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Industrial Electrical Engineering and Automation

Extending Wastewater Treatment Process Models for Phosphorous Removal and Recovery

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Preface

This short report summarizes the key findings and main conclusions of the PhD work by Dr Kimberly Solon, IEA, Lund University, presented in May 2017. It does not provide any complete background and description of the methodology of the work, instead the interested reader can access the complete PhD thesis:

“Extending Wastewater Treatment Process Models for Phosphorous Removal and Recovery”

via the web link https://www.iea.lth.se/publications/Theses/LTH-IEA-1082.pdf to discover all the details of the research.

1. Introduction

Water fulfils many functions in human society: domestic, industrial, agricultural, infrastructure, recreational, transportation use, energy use, etc. As a consequence of its usage, water becomes contaminated, which affects the water cycle and creates disturbances in natural functions (WWAP, 2016).

The contaminated water, or wastewater, contains significant amounts of pollutants, which results in oxygen depletion when discharged directly to surface waters. The wastewater composition largely varies depending on the area it is collected from. It generally constitutes contaminants such as solids, biodegradable and non-biodegradable (or slowly biodegradable) compounds, nutrients, toxic substances, pathogenic organisms, etc. Each of these different types of contaminations often requires different ways of treatment (physical, chemical, biological), thus a conventional wastewater treatment plant (WWTP), such as shown in Figure 1, also constitutes several stages wherein a certain type of pollutant is targeted to be removed in each stage. The main objective of wastewater treatment is to allow urban wastewater discharge into surface waters ensuring protection of public health and the environment (Pescod, 1992).

In the last ten years, there has been a rapid transition of WWTPs into water resource recovery facilities (WRRFs). Wastewater is now considered a resource from where nutrients, energy and water can be recovered. In line with this, plant-wide modelling of wastewater treatment processes needs to account for new processes and state variables. In this research work, emphasis is given to phosphorus removal and/or recovery. Wastewater contains significant amounts of phosphorus, which legislation requires to be reduced to legal limits before discharge onto surface waters due to the fact that it is also responsible for eutrophication. On the other hand, phosphorus is considered a limited resource and only an estimated 50-100 years is left before the known reserves of phosphate rock will be depleted (Herring & Fantel, 1993; Seyhan et al., 2012), with a more conservative estimate of up to 300 years according to Cordell & White (2011). Thus, phosphorus recovery from wastewater becomes a viable prospect to consider (Le Corre et al., 2009).

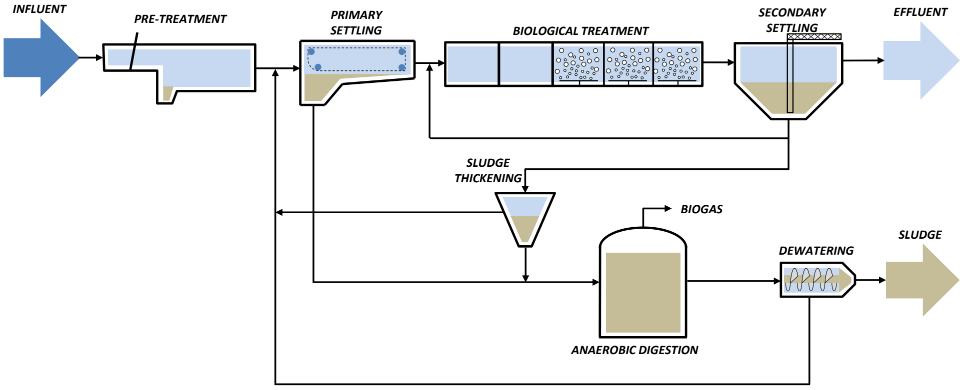

Figure 1. An example of a wastewater treatment plant configuration.

From a wastewater treatment modelling perspective, phosphorus removal and/or recovery requires an inevitable increase of model complexity in order to correctly describe phosphorus transformation processes. Since phosphorus occurs mostly as orthophosphates, such as PO_4^{3-} and HPO_4^{2-}, their valency suggests strong influence on ion pairing and ion activity, which affects pH and mineral precipitation (Tait et al., 2012). Phosphorus is also highly associated with iron as iron salts are commonly used to precipitate phosphorus (de-Bashan & Bashan, 2004; Gutierrez et al., 2010). The relationship of iron with sulfur is also significant because the former reduces phosphorus precipitation due to its preferential binding with sulfur (Kleeberg, 1997; Nürnberg, 1996) and results in release of phosphates. By itself, sulfur is also becoming important because of the adverse effects of sulfur compounds during plant operation, e.g. inhibitory effects of sulfide on some bacterial population and causing odour, corrosion and safety problems (Pol et al., 1998;

