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# Assessment of sludge management strategies in wastewater treatment systems using a plant-wide approach

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ABSTRACT

The objective of this paper is to use plant-wide modeling to assess the net impacts of varying sludge management strategies. Special emphasis is placed on effluent quality, operational cost and potential resource recovery (energy, nutrients). The study is particularly focused on a centralized bio-solids beneficiation facility (BBF), which enables larger, more capital intensive sludge management strategies. Potential barriers include the ability to process reject streams from multiple donor plants in the host plant. Cape Flats (CF) wastewater treatment works (WWTW) (Cape Town, South Africa) was used as a relevant test case since it is currently assessing to process sludge cake from three nearby facilities (Athlone, Mitchells Plain and Wildevoelvlei). A plant-wide model based on the Benchmark Simulation Model no 2 (BSM2) extended with phosphorus transformations was adapted to the CF design / operational conditions. Flow diagram and model parameters were adjusted to reproduce the influent, effluent and process characteristics. Historical data between January 2014 and December 2019 was used to compare full-scale measurements and predictions. Next, different process intensification / mitigation technologies were evaluated using multiple criteria. Simulation values for COD, TSS, VSS/TSS ratio, TN, TP, $NH_4^+/NH_3$, $H_xPO4^{3-x}$, $NO_x$ alkalinity and pH fall within the interquartile ranges of measured data. The effects of the 2017 severe drought on influent variations and biological phosphorus removal are successfully reproduced for the entire period with dynamic simulations. Indeed, 80% of all dynamically simulated values are included within the plant measurement uncertainty ranges. Sludge management analysis reveals that flow diagrams with thermal hydrolysis pre-treatment (THP) result in a better energy balance in spite of having higher heat demands. The flow diagram with THP is able to i) increase biodegradability/solubility, ii) handle higher sludge loads, iii) change methanogenic microbial population and iv) generate lower solids volumes to dispose by improving sludge dewaterability. The study also reveals the importance of including struvite precipitation and harvesting (SPH) technology, and the effect that pH in the AD and the use of chemicals (NaOH, MgO) may have on phosphorus recovery. Model-based results indicate that the current aerobic volume in the water line (if properly aerated) would be able to handle the returns from the sludge line and the contribution of a granular partial nitritation/Anammox (PN/ANX) reactor on the overall nitrogen removal would be marginal. However autotrophic N denitrification generates a much lower sludge production and therefore increases AD treatment capacity. The study shows for the very first time in Africa how the use of a (calibrated) plant-wide model could assist water utilities to decide between competing plant layouts when upgrading a WWTW.



## 1. Introduction

Sludge processing is an important part of water resource recovery facilities (WRRF) and it is focused on reducing volume and odors as well as to remove pathogens in order to make bio-solids (the final product) disposable and/or reusable. Sludge processing

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**Nomenclature**

| | |
|---|---|
| AD | Anaerobic digestion |
| ADM | Anaerobic Digestion Model |
| AER | Aerobic reactor |
| ANAER | Anaerobic reactor |
| ANOX | Anoxic reactor |
| ASM | Activated Sludge Model |
| ASR | Activated Sludge Reactors |
| BBF | Bio-solids beneficiation facilities |
| CAPEX | Capital expenditures |
| CF | Cape Flats |
| $CHEM_{MgO}$ | Chemical addition, MgO (kg/d) |
| $CHEM_{NaOH}$ | Chemical addition, NaOH (kg/d) |
| $CHEM_{struv}$ | Chemical recovery, struvite (kg/d) |
| CHP | Combined heat and power unit |
| CoCT | City of Cape Town |
| COD | Chemical oxygen demand (g/m$^3$) |
| $COD_{part}$ | Particulate chemical oxygen demand (g/m$^3$) |
| $COD_{sol}$ | Soluble chemical oxygen demand (g/m$^3$) |
| CSTR | Continuous stirred tank reactor |
| DB | Drying beds |
| MgO | Magnesium oxide |
| DEW | Dewatering |
| $DO_{operational}$ | Operational dissolved oxygen (g/m$^3$) |
| $E_{aeration}$ | Aeration energy (MWh/d) |
| $E_{consumption}$ | Energy consumption (MWh/d) |
| $E_{electricity,recovery}$ | Electrical energy, recovery (MWh/d) |
| $E_{heat,demand}$ | Heating energy, demand (MWh/d) |
| $E_{heat,recovery}$ | Heating energy, recovery (MWh/d) |
| $E_{mixing}$ | Mixing energy (MWh/d) |
| $E_{net}$ | Net Energy (MWh/d) |
| $E_{pumping}$ | Pumping energy (MWh/d) |
| Fe | Iron |
| FLOT | Flotation |
| FBDA | fine bubble diffused air |
| HRT | Hydraulic retention time (d) |
| $H_xPO4^{3-x}$ | Phosphates (g/m$^3$) |
| ISS | Inorganic suspended solids (g/m$^3$) |
| $ISS_0$ | Particulate inorganics with influent (g/m$^3$) |
| IWA | International Water Association |
| $K_H$ | Henry coefficient (m$^3$/atm.Kmol) |
| $L_{biofilm}$ | Granule radius, biofilm thickness (m) |
| LCA | Life cycle assessment |
| LCC | Life cycle costing |
| MLSS | Mixed liquor suspended solids (g/m$^3$) |
| N | Nitrogen |
| NaOH | Sodium hydroxide |
| $NH_4^+/NH_3$ | Ammonium/ammonia (g/m$^3$) |
| $NO_X$ | Nitrates (g/m$^3$) |
| OPEX | Operational expenditures |
| P | Phosphorus |
| PCM | Physico-Chemical Model |
| $pH_{operational}$ | Operational pH at the SPH reactor |
| $P_I$ | Partial pressure (atm) |
| PN/ANX | Partial nitritation / Anammox |
| PRIM | Primary clarifier |
| PWM | Plant Wide Model |
| $Q_{intr}$ | Internal recycle (m$^3$/d) |
| $Q_R$ | External recycle (m$^3$/d) |
| $Q_W$ | Waste flow (m$^3$/d) |
| $Q_p$ | Primary underflow (m$^3$/d) |
| $Q_{tck}$ | Thickening underflow (m$^3$/d) |
| $Q_{flot}$ | Flotation overflow (m$^3$/d) |
| $Q_{dew}$ | Dewatering underflow (m$^3$/d) |
| reAER | Re-aeration tank |
| S | Sulfur |
| $S_A$ | Soluble acidified compounds (g/m$^3$) |
| SC | Scenario |
| SEC | Secondary clarifier |
| $S_F$ | Soluble fermentable compounds (g/m$^3$) |
| $S_i$ | Soluble compound |
| $S_I$ | Soluble organic inerts (g/m$^3$) |
| SMS | Sludge management strategy |
| SP | Sludge production (T/d) |
| SPH | Struvite precipitation and harvesting |
| SRT | Solids retention time (d) |
| THK | Thickener |
| THP | Thermal hydrolysis pre-treatment |
| TKN | Total kjeldahl Nitrogen (g/m$^3$) |
| TN | Total nitrogen (g/m$^3$) |
| $T_{op}$ | Temperature operational (C) |
| TP | Total phosphorus (g/m$^3$) |
| TS | Total sulfur (g/m$^3$) |
| TSS | Total suspended solids (g/m$^3$) |
| $TSS_{overflow}$ | Total suspended solids in the overflow (g/m$^3$) |
| $TSS_{underflow}$ | Total suspended solids in the underflow (%) |
| $TSS_{operational}$ | Total suspended solids in the PN/ANX reactor (g/m$^3$) |
| $TSS_{recovery}$ | Total suspended solids recovery after SRH reactor |
| VSS | Volatile suspended solids (g/m$^3$) |
| WRRF | Water resource recovery facilities |
| WWTW | Wastewater treatment works |
| $X_B$ | Particulate organic biomass (g/m$^3$) |
| $X_i$ | Particulate compound |
| $X_I$ | Particulate organic inert (g/m$^3$) |
| $X_S$ | Particulate organic biodegradable (g/m$^3$) |
| $Z_i$ | Ionic species, calculated with the aqueous phase chemistry model |

trains involve a series of unit operations, namely thickening, treatment, dewatering and reject water handling. The treatment section (anaerobic & aerobic digestion, chemical stabilization, composting) is the central part of the process but may include pretreatment (thermal and/or enzymatic hydrolysis, pasteurization) and post-treatment steps (conditioning, gasification, drying, incineration). Another important aspect to consider is reject water resulting from sludge treatment, which will impose a substantial component of the hydraulic, organic and nitrogen/phosphorus load when returning to the water line. Technology selection is strongly influenced by expected effluent water quality, economic performance, beneficial use requirements (for sludge) and local conditions (WEF 2018, Tchobanoglous et al., 2013).

