15\right)\right)$

- $j = 8$: Hydrolysis of entrapped organic nitrogen

$$\rho_{8,\mathrm{as}} = k_{\mathrm{hT}}\frac{X_{\mathrm{S}}/X_{\mathrm{B,H}}}{K_{\mathrm{X}} + \left(X_{\mathrm{S}}/X_{\mathrm{B,H}}\right)}\left[\left(\frac{S_{\mathrm{O}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right) + \eta_{h}\left(\frac{K_{\mathrm{O,H}}}{K_{\mathrm{O,H}} + S_{\mathrm{O}}}\right)\left(\frac{S_{\mathrm{NO}}}{K_{\mathrm{NO}} + S_{\mathrm{NO}}}\right)\right]X_{\mathrm{B,H}}\left(X_{\mathrm{ND}}/X_{\mathrm{S}}\right)$$

Conversions rates (r_k) results from combinations of the basic processes with stoichiometric parameters according to eq. (20) (Alex et al., 2008):

- S_S (k= 2)

$$r_2 = -\frac{1}{Y_H}\rho_{1,as} - \frac{1}{Y_H}\rho_{2,as} + \rho_{7,as}$$

- X_I (k = 3)

$$r_3 = 0$$

- X_S (k = 4)

$$r_4 = (1 - f_P)\rho_{4,as} + (1 - f_P)\rho_{5,as} - \rho_{7,as}$$

- $X_{B,H}$ (k = 5)

$$r_5 = \rho_{1,as} + \rho_{2,as} - \rho_{4,as}$$

- $X_{B,A}$ (k = 6)

$$r_6 = \rho_{3,as} - \rho_{5,as}$$

- X_P (k = 7)

$$r_7 = f_P\rho_{4,as} + f_P\rho_{5,as}$$

- S_O (k = 8)

$$r_8 = -\frac{1 - Y_H}{Y_H}\rho_{1,as} - \frac{4.57 - Y_A}{Y_A}\rho_{3,as}$$

- S_{NO} (k = 9)

$$r_9 = -\frac{1 - Y_H}{2.86\,Y_H}\rho_{2,as} + \frac{1}{Y_A}\rho_{3,as}$$

- S_{NH} (k = 10)

$$r_{10} = -i_{XB}\rho_{1,as} - i_{XB}\rho_{2,as} - \left(i_{XB} + \frac{1}{Y_A}\right)\rho_{3,as} + \rho_{6,as}$$

- S_{ND} (k = 11)

$$r_{11} = -\rho_{6,as} + \rho_{8,as}$$

- X_{ND} (k = 12)

$$r_{12} = (i_{XB} - f_P i_{XP})\rho_{4,as} + (i_{XB} - f_P i_{XP})\rho_{5,as} - \rho_{8,as}$$

- S_{ALK} (k = 13)

$$r_{13} = -\frac{i_{XB}}{14}\rho_{1,as} + \left(\frac{1 - Y_H}{14 \cdot 2.86\,Y_H} - \frac{i_{XB}}{14}\right)\rho_{2,as} - \left(\frac{i_{XB}}{14} + \frac{1}{7Y_A}\right)\rho_{3,as} + \frac{1}{14}\rho_{6,as}$$

APPENDIX B - MASS CALCULATIONS

In order to carry out the mass calculations the molar mass for certain elements and molecules were needed (Table 1-B). The principal for the mass calculation is shown for iron and aluminum.