Zhang et al., 2008). Thus, the development of a plant-wide model for organics, nitrogen and phosphorus removal comes in several stages:

- the development of the aqueous phase chemical equilibria model to correctly describe and predict pH, speciation of the different compounds and precipitation reactions;
- extension of the biological models by taking into account new state variables; and,
- integration of the models into a plant-wide model with new unit processes for recovery, extended interfaces to link the different models together and new evaluation criteria (Jeppsson et al., 2013).

2. Biochemical Models for Wastewater Treatment

An overview of the standard models currently in use for modelling wastewater treatment plants (mainly biological processes) is mentioned below.

2.1. Activated Sludge Models

- ASM1: The first activated sludge model, ASM1 (Henze et. al., 1987), describes biological oxidation of carbon, nitrification and denitrification and is therefore used to simulate carbon and nitrogen removal in activated sludge systems.
- ASM2: It is an extension of ASM1 and includes biological and chemical phosphorus removal in addition to descriptions of carbon and nitrogen removal.
- ASM2d: It is developed as an extension to ASM2 (Henze et al., 1999) as understanding of the role of denitrification grew. This entails addition of two processes: (1) storage of inorganic phosphorus as poly phosphates and (2) anoxic growth of phosphorus accumulating organisms.
- ASM3: The Activated Sludge Model No. 3 (ASM3) (Gujer et al., 1999) tackles some of the limitations of ASM1, especially dealing with issues to facilitate model calibration. An important difference between ASM1 and ASM3 is in the COD flow.

Table 1. Overview of activated sludge models (Gernaey et al., 2004; Hauduc et al., 2013).

Model	**Substrates**	**Nitrification**	**Denitrification**	**Heterotrophic/ autotrophic decay**	**Hydrolysis**	**Bio-P**	**Denitrifying PAOs**	**Lysis of PAO/PHA**	**Fermentation**	**Chemical P removal**
ASM1	CN	X	X	DR, Cst	EA					
ASM3	CN	X	X	ER, EA	Cst					
ASM2	CNP	X	X	DR, Cst	EA	X		Cst	X	X
ASM2d	**CNP**	**X**	**X**	**DR, Cst**	**EA**	**X**	**X**	**Cst**	**X**	**X**

DR = death regeneration principle; EA = electron acceptor dependent; Cst = not electron acceptor dependent; C = carbon; N = nitrogen; P = phosphorus

Table 1 presents an overview of the different processes included in the IWA published ASMs showing important features of each model. These, together with the other described models, are commonly implemented and used in numerous simulation platforms and are used to a great extent for scientific research to study biological processes in real and hypothetical systems.

2.2. *Anaerobic Digestion Models*

ADM1: It is a structured model consisting of biochemical and physico-chemical processes aimed to help in the design, operation and optimization of full-scale anaerobic digestion plants (Batstone & Keller, 2003; Batstone et al., 2002). The biochemical processes of ADM1 are categorized into five key steps: disintegration, hydrolysis, acidogenesis, acetogenesis and methanogenesis, as shown in Figure 2.

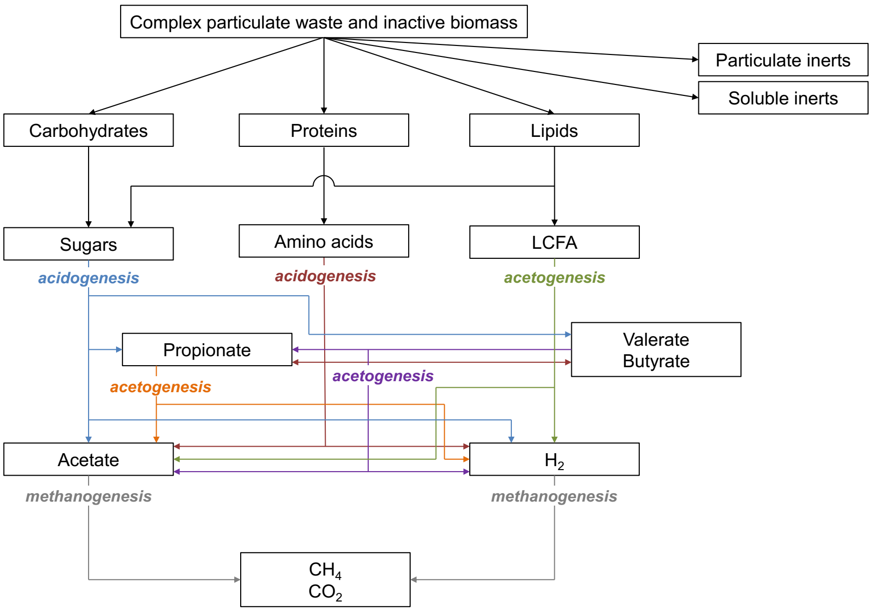

Figure 2. The anaerobic digestion process as described in Batstone et al. (2002).