The state of the art procedure to evaluate sludge treatment alternatives is traditionally carried out using simplistic design equations, rules of thumb or mathematical models through general (e.g. Matlab/Simulink) or specific (e.g. GPS-X, WEST-DHI, SUMO, BIOWIN) software simulation environments (Gernaey et al., 2004). These packages are extremely useful to evaluate promising technologies before full-scale implementation (Rieger et al., 2012). In this way, undesirable options may be identified at an early stage and only effective solutions will be put into practice. Indeed, the use of mathematical models has become a common practice in water/wastewater engineering with multiple applications in design (Flores-Alsina et al., 2012a), benchmarking (Copp, 2002;

Jeppsson et al., 2007), diagnosing (Rodriguez-Roda et al., 2002), and optimization (Rivas et al., 2008; Feldman et al., 2018).

An emerging (but challenging) best practice is the simultaneous consideration of water and sludge lines in plant-wide models. The recent developments within the IWA Task Group on Physico-chemical Modelling (Batstone et al., 2012) have generated multiple research outputs allowing a substantial advancement in that direction, more specifically, aqueous phase chemistry models (Solon et al., 2015; Lizarralde et al., 2015), precipitation frameworks (Barat et al., 2011; Kazadi-Mbamba et al., 2015a; Kazadi-Mbamba et al., 2015b; Bradley et al., 2019; Elduayen-Echave et al., 2019), solving routines (Flores-Alsina et al., 2015) and mass transfermodeling approaches (Lizarralde et al., 2018; Amaral et al., 2019; Baeten et al., 2020). As a result, it has been possible to predict the close interactions between phosphorus (P), sulfur (S) and iron (Fe) through the entire plant and expose long-term cyclic interactions within the treatment system (Solon et al., 2017; Kazadi-Mbamba et al., 2019). Anaerobic digestion is included in the current plant-widemodeling work, and has exposed critical interactions between sludge and water lines, particularly related to phosphorus and nitrogen cycling (Batstone et al., 2015b). This is emphasized where centralized bio-solids management is used, which can leverage large sludge input flows to justify capital intensive projects, but where the return loads are increased, possibly to the limits of the main line capacity.

In this paper, we present a model-based study of sludge management strategies (SMS) using the City of Cape Town (CoCT) municipality as a case study, where treatment and processing of wastewater sludges will be centralised in three regionalised locations: 1) Cape Flats (CF) WWTW (south), 2) Vissershok WWTW (North) and 3) Zandvliet WWTW (East). The CoCT refers to those as bio-solids beneficiation facilities (BBF). This was done by developing a model-based feasibility study of different treatment technologies to be implemented in the planned CF BBF, which will be located at the existing CF WWTW and will treat wastewater sludge from the CF WWTW itself, and from three other nearby WWTWs - Athlone (105,000 $m^3$/d design capacity); Mitchells Plain (35,000 $m^3$/d design capacity) and Wildevoelvlei (14,000 $m^3$/d design capacity). A mathematical model describing COD, TSS, N and P removal processes with the current design/operational conditions was constructed and predictions verified with influent/effluent/process data comprising the years from 2014 to 2019. Different stabilization, pre- and post-treatment units were added and compared to the base case scenario using multiple evaluation criteria. *This study present a series of novelties* compared to the state of the art work in this field.

1) A set of models describing sludge management strategies in wastewater treatment works (WWTW). Publications considering plant-wide aspects have usually focused on virtual case studies (Flores-Alsina et al., 2014a; Jia et al., 2020). There are only very few cases where full-scale systems have been successfully described (Kazadi-Mbamba et al., 2016; Hauduc et al., 2019; Vaneeckhaute et al., 2017) and all of them only allowed P recovery options (Marti et al., 2017; Lizarralde et al., 2019). No pretreatment methods and/or other reject water treatment methods, i.e. granular sludge, have been included and evaluated *within* a plant-wide context in a real case study.
2) A model library comprised of different sludge treatment technologies: thermal hydrolysis pre-treatment (THP), granular nitritation / anammox (PN/ANX) reactor and struvite precipitation and harvesting (SPR), easily linkable within the plant-wide approach, in order to simulate all units simultaneously. Previous investigations have been focused on analyzing these technologies separately (Wett et al., 2014; Vangsgaard et al., 2013; Galbraith et al., 2014) without paying special attention to PWM aspects such as model compatibility, overall model stiffness and computational efficiency.
3) A mass balance methodology is used to quantify the fate of COD, N and P through the plant This is accomplished for the different models (activated sludge, anaerobic digestion, pre-treatment, reject water), multiple interfaces, reactor designs (continuous stirred tank reactor, plug flow, granular) and the process configurations/treatment options evaluated within the study (Volcke et al., 2006). Plant-wide mass balances can be achieved when integrated methodologies / supermodels are accounted (Grau et al., 2009; Ekama, 2009; Barat et al., 2013; Fernandez-Arevalo et al., 2017; Hauduc et al., 2019) having to deal with the well-known problems of computational power and /or model transparency.
4) A holistic evaluation methodology, taking into account water, sludge and centrate process interactions applied to a real full-scale system. Special aspects such as energy expenditures (categorized in aeration, mixing, pumping, heating), use of different types of chemicals, sludge production and potential recovery (energy and nutrients) through the different flow diagrams is accounted for all the generated alternatives (Gernaey et al., 2014; Solon et al., 2017).

The paper details the development of the new PWM for this study by presenting sequentially the elements it is comprised of, as well as highlighting the integration/interfacing aspects. Model prediction capabilities are verified using full-scale data. The potential of the proposed approach is illustrated by comparing different SMS. Additional scenario analyses further explore the effect of selected operational settings (imported sludge loading, pH in the AD and struvite reactor, aerobic granular volume…) on the overall process performance. Lastly, opportunities and limitations that arise from utilization of the new models are discussed in detail.

## 2. Methods

### 2.1. Case study: Cape Flats

#### 2.1.1. Process description

The Cape Flats Wastewater Treatment Works (CF WWTW) is located adjacent to and south of the Zeekoevlei Nature Reserve, adjoining the suburb of Muizenberg in the south of Cape Town. The WWTW primarily treats wastewater of domestic origin, with a small portion of commercial/industrial wastewater (ca. 5%). The works are owned and operated by the City of Cape Town (CoCT). The plant was initially designed to treat an average dry weather flow (ADWF) of 150,000 $m^3$/d and consisted of six parallel modules (A,B,C,D,E,F), each with 25,000 $m^3$/d capacity. In 1999, an additional two modules with 25,000 $m^3$/d capacity were constructed (G,H). Currently, the plant has a total capacity of 200,000 $m^3$/d over eight parallel modules.

The treatment process used at the CF WWTW includes primary sedimentation (PRIM) followed by activated sludge reactors (ASR). An extensive maturation pond system is the final treatment step. Cape Flats WWTW was designed for nitrification, denitrification and for biological phosphorus removal. Thickened primary sludge (THK) and thickened biological sludge (FLOT) are anaerobically digested (AD). Currently, the digested sludge is dewatered in drying beds (DB). A schematic representation of the main units comprising the flow diagram is depicted in Fig. 1. The main design characteristics are summarized in Table 1.