Table 1-B *Molar mass for some chemical elements and molecules.*

Chemical element	Molar mass [g/mol]
Fe	55.9
Al	27.0
Cl	35.5
S	32.1
O	16.0
P	31.0
H	1.0
$FeCl_3$	162.2
$Fe_2(SO_4)_3$	399.9
$Fe(SO_4)$	151.9
$AlCl_3$	133.3
$Al_2(SO_4)_3$	342.2
$(FeOH)_3(PO_4)_2$	408.5
$Fe_3(PO_4)_2$	357.5
$(AlOH)_3(PO_4)_2$	322.0

Mass calculation - Iron

Remember that according to eq. (2) 1.5 mole iron is required to reduce 1 mole phosphorus and 0.5 mole precipitate is then formed.

$$\left(\frac{1.5}{31.0}\right) \cdot 55.9 = 2.7\ g\ Fe/g\ P$$

$$\left(\frac{0.5}{31.0}\right) \cdot 408.5 = 6.6\ g\ precipitate/g\ P$$

Mass calculation - Aluminum

Remember that according to eq. (4) 1.5 mole aluminum is required to reduce 1 mole phosphate and 0.5 mole precipitate is then formed.

$$\left(\frac{1.5}{31.0}\right) \cdot 27.0 = 1.3\ g\ Al/g\ P$$

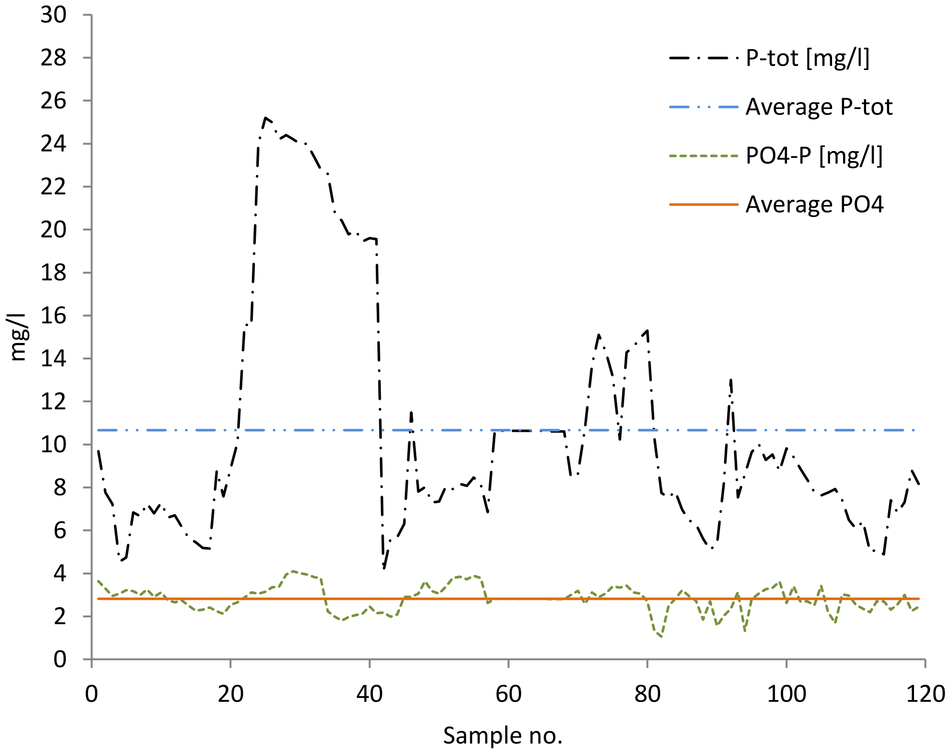
$$\left(\frac{0.5}{31.0}\right) \cdot 322.0 = 5.2\ g\ precipitate/g\ P$$