In order to extend these models to enhance their ability to predict phosphorus removal and recovery, ASM2d and ADM1 models are chosen as the starting points. A plant-wide framework for modelling phosphorus is developed by: i. modelling the physico-chemistry in wastewater; ii. including additional processes dealing with phosphorus, iron and sulphur in ASM2d and ADM1 models; and, iii. developing interfaces between the different models in a plant-wide context for easy integration and holistic analysis.

3. Physico-Chemical Framework for Wastewater Treatment Models

Physico-chemical processes are non-biologically mediated. They are categorized as either liquid-liquid, gas-liquid or liquid-solid processes (Batstone et al., 2012).

3.1. Liquid-Liquid Processes

Acid base reactions: Stumm & Morgan (1996) give the general principle of chemical equilibrium dissociation reactions:

$$HA \leftrightarrow H^{+} + A^{-} \qquad (1)$$

where, HA is an acid dissociating into a conjugate base, A^{-}, and a hydrogen ion, H^{+}. The chemical equilibrium can be solved either by ordinary differential equations (ODEs) or algebraic equations (AEs). The dissociation processes of acid-base reactions as well as that of ion pairing reactions can be described using ODEs with given high kinetic rate constants to show that these reactions occur more or less instantaneously (Musvoto et al., 1997, 2000), or separately, calculated as AEs at each time step.

Ion speciation/pairing: In some cases, there are also non-electrostatic interactions between ions, which form ionic complexes as new chemical species. These ion pairs or ion complexes are different from the free ions (such as a hydrogen phosphate ion, HPO_4^{2-}, which is different from free orthophosphate, PO_4^{3-}) in solution. The most common ion pairs present in wastewater are set up to describe ion-pairing behaviour. This is implemented in a similar fashion as weak acid-base reactions where an algebraic procedure (Ikumi et al., 2011; Serralta et al., 2004) is used based on the assumption that ion pairs are in a state of equilibrium at all times.

Ion activity: The effect of ionic strength, also known as ion activity ($S_{\{i\}}$), is defined as the effective concentration of any particular kind of ion in solution and is caused by electrostatic interactions between ions. It is calculated by multiplying the concentration of ion i ($S_{[i]}$) by a correction factor, which is called the activity coefficient (γ_i) (Stumm & Morgan, 1996):

$$S_{\{i\}} = \gamma_i \cdot S_{[i]} \tag{2}$$

The current physico-chemical models applied to wastewater treatment process modelling have used the Davies equation to describe the activity of the components. This equation is simple and does not need other constants, unlike the extended and WATEQ Debye-Hückel equations. In addition, the Davies equation is valid for a larger range of ionic strength.

$$\log \gamma_i = -A \cdot z_i^2 \cdot \left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.3 \cdot I \right) \tag{3}$$

3.2. Liquid-Solid Processes

Precipitation and redissolution: Opposite to liquid-liquid processes, liquid-solid processes are assumed to occur slowly and take time to reach equilibrium. In order to model precipitation reactions, the possibility of precipitation is calculated first by testing if the solution is supersaturated or not. The Saturation Index (SI) indicates if a solution is in equilibrium, undersaturated or supersaturated with respect to a mineral (i.e. whether mineral precipitation might occur or not) (Merkel & Planer-Friedrich, 2005; Stumm & Morgan, 1996). If $SI < 0$, the liquid phase is undersaturated, thus a mineral might dissolve into the liquid phase. If $SI = 0$, the liquid phase is saturated or at equilibrium while if $SI > 0$, the liquid phase is supersaturated and mineral precipitation might occur. It is calculated as:

$$SI = \log \frac{IAP}{K_{SP}} \tag{4}$$

where, IAP is the ion activity product and K_{SP} is the solubility product constant of the mineral. Note that SI only indicates what could happen thermodynamically. However, it does not indicate the rate by which the process will proceed.