#### 2.1.2. Historical data

The measured data used in this study comprises the historical data between January 2014 and December 2019 (5 years, 1 sample per week). Samples were taken from 22 locations: 1 point at

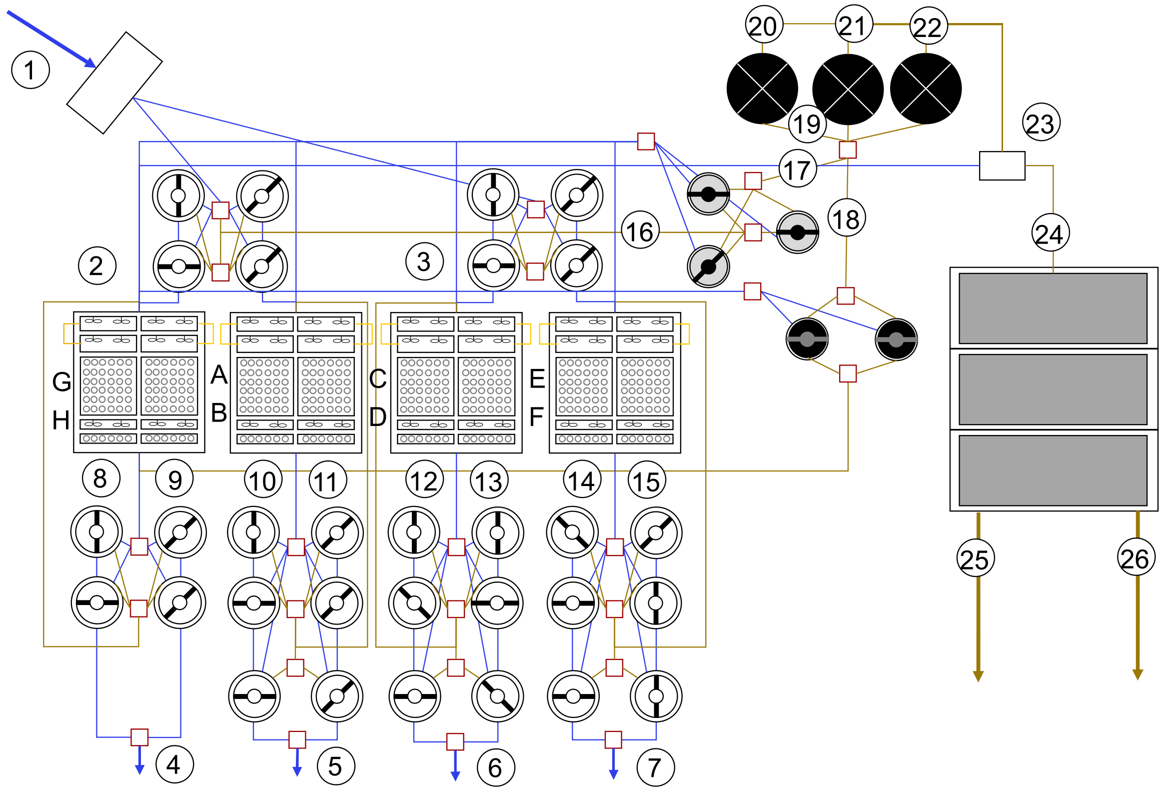


**Fig. 1.** Flow diagram of Cape Flats WWTW (adapted from Google Earth): 1) influent / raw wastewater, 2 and 3) effluent of primary clarification, 4–7) effluent of secondary clarification, 8–15) outflow of activated sludge section, 16) underflow of primary clarification, 17) underflow of primary sludge thickener, 18) overflow of secondary sludge dissolved air flotation unit, 19) influent of anaerobic digestion, 20–21) effluent of anaerobic digestion, 23) mechanical dewatering (non-active), 24) drying beds, 25) sludge to disposal and 26) reject water.

**Table 1**
Main design characteristics of Cape Flats WWTW.

| Tank | ID | Height/depth (liquid) m | Volume $m^3$ | Diameter M |
|---|---|---|---|---|
| Primary clarification | PRIM 1–8 | 3.4 | 1413 | 23 |
| Anaerobic reactors (A-F) | ANAER 1,2,3,4,5,6 | 10 | 1042 | – |
| | ANAER 7,8 | 10 | 1382 | – |
| ANOXIC reactors | ANOX 1,2,3,4,5,6 | 10 | 2301 | – |
| | ANAER 7,8 | 10 | 2916 | – |
| AEROBIC reactors | AER 1,2,3,4,5,6 | 10 | 7360 | – |
| | AER 7,8 | 10 | 7522 | – |
| Post ANOXIC reactors | postANOX 1,2,3,4,5,6 | 10 | 2600 | – |
| | postANOX 7,8 | 10 | 2456 | – |
| *Re*-aeration reactors | reAER 1,2,3,4,5,6 | 10 | 1040 | – |
| | reAER 1,2,3,4,5,6 | 10 | 1074 | – |
| Secondary clarifiers | SEC 1–18 | 4 | 2024 | 26 |
| | SEC 19–22 | 4 | 3019 | 31 |
| Thickeners | THK 1–3 | 3.5 | 921 | 18 |
| Flotation | FLOT 1,2,3 | 2 | 234 | 12 |
| Anaerobic digester | AD1,2,3 | 20 | 6300 | 20 |

the raw wastewater inlet, 2 points at the primary effluent (module A-D & module E-H), 4 points at the secondary effluent (module A-B, C-D, E-F & G-H), 8 points at the activated sludge section (module A-H), 1 point at the combined primary clarifier underflows, 1 point at the thickener sludge underflow, 1 point at the dissolved air flotation overflow, 1 point at the combined entrance of the anaerobic digesters, 3 points at the effluent of the anaerobic digesters. Measurements involved the determination of: pH, TSS, VSS, COD, TN and TP. These analyses were complemented with filtered (0.45 Mm) samples for quantifying $NH_4^+/NH_3$, $H_xPO_4^{3-x}$, alkalinity and $NO_x$ (solution) (see Table 2). Standard methods were used for the experimental determination of the different process parameters.

*2.2. Sludge management strategies*

The *first sludge management strategy (SMS0)* explores the future potential of using Cape Flats as Bio-solids Beneficiary Facility (BBF) with the current flow diagram. The external (imported) sludge from nearby WWTWs: 1. Mitchells Plain (primary sludge, dewatered and secondary sludge, dewatered), and 2. Wildevoelvlei (secondary sludge, dewatered) will be trucked to the Cape Flats BBF blended with the indigenous CF sludge before anaerobic digestion (see quantities in Table 3). Primary and secondary sludge from the third donor WWTW (Athlone WWTW) is already introduced to CF via sewer pipes (i.e. Athlone sludge is re-introduced to the sewer to gravitate to CF with raw wastewater). It is assumed

**Table 2**
Sampling points and main analytical measurements for each sample. For the location of sampling points refer to Fig. 1.

| | | 1 | 2,3 | 4- 7 | 8–15 | 16 | 17 | 18 | 19 | 20–22 |
|---|---|---|---|---|---|---|---|---|---|---|
| TSS | $g/m^3$ | X | X | X | X | X | X | X | X | X |
| VSS/TSS | % | X | X | X | X | X | X | X | X | X |
| COD | $g/m^3$ | X | X | X | | | | | | |
| TN | $g/m^3$ | X | X | X | | | | | | |
| $NH_4^+/NH_3$ | $g/m^3$ | X | X | X | | | | | | |
| $NO_x$ | $g/m^3$ | X | X | X | | | | | | |
| TP | $g/m^3$ | X | X | X | | | | | | |
| $H_xPO_4^{3-x}$ | $g/m^3$ | X | X | X | | | | | | |
| pH | – | X | X | X | X | | | | | X |
| Alkalinity | $g/m^3$ | X | X | X | X | | | | | X |

that there is a combined heat and power (CPH) recovery unit and the stabilized sludge is mechanically dewatered to up to 27% dry matter. Reject water will be recycled back to the main line aerobic zone. *Sludge management strategy 1 (SMS1)* upgrades the AD section with three additional reactors (= double volume). In strategy 2 (*SMS2*) thermal hydrolysis pre-treatment (THP) is added, consisting of 3 units: pulper, reactor and flash tank. Temperature and pressure is increased gradually (up to 180 °C and 6 bar) in the pulper tank to facilitate the cell breakage in the flash tank. Sludge temperature is reduced to mesophilic conditions ($T$ = 35 °C) and heat is partially recovered through heat exchangers before entering the AD. The process flowsheet will also include a dewatering system before THP to reach a target TSS concentration of 16% following manufacturing recommendations (Barber 2016). Dilution water will be used to control the $NH_3$ concentration in the AD and reduce the TS post PHT to 9%. Sludge from the final dewatering was assumed to be up to 30% dry matter (see Table 3). *Sludge management strategy* 3 and 4 account for reject water treatment in *SMS2*. The third

**Table 3**
Influent sources, technical improvements, and operational modifications included in the default CF layout to be considered during the evaluation of sludge management strategies (SMS).