APPENDIX C - MEASUREMENTS

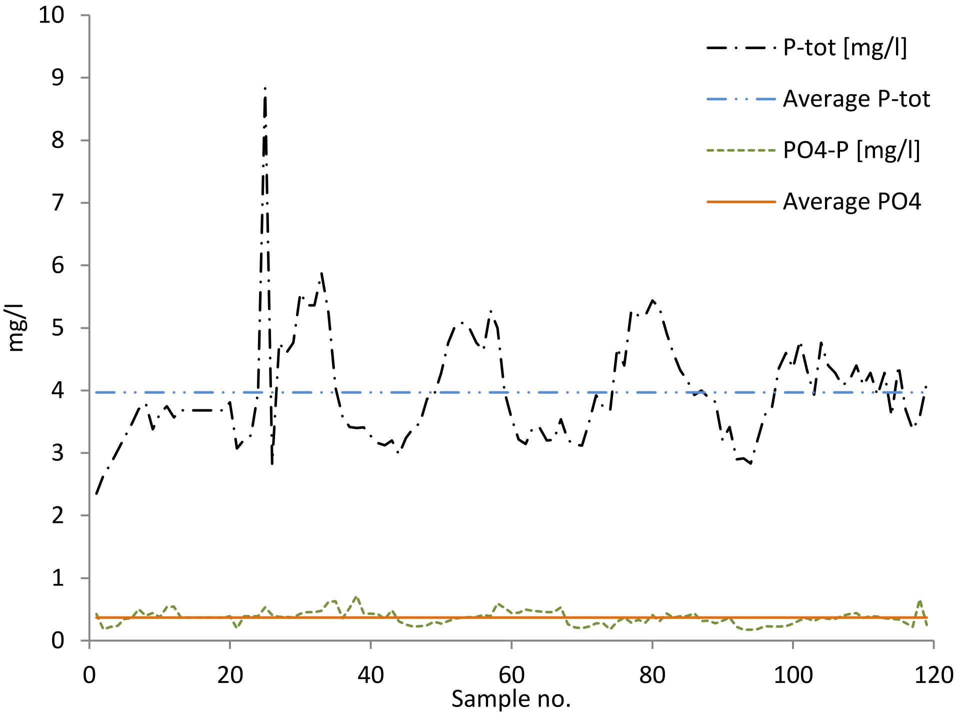
All data used in the theses were from Henriksdals WWTP in Stockholm and received from IVL Swedish Environment Institute.

The data is from a measurement campaign the 26th of June to 1st of July 2005. Samples were taken from three positions in the WWTP:

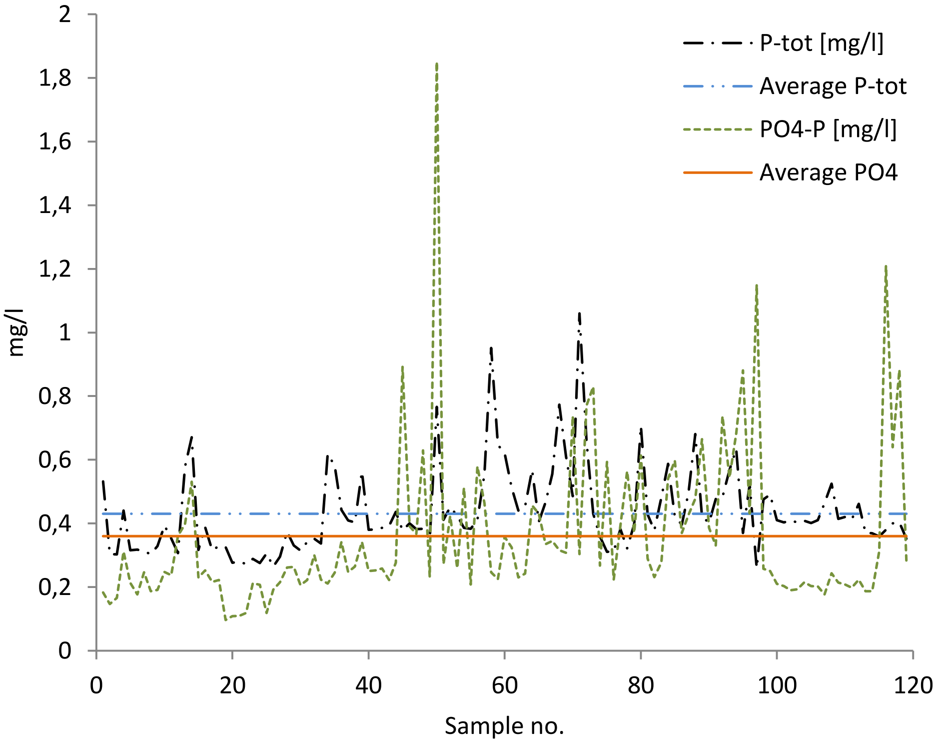
A. in incoming water



B. in water leaving the primary precipitation step



C. in water leaving the secondary sedimentation



APPENDIX D - CODE

Initial file for the precipitation module:

```
% This initialization file will set parameters and initial values for
% the primary precipitation module. The initial values are based on BSM2 open-loop
results using the constant
% input file.

% Precipitation chemical which needs to be added for each gram of phosphate that is
removed
K_chemical = 2.7;  %Fe
%K_chemical = 7.9;  %FeCl3
%K_chemical = 1.3; %Al
%K_chemical = 6.5; %AlCl3
%K_chemical = 19.4; %Fe2(SO4)3
%K_chemical = 7.4; %FeSO4
%K_chemical = 16.6; %Al2(SO4)3

% Precipitate formed for each gram of phosphate that is removed
K_sludge = 6.6; %Fe
%K_sludge = 6.6; %FeCl3
%K_sludge = 5.2; %Al
%K_sludge = 5.2; %AlCl3
%K_sludge = 6.6; %Fe2(SO4)3
%K_sludge = 5.8; %FeSO4
%K_sludge = 5.2; %Al2(SO4)3

% Controller parameters
PO4P_ref = 0.4;
PO4P_K = -1.40; % -2.80; % -0.93;
PO4P_Ti = 0.01;
qfoffset = 6.39;
PO4P_Tt = 0.008;
qfmax = 30;
qfmin = 0;

% Initial values
S_I_F =  28.20;
S_S_F =  59.47;
X_I_F =  94.23;
X_S_F =  356.91;
X_BH_F = 51.77;
X_BA_F = 0.043;
X_P_F = 0.272;
S_O_F =  0.0283;
S_NO_F = 0.07399;
S_NH_F = 37.66;
S_ND_F = 5.5537;
X_ND_F = 15.82;
S_ALK_F = 7.8935;
TSS_F = 427.74;
Q_F = 21086.338;
T_F = 14.8581;
S_D1_F = 2.7675;
S_D2_F = 0;
S_D3_F = 0;
X_D4_F = 0;
X_D5_F = 7.7305;

XINIT_F = [ S_I_F  S_S_F  X_I_F  X_S_F  X_BH_F  X_BA_F  X_P_F  S_O_F  S_NO_F  S_NH_F
S_ND_F  X_ND_F  S_ALK_F TSS_F Q_F T_F S_D1_F S_D2_F S_D3_F X_D4_F X_D5_F ];

PAR_F = [ K_chemical K_sludge ];
```