In this study, the rate of crystallization (r_i) used is presented by Kazadi Mbamba et al. (2015a), which has been adapted from the crystallization rate presented by Nielsen (1984):

$$r_i = k_{cryst} \cdot X_{cryst} \cdot \left[\left(\frac{\{M^{v+}\}^x \cdot \{A^{v-}\}^y}{K_{SP}} \right)^{\frac{1}{v}} - 1 \right]^n \tag{5}$$

where, k_{cryst} is the precipitation rate constant, X_{cryst} is the concentration of the precipitate and n is a constant typically equal to 2. Redissolution, on the other hand, can be considered as the inverse of the precipitation kinetics. In line with this, the dissolution rate equation is expressed as:

$$r_{\mathrm{i}} = -k_{\mathrm{diss}} \cdot X_{\mathrm{cryst}} \cdot \left[\left(\frac{\{\mathrm{M}^{\mathrm{v}+}\}^{x} \cdot \{\mathrm{A}^{\mathrm{v}-}\}^{y}}{K_{\mathrm{SP}}} \right)^{\frac{1}{\mathrm{v}}} - 1 \right]^{\mathrm{n}} \tag{6}$$

where, k_{diss} is the dissolution rate constant.

3.3. Liquid-Gas Processes

Stripping/Volatilization and absorption: Mass transfers between the liquid phase and gas phase are modelled to describe the dissolution of gaseous components formed during biological reactions into the aqueous phase (i.e. absorption) as well as the mass transfers of the dissolved forms of these gaseous components into the gas phase (i.e. volatilization – due to natural phenomenon or stripping – due to a mechanical device). Derived from Fick's first law (Fick, 1855), the equation below is a very common form of the kinetic rate equation for the liquid-gas transfer:

$$r_{\mathrm{i,G/L}} = k_{\mathrm{L}} \cdot a \cdot \left(K_{\mathrm{H,i}} \cdot P_{\mathrm{i}} - C_{\mathrm{i}} \right) \tag{7}$$

where $r_{\mathrm{i,G/L}}$ is the mass transfer rate between the gas and liquid phase, k_{L} is the mass transfer rate, a is the contact area between the liquid and the gas phase, $K_{\mathrm{H,i}}$ is the Henry's constant, P_{i} is the partial pressure and C_{i} is the dissolved concentration of the gaseous component. The common gaseous components, which are considered during modelling of stripping processes in wastewater treatment, are oxygen, carbon dioxide, ammonia, nitrogen, nitrous oxide, hydrogen and methane.

4. Extensions to Biological Models

4.1. Phosphorus Transformations

ASM2d: The activated sludge configuration is modified from the Ludzack-Ettinger process to include an anaerobic section in order to promote phosphorus release under anaerobic conditions and uptake by phosphorus accumulating organisms in the subsequent anoxic and aerobic zones (Figure 3).

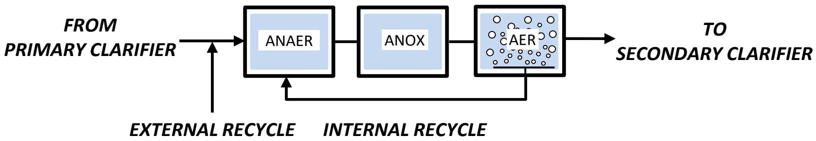

Figure 3. Activated sludge layout with anaerobic/anoxic/aerobic (A_2O) configuration

In addition, the simple chemical transformations in ASM2d are removed as a full physico-chemical model is now included. Also, new state variables for S and Fe are added. An important aspect of the model is defining the phosphorus content of all soluble and particulate components in the ASM2d through elemental balances as described by Takács & Vanrolleghem (2006).

ADM1: Modelling of phosphorus is one of the major limitations of the ADM1 (Batstone et al., 2015). The main concept for integrating phosphorus in ADM1 is to assume that the phosphorus-related microorganisms are still active when they reach the anaerobic digester (Ikumi et al., 2014; Wang et al., 2016). In order to handle this, some of the ASM2d processes (Henze et al., 1999), those which occur in anaerobic conditions, are included as additional processes in ADM1. An important aspect of phosphorus modelling is its effect on pH. In ADM1, the most important ions are tracked, except the phosphorus-related ones. It should be noted that a prerequisite to adding phosphorus and its precipitation kinetics requires taking into account physico-chemical effects, such as ion activity correction, ion pairing behaviour and relevant weak acid-base reactions.