| | Sludge management strategy |
|---|---|
| ***Additional sludge loads*** | |
| Mitchells Plain (primary) =10 Tons TSS/d<br>Mitchells Plain (secondary) = 28 Tons TSS/d<br>Wildevoelvlei (secondary) = 4 Tons TSS/d | *SMS0, SMS1, SMS2, SMS3, SMS4* |
| ***Primary clarifier efficiency*** | |
| $TSS_{primary}$ = 50% | *SMS0, SMS1, SMS2, SMS3, SMS4* |
| ***Improved aeration system*** | |
| $DO_{aeraion}$=2 $g/m^3$ and $DO_{re\text{-}aeration}$ =1.5 $g/m^3$ | *SMS0, SMS1, SMS2, SMS3, SMS4* |
| ***Pre-dewatering*** | |
| $TSS_{underflow}$ = 16% | *SMS2, SMS3, SMS4* |
| ***Thermal hydrolysis pre-treatment*** | |
| $T_{pulper}$ = 100 °C, $P_{pulper}$ = 1 bar, $T_{reactor}$ = 180 °C, $P_{pulper}$ = 6 bar,<br>$T_{reactor}$ = 100 °C, $P_{pulper}$ = 1 bar, $TSS_{output}$ = 9%<br>(*by water dilution) | *SMS2, SMS3, SMS4* |
| ***Upgraded Anaerobic digestion volume*** | |
| HRT = 30 days | *SMS1* |
| ***Sludge dewatering after PHT*** | |
| *SMS2, SMS3, SMS4* | *SMS2, SMS3, SMS4* |
| ***Sludge dewatering after conventional AD*** | |
| $TSS_{underflow}$ = 27% | *SMS0, SMS1* |
| ***Partial Nitration / Anammox*** | |
| HRT = 1 day,<br>$TSS_{operational}$ = 20,000 $g/m^3$<br>$DO_{operational}$ = 0.5 g/m3<br>$L_{biofilm}$ = 0.001 m | *SMS3* |
| ***Struvite reactor*** | |
| HRT = 0.5 day; $PH_{operational}$ = 9; Addition of MgOH (25%) and NaOH (25%) | *SMS4* |
| ***P harvesting system*** | |
| $TS_{underflow}$ = 30%<br>$TS_{recovery}$ = 98% | *SMS4* |

strategy (*SMS3*) is based on adding an aerobic granular sludge reactor running partial nitritation / Anammox (PN/ANX) and the fourth strategy (*SMS4*) incorporates a struvite precipitation and harvesting (SPH) unit. It is important to point out that primary TSS removal efficiency in PRIM1–8 is reduced in order to maximize denitrification / P release in the activated sludge in all evaluated scenarios. A substantial upgrade in the blower systems is assumed in both aerobic (AER1–8) and re-aeration (reAER1–8) zones to increase dissolved oxygen (DO) distribution within the tanks. More information about the different scenarios and assumptions made can be found in Table 3. Flow diagrams of each alternative can be found in the Supplemental Information (Figures S1–4).

### 2.3. Mathematical models

#### 2.3.1. Biological models

A modified version of the Activated Sludge Model (ASM) No 2d was used to describe the main reactions in the water line (Henze et al., 2000). The model was upgraded to account for: i) the role of Mg and K during the formation of polyphosphates, ii) electron acceptor dependency during microbial decay, and iii) S and Fe oxidation / reduction reactions. The sludge line was approximated using the Anaerobic Digestion Model (ADM) no 1 (ADM1) (Batstone et al., 2002). The model was extended to describe P, S and Fe reactions according to Flores-Alsina et al. (2016) and Ikumi and Harding (2020). It also includes special $NH_3$ inhibition functions and acetate oxidizing processes as described in Wett et al. (2014). Both ASM and ADM explicitly differentiate between organic (VSS) and inorganics (ISS) fractions in total suspended solids (TSS) (Ekama and Wenzel, 2004; Ekama et al., 2006). More information about both ASM and ADM models can be found in Solon et al. (2017).

#### 2.3.2. Physico-chemical model (PCM)

A common physico-chemical framework was implemented in both ADM and ASM. The model simulates the acid-base system and is thereby able to predict pH (Solon et al., 2015). It also corrects for ionic strength (I) via the Davies approach to consider chemical activities instead of molar concentrations and hence performs all the calculations under non-ideal conditions (Flores-Alsina et al., 2015). Multiple mineral precipitation potential is described in the model based on Saturation Index calculations (SI) (Kazadi Mbamba et al., 2015a,b). Mass transfer between the liquid and the gas phase is accounted for selected compounds ($i = S_{O2}$, $S_{N2}$, $Z_{CO2}$, $Z_{NHX}$, $S_{CH4}$, $S_{H2}$). The transport rates are formulated as a function of the difference between the saturation concentration and the actual concentration of the gas dissolved in the liquid (Batstone et al., 2012). The saturation concentration of the gas in the liquid is given by Henry's law of dissolution, which states that the saturation concentration is equal to the product of Henry's constant ($K_H$) multiplied by the partial pressure of the gas ($P_i$). All constants are temperature corrected.

#### 2.3.3. Sludge pre-treatment models: thermal hydrolysis

Thermal hydrolysis was described accounting for pasteurization, solubilisation and viabilization (see Wett et al., 2014; Aichinger et al., 2019). Pasteurization includes decay of all living microorganisms (=cell breakage). These are converted into different biodegradable (proteins, carbohydrates and lipids) and unbiodegradable (soluble and particulate inerts) compounds. In solubilisation, all biodegradable material is hydrolysed into smaller monomers i.e. amino acids, sugars and fats. There is an important fraction (60%) that is further converted into volatile fatty acids (VFA) (Batstone et al., 2009). Finally, in viabilization a fraction of unbiodegradable particulates is transformed into biodegradable organic particulates. All three processes involve a substantial release of alkalinity, $NH_4^+/NH_3$ and $H_xPO_4^{3-x}$. The process also accounts for the formation of dissolved organic non-biodegradable N (DON) and P (DOP) compounds which are mainly associated with $S_I$ and $X_I$. Details about the stoichiometry of the reactions can be found in Batstone et al. (2002). Mass balances are constructed and verified to ensure continuity of COD, C, N & P.

#### 2.3.4. Sludge post-treatment models: partial nitritation/ anammox & struvite precipitation

The PN/ANX granular reactor is approximated using the multi-scale approach proposed by Feldman et al. (2017). The model accounts for Ammonium/Nitrite Oxidizing Bacteria (AOB/NOB), Anammox Bacteria (ANX) and Ordinary Heterotrophic Bacteria (OHO). It also considers methane oxidation (MOB), denitrifying anaerobic methane oxidation (DAMO) and both physico-chemical and biological S removal processes. Granules are described as 1-dimensional biofilm systems. Solubles penetrate through diffusion and particulates propagate by convective movement (Wanner et al., 2006). Struvite precipitation is described using the same PCM as described above. A PI controller maintains the pH at 9.5 by adding NaOH. There is a constant dosage of Mg to promote saturation conditions. The crystalized P is separated from the main stream in an ideal splitter (Jeppsson et al., 2007). Details about how to model the side-stream technologies can be found in Solon et al. (2017) and Flores-Alsina et al. (2019).

#### 2.3.5. Dynamic influent generator

The model modules for: (1) flow rate generation (FLOW); (2) chemical oxygen demand (COD), N and P generation (POLLUTANTS); (3) temperature profile generation (TEMPERATURE); and, (4) sewer network and first flush effect (TRANSPORT) defined in Gernaey et al. (2011) are used to generate the WWTW influent dynamics (12 months period of output data for the evaluation period with a 15 min sampling interval). In addition, cation and anion profiles had to be added. The resulting pH is close to neutrality (pH ~ 7.3). More information about the flow rate pollution dynamics and how they are handled by the influent generator can be found in Gernaey et al. (2011) and Flores-Alsina et al. (2014b).

#### 2.3.6. Ancillary models

Primary and secondary clarifiers, flotation and thickening, dewatering and struvite harvesting are described as ideal splitters (Jeppsson et al., 2007). These models are adjusted to reflect the experiments carried out by Ekama et al. (2006) where organic and inorganic compounds show different settling velocities/separation efficiencies

#### 2.3.7. Model interfaces

The plant-wide model includes different types of interfaces. First, the interface between the models for the water (ASM) and the sludge (ADM) line (and vice versa), as well as interfaces between the model for the reject water treatment unit (PN/ANX) and both ADM and ASM. All interfaces ensure continuity in mass and avoid component leaks. Second, there is also an interface between ASM, ADM and PN/ANX with the PCM. The outputs of the ASM/ADM/PN/ANX interface at each integration step are used as inputs for the PCM module to estimate pH and ion speciation/pairing (PMC module works as a sub-routine). The precipitation/stripping/inhibition equations are embedded within the AD/AS/PN/ANX ordinary differential equations (ODE) model structure and are therefore included in the overall mass balance. More information about model interfaces can be found in Solon et al. (2017).