C-file (S-function) for the precipitation module:

```c
/*
 * This function, precipitation_bsm2.c, is a C-file S-function implementation of
 * primary precipitation.
 */

#define S_FUNCTION_NAME precipitation_bsm2

#include "simstruc.h"
#include <math.h>

#define XINIT ssGetSFcnParam(S,0)   /* Initial stage */
#define PAR_F ssGetSFcnParam(S,1) /* Parameters for primary precipitation */
/*
 * mdlInitializeSizes - initialize the sizes array
 */

static void mdlInitializeSizes(SimStruct *S)
{
     ssSetNumContStates(    S, 21);     /* number of continuous states */
     ssSetNumDiscStates(    S, 0);      /* number of discrete states */
     ssSetNumInputs(        S, 22);     /* number of inputs */
     ssSetNumOutputs(       S, 23);     /* number of outputs */
     ssSetDirectFeedThrough(S, 1);      /* direct feed-through flag */
     ssSetNumSampleTimes(   S, 1);      /* number of sample times */
     ssSetNumInputArgs(     S, 2);      /* number of input arguments */
     ssSetNumRWork(         S, 0);      /* number of real work vector elements */
     ssSetNumIWork(         S, 0);      /* number of integer work vector elements */
     ssSetNumPWork(         S, 0);      /* number of pointer work vector elements */

}

/*
 * mdlInitializeSampleTimes - initialize the sample times array
 */

static void mdlInitializeSampleTimes(SimStruct *S){
     ssSetSampleTime(S, 0, 0.0);     /*  ssSetSampleTime(S, 0, CONTINUOUS_SAMPLE_TIME)
*/
     ssSetOffsetTime(S, 0, 0.0);
}

/*
 * mdlInitializeConditions - initialize the states
 */

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

for (i = 0; i < 21; i++) {
    x0[i] = mxGetPr(XINIT)[i];
}

}

/*
 * mdlOutputs - compute the outputs
 */

static void mdlOutputs(double *y, const double *x, const double *u, SimStruct *S, int
tid)
{
  double K_chemical, K_sludge;

K_chemical = mxGetPr(PAR_F)[0];
K_sludge = mxGetPr(PAR_F)[1];
```

```
y[0]=u[0];
y[1]=u[1];
y[2]=u[2];
y[3]=u[3];
y[4]=u[4];
y[5]=u[5];
y[6]=u[6];
y[7]=u[7];
y[8]=u[8];
y[9]=u[9];
y[10]=u[10];
y[11]=u[11];
y[12]=u[12];
y[13]=u[13];
y[14]=u[14];
y[15]=u[15];

y[16]=u[16]-u[21]/K_chemical;

      if (y[16] < 0.0){
         y[16] = 0.0;
      }

y[17]=u[17];
y[18]=u[18];
y[19]=u[19]+u[21]+(u[16]-y[16])*K_sludge; // added precipitation chemicals + formed precipitate
y[20]=u[20]+(u[16]-y[16]); // Effluent particulate phosphorus

y[21]=u[21]; // Amount precipitation chemicals added, not used later
y[22]=(u[16]-y[16])*K_sludge; // Effluent sludge, not used later

}


/*
 * mdlUpdate - perform action at major integration time step
 */

static void mdlUpdate(double *x, const double *u, SimStruct *S, int tid){

}
/*
 * mdlDerivatives - compute the derivatives
 */
static void mdlDerivatives(double *dx, const double *x, const double *u, SimStruct *S, int tid)
{
  int i;

 for (i = 0; i < 21; i++) {       //can instead be set to zero or removed and insert numbers constants set to zero as states not used
      dx[i] = u[i];
  }
}
/*
 * mdlTerminate - called when the simulation is terminated.
 */
static void mdlTerminate(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
```

APPENDIX E - ASM1 PARAMETERS

The parameters in ASM1 calibrated against Henriksdals WWTP (Table 1-E).

Table 1-E *Stoichiometric and kinetic parameters in the ASM1 model and secondary sedimentation, parameters received from the thesis done at IVL (Hellstedt, 2005).*

Parameter	Value	Comment
ASM1:		
b_{HT}	0.04	See section 2.4.5
b_{AT}	0.2	See section 2.4.5
K_S	30	See section 2.4.5
$K_{O,H}$	0.9	See section 2.4.5
K_{NO}	0.3	See section 2.4.5
$K_{O,A}$	0.2	See section 2.4.5
K_{NH}	0.3	See section 2.4.5
K_X	0.05	See section 2.4.5
k_{hT}	3.5	See section 2.4.5
k_{aT}	0.0006	See section 2.4.5
η_g	0.8	See section 2.4.5
η_h	0.3	See section 2.4.5
μ_{HT}	0.5	See section 2.4.5
μ_{AT}	0.57	See section 2.4.5
f_p	0.08	See section 2.4.5
i_{XB}	0.086	See section 2.4.5
i_{XP}	0.06	See section 2.4.5
Y_H	0.5	Heterotrophic yield
Y_A	0.26	Autotrophic yield
Secondary sedimentation:		
r_h	0.00028	Settling parameter characteristic of the hindered settling zone.
r_p	0.006	Settling parameter characteristic of low solids concentration
$feedlayer$	4	Layer where the flow is feed to the settler.