4.2. *Sulfur Transformations*

ASM2d: The ASM2d is modified to include sulfur transformations in the biological reactor. Since the activated sludge configuration includes an anaerobic section, applicable oxidation and reduction reactions of sulfur depending on whether it is in the anaerobic zones or in the aerobic/anoxic zones, respectively, are included. Hydrogen sulfide inhibition is taken into account during growth of heterotrophic organisms, phosphorus accumulating organisms, nitrifiers and sulfate-reducing bacteria (SRB). The inhibition is due to toxicity of several bacterial groups, including the SRB themselves, to sulfide. Hydrogen sulfide stripping is also included.

ADM1: Sulfate reduction process carried out by four groups of microorganisms: hydrogenotrophic sulfate-reducing bacteria (X_{hSRB}), propionate-degrading sulfate-reducing bacteria (X_{pSRB}), butyrate-degrading sulfate-reducing bacteria (X_{bSRB}) and acetotrophic sulfate-reducing bacteria (X_{aSRB}) are included. Hydrogen sulfide inhibition is taken into account in the acetogenesis and methanogenesis stages, as well as for the growth of SRB. The inhibition as described by Chen et al. (2008) is a result of competition for common substrates and also due to toxicity of several bacterial groups, including the SRB themselves, to sulfide. In addition to biochemical conversions, possible precipitation of sulfur with iron as ferrous sulfide (FeS) is included in the extended ADM1.

4.3. *Iron Transformations*

ASM2d: The ASM2d is modified to include iron transformations in the biological reactor. In this model, only Fe(II) oxidation using either oxygen or nitrate as electron acceptors is included. This is assumed to be a purely chemical reaction resulting in oxidation of Fe(II) to hydrous ferric oxide, $Fe(OH)_3$ (XHFO). In addition, reduction of hydrous ferric oxide to Fe(II) using inorganic sulfides and acetate are also included. The hydrous ferric oxide model (Smith et al., 2008) describes how the precipitation of XHFO provides a number of adsorption sites for ions on its surface.

ADM1: The process of Fe(III) reduction is added as a process to ADM1. Fe(III), in the form of hydrous ferric oxides ($X_{\mathrm{HFO,L}}$, $X_{\mathrm{HFO,H}}$), is reduced to Fe(II) using hydrogen and sulfide as electron donor. In addition to biochemical conversions, precipitation of iron with sulfur and phosphate is included in the extended ADM1. Possible precipitates considered are ferrous sulfide (FeS) and ferrous phosphate ($Fe_3(PO_4)_2$).

5. Plant-Wide Modelling with P, S and Fe Transformations

5.1. *Plant Layout and Influent*

The models representing the wastewater treatment unit processes are implemented in a plant layout that is a modification of the BSM2 plant. It consists of: primary clarifier, activated sludge unit, secondary settler, sludge thickener, anaerobic digester, storage tank and dewatering unit. The main modification with respect to the original design of the BSM2 plant layout is on the activated sludge configuration. An anaerobic/anoxic/aerobic (A_2O) configuration (Figure 4) is implemented replacing the modified Ludzack-Ettinger process. An anaerobic section is added, preceding the anoxic and aerobic sections, to promote anaerobic phosphorus release and to provide the phosphorus accumulating organisms with a competitive advantage over other bacteria.

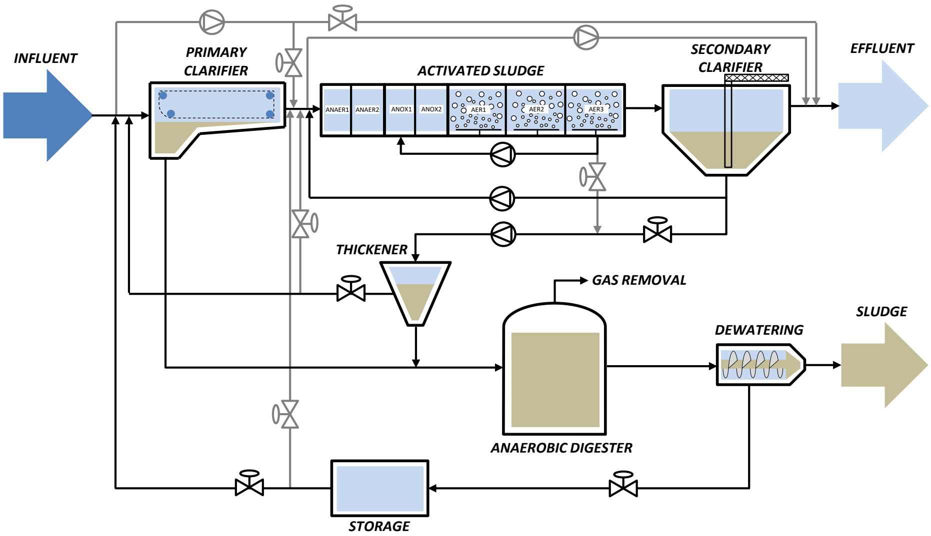

Figure 4. BSM2-P plant layout.