### 2.4. Evaluation criteria

To assess the performance of the different treatment options, a set of evaluation criteria was selected following Jeppsson et al. (2013). Different effluent quality criteria, such as chemical oxygen demand (COD), total (TSS)/volatile suspended solids (VSS), total Kjeldahl nitrogen (TKN), total nitrogen (TN) and total phosphorus (TP) and phosphates ($H_xPO_4^{3-x}$) were calculated from ASM/ADM state variables (Henze et al., 2000) to assess the pollution removal efficiency of the system. Energy recovery in the AD was calculated by using the energy content of the methane gas (50.014 MJ (kg $CH_4$)$^{-1}$) and assuming a 39% and 45% efficiency for electricity ($E_{electricity,rec}$) and heat generation ($E_{heat,rec}$) respectively. The heating demand ($E_{heat,demand}$) was calculated from the quantity of water entering into the AD or the THP until reaching the desired operational ($T_{op}$) temperature (35 or 160 deg. C, respectively). Aeration energy ($E_{aeration}$) was calculated imposing an energy expenditure equal to 1.8 kg (-COD) (kWh)$^{-1}$. Pumping energy ($E_{pumping}$) was calculated as the weighted averaged sum of internal ($Q_{INTR}$) and external recycle ($Q_R$) and waste flow ($Q_W$) and different underflows ($Q_{prim}$, $Q_{thick}$, $Q_{flot}$, $Q_{dew}$) The difference between $E_{electricity,rec}$ + $E_{heat,rec}$ - $E_{aeration}$ – $E_{pumping}$ – $E_{mixing}$- $E_{heat,demand}$ is the net energy generated ($E_{net}$). Additional criteria such as quantity of sludge production (SP), use of chemicals ($CHEM_{MgO}$& $CHEM_{NaOH}$) and nutrient recovery ($CHEM_{struv}$) were quantified as described in Solon et al. (2017).

## 3. BASE case model validation

### 3.1. Influent characteristics

The assumed total load arriving to the CF WWTW is the following: COD = 107 T/d, TN = 8.5 T/d; TP =3.8 T/d, TS = 1.3 T/d and flow-rate = 110,000 $m^3$/d· It is important to highlight that simulations were not done at the full design capacity, but at the current operational point (see Section 2.1). Parameters reported in Gernaey et al., 2014 were used to characterize the influent fractions. The $COD_{part}$ was estimated from the VSS measurements. $COD_{sol}$ was calculated as difference between COD and $COD_{part}$. The $S_I$ and $X_I$ were estimated assuming 90% biodegradability for both soluble and particulate fractions (based on personal communication with plant operators). Hence, it was possible to quantify $S_F$+ $S_A$ and $X_S$. Finally, 60% of the biodegradable soluble COD was assumed to be in form of volatile fatty acids (VFA). Default values in the BSM2 model for N and P content in $S_I$, $S_F$, $X_S$, $X_I$ and $X_B$ were used to allocate the biodegradable and non-biodegradable fractions. These considerations were verified with TN, TP, $NH_x$ and $H_xPO_4^{3-x}$ measurements. The difference between VSS and TSS was allocated directly to $ISS_0$. The cationic/anionic composition was adjusted to match an influent pH of 7.3. Alkalinity measurements define the buffer capacity. Ionic strength is correlated with influent conductivity measurements. More information can be found in Table S1 in the Supplementary information section.

### 3.2. Default design / operational conditions

#### 3.2.1. Primary clarifiers

The model was adjusted to reflect the primary clarification efficiency at Cape Flats Wastewater Treatment Works (CF WWTW). Both historical data and computer simulations show that the primary clarifier is designed / operated to present an overflow TSS removal efficiency of 80% and an underflow TSS concentration up to 2% (See Fig. 2a). The higher than expected values are due to the arrival of primary and secondary sludge from the nearby Athlone WWTW in the raw wastewater. The sludge from Athlone is reintroduced into the sewer network to be treated at the Cape Flats Settling characteristics were adjusted to reflect the sedimentation differences between the VSS and ISS fractions (see VSS/TSS ratio in Fig. 2b). Additional simulations show good prediction capabilities for COD, TN and TP at the effluent primary clarification (PRIM) (see Fig. 2c,d,e,f,g). In terms of mass balances, both model and data show that the primary clarifier lets 36, 70 and 70% of the influent total COD, TN and TP loads to pass to the overflow stream. Additional calculations confirmed that the underflow is taking the remaining 64, 30 and 30%. pH and alkalinity simulations/measurements are not substantially affected (primary clarification tank is assumed to be non-reactive) (see Fig. 2i and j).

#### 3.2.2. Activated sludge reactors and secondary clarifiers

The virtual and the full-scale reactors are operated to maintain an MLSS concentration of 5300 mg/L by wasting excess activated sludge from the last reactor (reAER) (See Fig. 2a) (SRT ≈ 20 days). There is an internal recycle from the aerobic (AER) to the anoxic (ANOX) section with a flow rate that is in a 6:1 ratio to the influent flow. The TSS is recirculated from the secondary clarifier (SEC) to the first anoxic reactor with a flow rate that is proportional to the influent flow rate at a concentration of 7500 mg/L. The same strategy as in the primary clarifier (PRIM) is applied to differentiate the settlability of VSS and ISS (See Fig. 2b). Aeration is regulated to maintain constant oxygen concentration within the aerobic section (AER) (DO = 0.5 g/$m^3$). This was done to take aeration problems into account experienced onsite at Cape Flats Wastewater Treatment Works, particularly during 2015&2016 as well as 2018&2019. Old and inefficient aeration blowers were replaced in 2016, and the fine bubble diffuser installations in all bioreactors were replaced from 2019 onwards. This meant aeration was not optimal during and before the periods mentioned, and from 2019 two bioreactors were taken offline in turn, to replace the fine bubble diffused air (FBDA) installations. Simulation results show that the model is capable of predicting effluent quality for COD, TSS, N and P. Mass balances reveal that 30% of the incoming COD is removed aerobically/anoxically, 23% of N leaves with the effluent, 36% of N is nitrified/denitrified and converted to $N_2$ in the aerobic /anoxic/re-aeration zones and 41% of N ends up being part of the sludge. When it comes to P, there is an effluent / sludge partitioning ratio of 35% / 65% (see Fig. 2c, d, e, f and g). The pH simulations/measurements are slightly increased due to $CO_2$ stripping in the last aerated reactor. The default parameter values in the ASM2d model (Henze et al., 2000) were used to run these simulations. The secondary clarifier was assumed to have 98% TSS removal efficiency. The same principle with respect to VSS and ISS settling velocities as described in 3.2.1 is applied here (see Fig. 2i and j).

#### 3.2.3. Thickening and flotation of primary and secondary sludge

Simulation results show that thickening and flotation models can describe primary and secondary sludge compaction. In the flotation units, the increase in the VSS/TSS ratio is especially noticeable as it is evident in both data and model predictions (See Fig. 2a and b). For the sake of simplicity, flotation units were assumed to be non-reactive. There was empirical evidence (data not shown) that the previously accumulated PP is released, and is returned to the AS section via the recycle. Nevertheless, it did not have a major effect on effluent quality and the model could predict P without accounting for this process (data not shown). Other studies dealing with reactor with shorter HRT have demonstrated that impact of reactive units may be quite significant (Flores-Alsina et al., 2012b; Guerrero et al., 2013).

#### 3.2.4. Anaerobic digestion

Thickening and flotation sludge are blended and introduced to the Anaerobic Digester (AD). Temperature is increased to 35 °C to

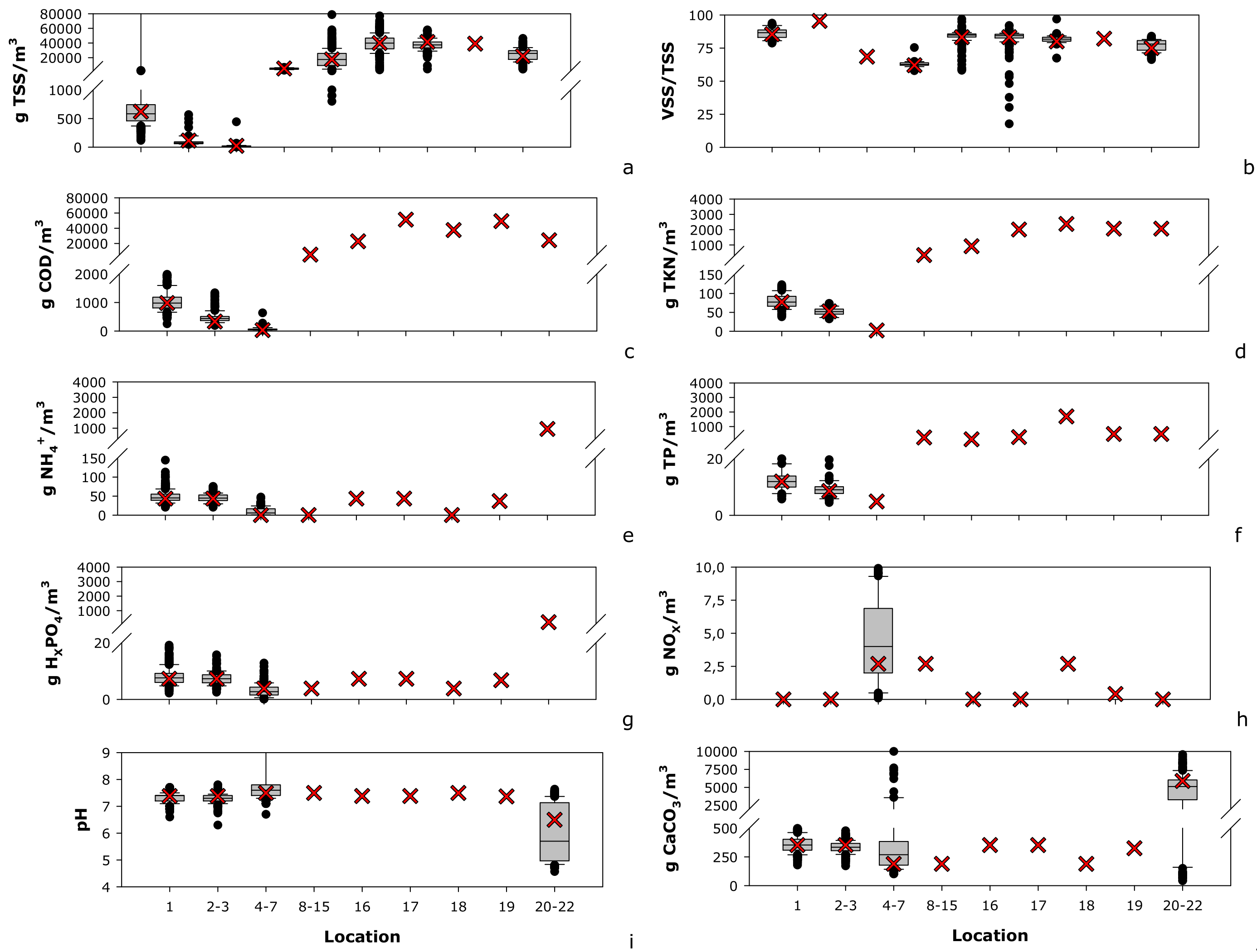


**Fig. 2.** Plant-wide measurements (box plots) and model simulations (X) for selected variables at different plant locations. 1) influent / raw wastewater, 2 and 3) effluent of primary clarification, 4–7) effluent of secondary clarification, 8–15) outflow of activated sludge section, 16) underflow of primary clarification, 17) underflow of primary sludge thickener, 18) overflow of secondary sludge dissolved air flotation unit, 19) influent of anaerobic digestion, 20–21) effluent of anaerobic digestion (see **Fig. 1** for details).

maintain mesophilic conditions. The sludge retention time (SRT) is 25 days. Fermenters and acidogenic bacteria mediate the VSS destruction (50%), release of alkalinity and decrease of pH (6.8), as shown in both simulation and plant measurements (See Fig. 2a, b, i and j). Default values of (kinetic) model parameters were reduced in order to mimic bad isolation and mixing conditions within the reactor, plus some additional problems in maintaining operational temperature, based on personal communication with plant operators (see Table S2 Supplemental information). Model predictions suggest that 36.5% of the incoming COD is captured as $CH_4$. The calculated methane yield is 390 ($Nm^3$ $CH_4$/ton COD converted). Digested sludge is sun dried (see Fig. 1).

### 3.3. Dynamic influent generation and effluent phosphorus prediction

The BSM2 influent generator blocks FLOW, POLLUTANTS, TEMPERATURE and TRANSPORT were adapted to describe CF dynamics. In the FLOW block dry weather conditions, 56% was assumed to originate from households (*HH)* and industrial wastewater (*IndS*). Specifically, 82% of this dry weather flow fraction is produced by *HH*, whereas the other 18% represents *IndS* wastewater. The remaining 44% of the influent flow rate (dry weather conditions) originates from groundwater infiltration. The latter was adjusted to reproduce the evapotranspiration regimes in the Southern hemisphere. Wet weather conditions were reproduced using a rainfall data profile. Default loading values were used to quantify concentrations (POLLUTANTS) (see values in Gernaey et al., 2011). For example, Fig. 3 shows the predicted / measured influent profiles for flow rate, COD, N and P. It is important to highlight that, in order to reproduce the effect that the severe drought in Cape Town had on influent dynamics (from 2017 onwards), the quantity of water produced per inhabitant had to be reduced by 50% (QperPE is reduced from 150 L/day/PE to 75 L/day/PE). The pollution load remains the same, but the pollutant concentration is increased due to the lower flow rate. The default parameters for the TEMPERATURE block are used assuming a maximum and minimum value of 20 and 10 deg. C respectfully. The same procedure to change to the Southern hemisphere is applied here. A relatively long hydraulic retention time (HRT) (> 8 h) is assumed in the sewer network (TRANSPORT). A 98% (flow rate), 89% (COD), 80% (TN) and 80% (TN) of the simulated values are included within the defined uncertainty range for the plant measurements (+ 50% variation). For more information about model parameters and influent generator adjustments, consult the work published by Gernaey et al. (2011) and Flores-Alsina et al. (2014b).

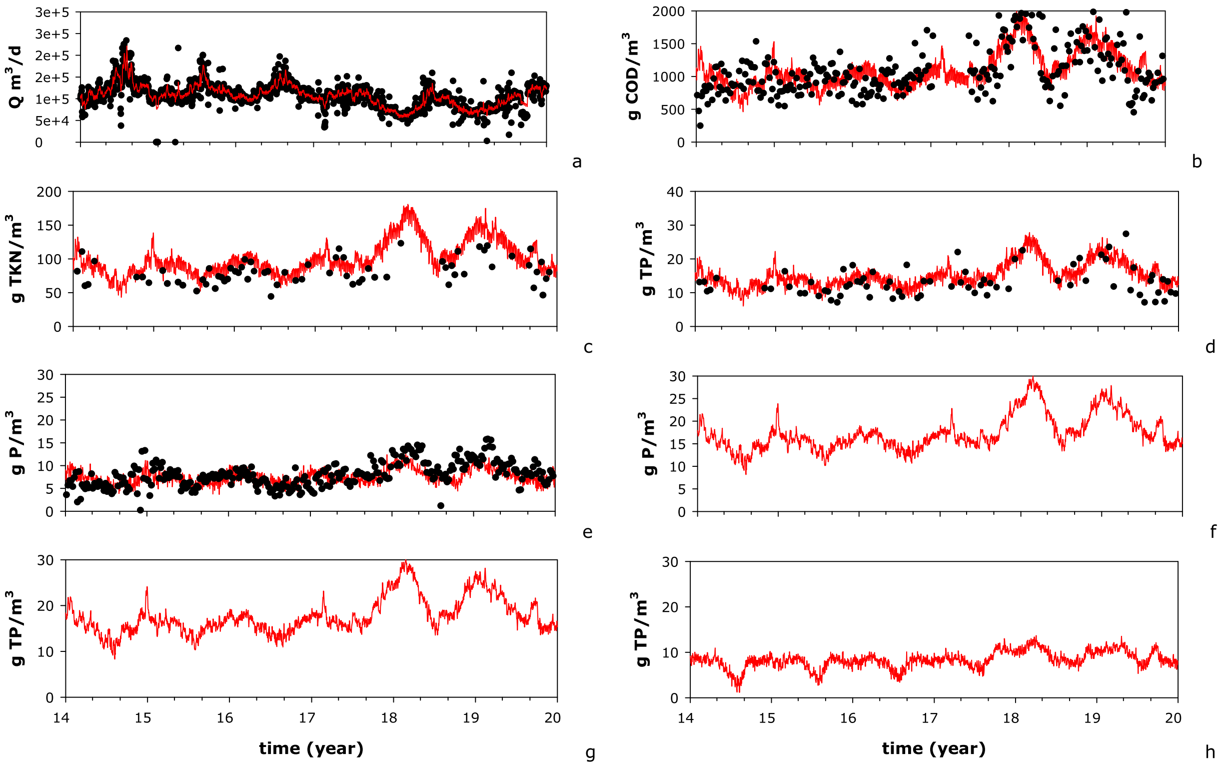


**Fig. 3.** Influent (a,b,c,d) and effluent (e,f,g,h) measurements/predictions for influent flow rate (a), total COD (b), total nitrogen (c) and total phosphorus (d,e,f,g,h). Phosphorus predictions include the base case (e) and three different scenarios: f) SMS1 (2 AD), g) SMS2 (THP) and h) SMS4 (THP+SPH).