Model-based influent scenario generation as described in Gernaey et al. (2011) is utilized to create a dynamic wastewater influent to simulate the treatment plant performance. The resulting daily average influent mass flow rates are presented in Table 2.

Table 2. Daily average influent mass flow rates.

Mass flow rates	Value	Unit
COD	8 386	kg COD.d^{-1}
N	1 014	kg N.d^{-1}
P	197	kg P.d^{-1}
S:COD	0.003	kg S.kg COD-1

5.2. Interfaces

<u>ASM-PCM interface</u>: The default implementation of the ASM2d was adjusted in order to include the PCM. The main modifications are:

i. the use of inorganic carbon (S_{IC}) instead of alkalinity (S_{ALK}) as a state variable;

ii. the inclusion of mass transfer equations for CO_2, H_2S, NH_3 and N_2 (Batstone et al., 2012; Lizarralde et al., 2015);

iii. consideration of multiple cations (S_K, S_{Na}, S_{Ca}, S_{Mg}) and anions (S_{Cl}), which are tracked as soluble/reactive states; and,

iv. omission of chemical precipitation using metal hydroxides (X_{MeOH}) and metal phosphates (X_{MeP}) since the generalised kinetic precipitation model is used instead (Hauduc et al., 2015; Kazadi Mbamba et al., 2015a; 2015b).

The outputs of the ASM2d at each integration step are used as inputs for the aqueous phase module to estimate pH and ion speciation/pairing while precipitation and stripping equations are formulated as ordinary differential equations and included in the system of ODEs in the ASM2d.

<u>ADM-PCM interface</u>: The ADM is slightly modified to account for the updated physico-chemical model and new processes. The main modifications are:

i. the original pH solver proposed by Rosén et al. (2006) is substituted with the physico-chemical model;

ii. C, N, P, O and H fractions are updated and taken from de Gracia et al. (2006);

iii. the original ADM1 pools of undefined cations (S_{cat}) and anions (S_{an}) are substituted for specific compounds as in the ASM-PCM interface; and,

iv. the existing gas-liquid transfer equations are extended to include H_2S and NH_3.

Similar to the ASM-PCM interface, the outputs of the ADM at each integration step are used as inputs for the aqueous phase module to estimate pH and ion speciation/pairing while precipitation and stripping equations are formulated as ordinary differential equations and included in the system of ODEs in the ADM.

ASM-ADM-ASM interface: The continuity-based interfacing method (CBIM), described in Volcke et al. (2006), Zaher et al. (2007) and Nopens et al. (2009), is used for creating the interfaces between ASM-ADM-ASM to ensure elemental mass and charge conservation. The ASM-ADM-ASM interfaces consider instantaneous processes and state variable conversions.

5.3. Other Unit Processes

Aside from the activated sludge units and the anaerobic digesters, other process models included are primary clarifier, secondary settler, thickener and dewatering units. Thickener and dewatering units are considered as reactive. The gas stripping unit is modelled based on Kazadi Mbamba et al. (2016) while the crystallization unit is described using the multiple mineral precipitation model as presented in Kazadi Mbamba et al. (2015b).

5.4. Extended Evaluation Criteria

To assess the performance of combined C, N and P control strategies, an updated set of evaluation criteria is necessary (Jeppsson et al., 2013; Solon & Snip, 2014). This allows for simplification of the large output dataset into a more manageable set of comparable numbers. The effluent concentrations over the evaluation period should, at all times, obey the concentration limits given in Table 3.

Table 3. Effluent quality limits.

Variable	Value	Unit
N_{total}	< 18	g N.m^{-3}
COD_{total}	< 100	g COD.m^{-3}
S_{NH}	< 4	g N.m^{-3}
TSS	< 30	g SS.m^{-3}
BOD_5	< 10	g BOD.m^{-3}
P_{total}	< 2	g P.m^{-3}

Additional consideration has been necessary to include effluent violations (frequency and magnitude) and percentiles related to P.