Regarding effluent phosphorus predictions, Fig. 3 shows that the model was also able to predict P removal resulting from the historical mode of operation. In this case, 87% of the simulated values are within the uncertainty range defined for the plant measurements (+ 50% variation). Both simulations and plant measurements show a relatively low P removal efficiency. This is attributed to the lack of volatile fatty acids in the anaerobic section (ANAER1–8), which does not allow Phosphorus Accumulating Organisms (PAO) to store sufficient poly–hydroxy–alkanoates (PHA). As a consequence PAO are not able to use these internal storage products in the following anoxic / aerobic sections for growth of new biomass and uptake of P from the water phase. Furthermore, the model also managed to account for the effect of temperature on PAOs i.e. low activity in winter and high activity in summer (Henze et al., 2000). No variation in model parameters (Section 3.2) was assumed in dynamic conditions. Default temperature corrections were used (see Henze et al., 2000). Additional elements concerning biological phosphorus removal are explored in the following sections of the paper.

## 4. Sludge managament strategies

### 4.1. Mass balancing

The arrival of dewatered sludge from Mitchells Plain and Wildevoelvlei WWTWs to Cape Flats WWTW means an increase of the solids load with 32 t dry solids/day (see Table 3). The CF plant acting as bio-solids beneficiation facilities (BBF) was simulated assuming five different sludge management strategies (*SMS 0, 1, 2, 3 & 4*) as described in Table 3. The results of the analysis of the different technological solutions are summarized in both Fig. 4 and Table 4. More specifically, Fig. 4 depicts the main mass balances (normalized to 1) for COD, N and P. Computer simulations revealed that sludge management strategies with an implemented THP would allow a much higher (≈1.2 times) COD recovery (as

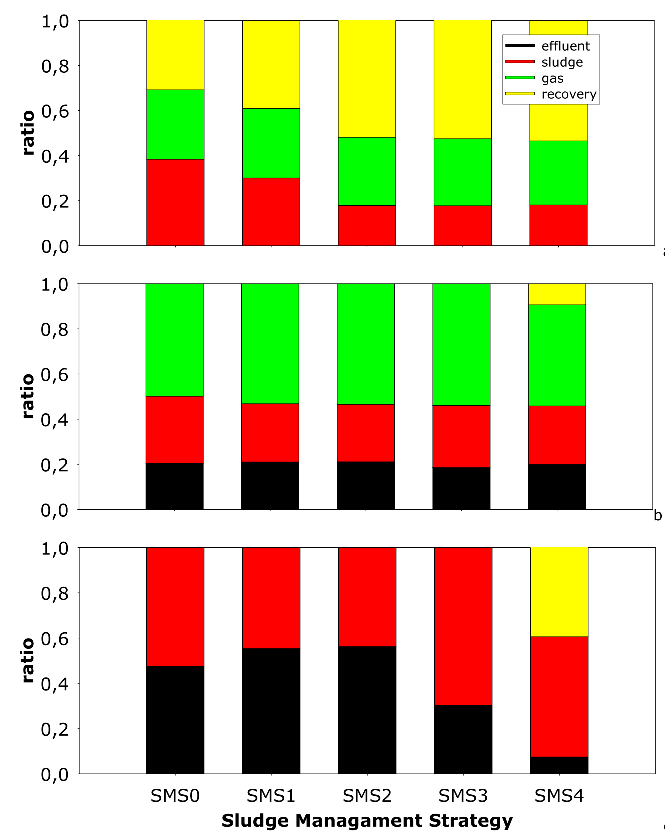


**Fig. 4.** COD (a) N (b) & P (c) mass balances for the evaluated sludge management strategies. More details can be found in Table 3. SMS0 = base case including internal recycle + imported sludge. SMS1 = SMS0 + double volume anaerobic digester. SMS2 = SMS0 + THP. SMS3 = SMS0 + THP + PN/ANX. SMS4 = SMS0 + THP + SPH.

$CH_4$) compared to a conventional digestion process (see Fig. 4a). In terms of organic fraction (VSS/TSS) after digestion, THP decreases from 68% to 55%. In addition, the higher N release from proteins in THP options, favors acetate oxidizers (instead of acetoclastic methanogens) producing additional hydrogen and carbon dioxide (Westerholm et al., 2020). As a result, there will be a population shift towards hydrogenotrophic archaea, which are less sensitive to $NH_3$ (see microbial distribution for THP options in supplemental information section Figure S5). When it comes to N, mass balances revealed two different points. Firstly, the formation of soluble inerts ($S_I$) and dissolved organic nitrogen (DON) related to $S_I$ in all flow diagrams with thermal hydrolysis pretreatment (THP) does not impact the overall nitrogen removal compared to their competing options. Secondly, partial nitration/anammox (PN/ANX) technology yields only a marginal difference with respect to the options without extra treatment (*SMS 0, 1, 2 & 4*). In all cases, the model suggests that there is enough nitrification / denitrification capacity in the current water line (as long as sludge retention time and dissolved oxygen are maintained at suitable levels). The layout with PN/ANX, changes the way N is denitrified in the plant compared to the other scenarios. Around 65% is heterotrophic and 35% is autotrophic while for the competing options denitrification is 100% heterotrophic (see microbial distribution for SMS3 in the supplemental information section Figure S7). Interestingly, the flow diagram with struvite precipitation captures 10% of the incoming N (influent + external) instead of being lost to the air (see Fig. 4b). Regarding P, simulations indicated that, as a result of the PN/ANX implementation, there is a reduction of $NO_X$ in the aerobic zone (AER1–8) being recycled to anaerobic reactors (ANAER1–8). Consequently, there is lower competition between OHO and PAO. This is translated into a major accumulation of PP and a higher fraction of P sent to the sludge line. Another important point that was extracted from this analysis is the need to include a struvite precipitation and harvesting (SPH) reactor in order to remove P to acceptable levels (> 90% removal). This is mainly due to the disintegration of PP in the anaerobic digester (AD) and the subsequent return to the activated sludge section via the centrate, i.e. P is pumped back and forth from the water to the sludge line unless it is effectively captured (see Fig. 4c).

### 4.2. Evaluation criteria

Similar conclusions as in 4.1 can be reached when considering the criteria used to assess effluent quality, operational cost and potential resource recovery (energy / nutrients) summarized in Table 4. Reject water treatment seems to be the only option to lower effluent P levels. This reduction is caused by different mechanisms. In the option with THP+PN/ANX (*SMS3*) it is due to an increase of autotrophic denitrification in the sludge line, which decreases the N load in the activated sludge (AS) section (giving a competitive advantage to PAOs). In THP +SPH (*SMS4*) it is by capturing and harvesting part of the N and P into inorganic precipitates. This is further explored in the following section. When it comes to costs, partial nitritation gives the lowest $E_{aeration}$ consumption since part of the $NH_x$ is only oxidized to $NO_2^-$. The highest $E_{mixing}$ is caused by the larger HRT assumed when the anaerobic volume is doubled (see Table 3). The extra pumping for struvite harvesting increases $E_{pumping}$ values. Strategies with a THP seem to have a better energy balance ($E_{net}$), even though the heating demands to reach operational temperature ($T_{op}$) in the flash reactor are the highest. Alternatives with conventional AD (*SMS1*) have worse dewaterability and higher solids production as indicate by sludge production (SP) values. The reduction of the OHO activity versus ANX (with lower yields) is the cause of lower SP values in PN/ANXP recovery (compared to its competing options) as $CHEM_{struvite}$ (39% of the influent P) implies periodic purchase of chemicals as a trade-off ($CHEM_{MgO}$ + $CHEM_{NaOH}$), although struvite can be sold as fertilizer (assuming that there is a market for it). Further interactions are analyzed in the following section.