The Effluent Quality Index (*EQI*) reflects the amount of pollution discharged onto surface waters averaged over the period of observation based on a weighting of the effluent loads of compounds that have a major influence on the quality of the receiving water and are usually included in the legislation. The *EQI* is updated to include the additional P load, both organic and inorganic.

Another criterion is the Operational Cost Index (*OCI*). It is given as the weighted sum of costs related to sludge production, aeration, pumping, external carbon source, mixing, heating and the benefit of methane production. Because of the modifications to the plant layout and operation, additional costs are considered, such as those relating to the additional recycles (anoxic, anaerobic), aerators (CO_2 stripping) and chemicals (for chemical P precipitation and/or recovery).

6. Scenario Analysis

The plant-wide model is tested and used to analyse and compare several operational strategies aimed at phosphorus removal and recovery. Four dynamic scenarios are analysed:

i. A_0 – default, open loop configuration (i.e. no control);

ii. A_1 – cascade ammonium and wastage controller;

iii. A_2 – cascade ammonium and wastage controller + iron addition (i.e. chemical P precipitation) in the activate sludge section; and,

iv. A_3 – cascade ammonium and wastage controller + struvite recovery.

The default configuration without any control (A_0) represents the reference operational conditions with which the different operational/control/recovery strategies are implemented, simulated and evaluated.

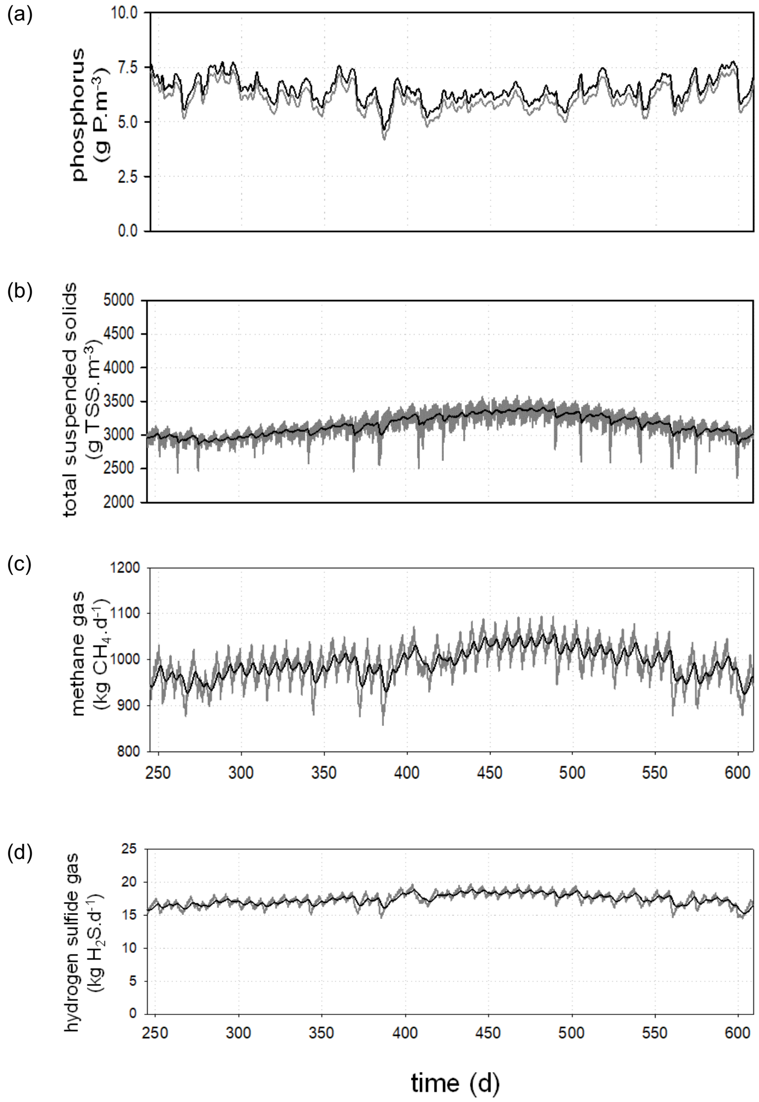

Figure 5. Dynamic profiles for the default open loop scenario (A_0) showing: (a) effluent P (inorganic phosphorus (grey) and TP (black)), (b) TSS in AER3, (c) methane gas production and (d) hydrogen sulfide gas production. An exponential smoothing filter (time constant = 3 days) is used to improve visualization of the data. Raw data is presented in grey (in (b), (c), (d)).

Dynamic profiles can be obtained using the model and some selected output variables are shown in Figure 5. All of the proposed alternatives (A_1, A_2 and A_3) result in significant improvements compared with the open loop configuration (A_0). The implementation of controllers for a better aeration strategy and sludge wasting scheme (A_1) results in a favourable alternative. Simulation results also show that this option leads to larger N and P effluent reductions, but is also a more cost-effective way to operate the plant. Both A_2 and A_3 also substantially reduce the quantity of effluent P. However, A_3 considers a modification of the plant layout by addition of a recovery unit. Capital costs for the crystallizer, stripping unit, blowers, civil, electrical and piping works should be included in order to make a more complete techno-economic assessment. On the other hand, A_2 can be set up with an extra dosing tank. Even though the potential benefit that comes from struvite recovery is very uncertain and these results should be taken with care, the cost for each kg N and P removed is much higher for A_2 (see N_{removed}/OCI and P_{removed}/OCI values in Table 4).

The model shows the importance of linking the P with the S and Fe cycles. This is a perfect starting point for evaluating and developing control strategies for wastewater treatment plants with focus on resource recovery (Solon et al., 2017). The sub-models included can be used as modelling tools to simulate particular processes. For example, the ADM1 model can be used independently as well as the ASM2d, both of which are extended with P, S and Fe related conversions. On the other hand, the model extensions could also be applied to integrated urban water systems wherein it is important to track the chemicals added in the sewer network and how it could impact the downstream WWTP processes.

Table 4. Evaluation criteria for the evaluated control/operational strategies.

Operational alternatives →	**A_0**	**A_1**	**A_2**	**A_3**	**Unit**
N_{Kjeldahl}	3.5	3.6	3.6	3.7	g N.m^{-3}
N_{total}	11.2	9.2	9.1	8.5	g N.m^{-3}
P_{inorg}	5.95	2.9	0.9	0.6	g P.m^{-3}
P_{total}	6.4	3.7	1.7	1.5	g P.m^{-3}
EQI	18 234	12 508	8 237	7 766	kg pollution.d^{-1}
TIV S_{NHX} (= 4 g N.m^{-3})	0.95	0.07	0.08	0.08	%
TIV N_{total} (= 14 g N.m^{-3})	0	0	0	0	%
TIV P_{total} (= 2 g N.m^{-3})	100	75	13.4	15.7	%
AE	4 000	3 146	3 218	3 194	kWh.d^{-1}
$E_{\text{production}}$	5 955	6 054	6 150	6 038	kWh.d^{-1}
SP_{disposal}	3 461	3 538	3 730	3 487	kg TSS.d^{-1}
M_{FeCl3}	-	-	169	-	kg Fe.d^{-1}
$M_{\text{Mg(OH)2}}$	-	-	-	40	kg Mg.d^{-1}
$S_{\text{recovered}}$	-	-	-	206	kg struvite.d^{-1}
OCI	10 201	9 495	13 770	8 912	-
G_{CH4}	992	1 009	1 025	1 006	kg CH_4.d^{-1}
G_{H2S}	17.4	19.2	12.1	19.2	kg H_2S.d^{-1}
N_{removed}/OCI	0.079	0.089	0.062	0.097	kg N (removed).OCI^{-1}
P_{removed}/OCI	0.007	0.013	0.012	0.019	kg P (removed).OCI^{-1}

7. Key Contributions

The key contributions of this research to the state of knowledge are stated below.

- A versatile/general module which takes into account ion activity corrections and ion pairing is developed. This can be easily added to different activated sludge (AS) and anaerobic digestion (AD) models and can reliably predict pH and speciation of components under anaerobic, anoxic and aerobic conditions in AS and AD models.
- Phosphorus, sulfur and iron transformations under anaerobic, anoxic and aerobic conditions are added to ASM2d for plant-wide phosphorus modelling and simulation.
- An extension of ADM1 with sulfate reduction, iron reduction and phosphorus transformations is developed for plant-wide phosphorus modelling and simulation. In addition, model interfaces are developed to link the extended ASM2d and ADM1 variables.
- A platform for control strategy development, testing and evaluation for wastewater treatment plants designed for carbon, nitrogen and phosphorus removal and/or recovery is presented.
- Multi-criteria (economic/environmental) analysis of the results is provided taking into account phosphorus-related components and cost of chemicals/price of resource for effluent quality and operational cost evaluation, respectively.

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