### 4.3. Dynamic analysis of P removal processes

Fig. 3 reveals the effect on effluent P removal of recycling anaerobic digester centrate (in the baseline scenario centrate was not returned). More specifically, P accumulated in the Activated Sludge Section is released in the anaerobic digester when PAO decay. A fraction of this P ends up as organic particulates (biomass, lipids, inerts) (Ikumi and Harding, 2020). Another fraction forms inorganic precipitates such as struvite and calcium phosphate. The latter will strongly depend on the cations present in the anaerobic digester (particularly calcium and magnesium) (Kazadi-Mbamba et al., 2015b). The major soluble part is sent back to the water line via the centrate. It is important to highlight that the formation of P compounds linked to non-biodegradable organic compounds (soluble and particulate) during THP does not have an effect on the overall P removal efficiency (see Fig. 3f and g). As shown in the previous section, the only way to substantially reduce P levels in the effluent, is to promote the quantity of P bound to inorganic material in the centrate, which is promoted in the *SMS4* scenario (THP + SPH), where external Magnesium is added and phosphate captured as struvite. Nevertheless, the effluent should be further optimized. The effect of calcium addition and pH in both the AD and SPH reactor is further explored in the following section of the paper.

**Table 4**
Evaluation criteria used to assess effluent quality, operational cost and potential resource recovery (energy/nutrients) for the different sludge management strategies that have been simulated.

| | SMS0 | SMS1 (2AD) | SMS2 (THP) | SMS3 (THP + PN/ANX) | SMS4 (THP + SPH) | |
|---|---|---|---|---|---|---|
| Effluent TKN | 2.1 | 2.1 | 2.1 | 4.4 | 2.1 | $g/m^3$ |
| Effluent TN | 5.5 | 6.1 | 6.2 | 5.7 | 5.1 | $g/m^3$ |
| Effluent $H_xPO_4^{3-x}$ | 9.2 | 11.1 | 11.6 | 3.6 | 1.2 | $g/m^3$ |
| Effluent TP | 10.1 | 11.6 | 12.2 | 6.3 | 2.3 | $g/m^3$ |
| Aeration energy ($E_{aeration}$) | 34.8 | 35.3 | 35.2 | 32.8 | 33.5 | MWh/d |
| Mixing energy ($E_{mixing}$) | 7.9 | 10.2 | 7.9 | 7.9 | 7.9 | MWh/d |
| Pumping energy ($E_{pumping}$) | 6.5 | 6.4 | 6.6 | 6.3 | 6.7 | MWh/d |
| Heating demand ($E_{heat,demand}$) | 60.5 | 58.9 | 77.5 | 76.7 | 78.4 | MWh/d |
| Electricity production ($E_{electricity,rec}$) | 66.5 | 84.1 | 108.9 | 108.7 | 108.3 | MWh/d |
| Heat production ($E_{heat,rec}$) | 77.8 | 98.5 | 127.6 | 127.4 | 126.9 | MWh/d |
| Energy consumption ($E_{consumption}$) | 109.7 | 110.8 | 127.2 | 123.7 | 126.5 | MWh/d |
| Energy net ($E_{net}$) | 34.6 | 71.8 | 109.3 | 112.4 | 108.7 | MWh/d |
| Sludge production (SP) | 51.1 | 43.2 | 30.2 | 22.6 | 30.5 | T TSS/d |
| Chemicals usage, Mg ($CHEM_{MgO}$) | – | | | | 492.8 | kg/d |
| Chemical usage, Na ($CHEM_{NaOH}$) | – | – | | | 663.1 | kg/d |
| Chemicals recovered, struvite ($CHEM_{struv}$) | – | – | | | 668.2 | kg/d |

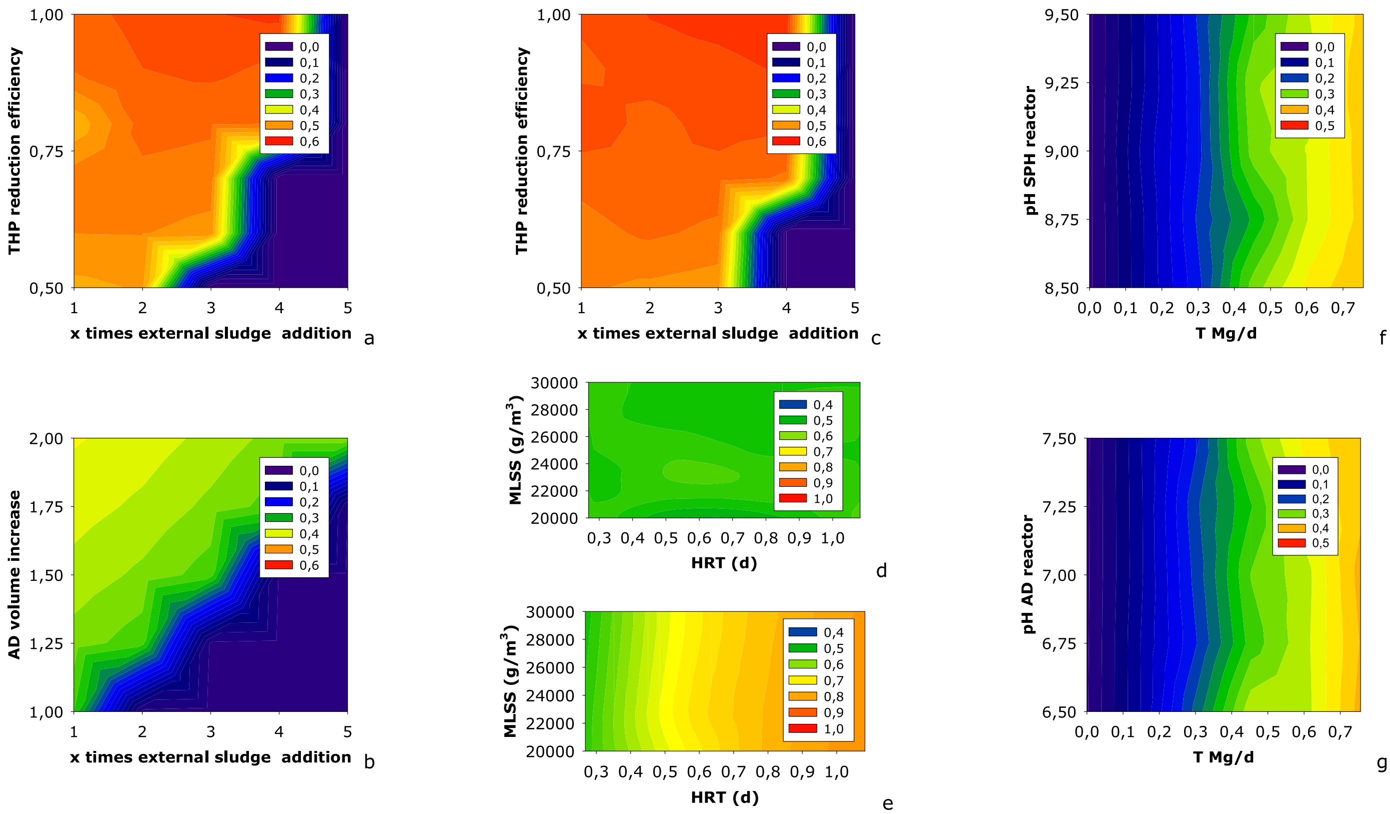


**Fig. 5.** Effect of operational conditions on: 1) COD recovery for *SMS1* and *SMS2* (a,b), 2) COD recovery for SMS3 (c), 3) N removal for *SMS3* (d,e) and 4) P recovery for *SMS4* (f,g). SMS0 = base case including internal recycle (a), i.e. when AD volume increase is 1. SMS1 = SMS0 + double volume anaerobic digester (a,b). SMS2 = SMS0 + THP (a,b). SMS3 = SMS0 + THP + PN/ANX (c,d,e). SMS4 = SMS0 + THP + SPH (f,g).

## 5. Additional simulations

### *5.1. Effect of (imported sludge) loading on energy recovery*

In this section, the effect of increasing the imported sludge contribution on two of the proposed sludge strategies is evaluated. In the first case, the thermal hydrolysis pretreatment (THP) capabilities to solubilize biodegradable organics are modified, as well as the $NH_x$ inhibition values. Default parameter values were multiplied by a factor ranging from 1 to 0.5 (where 1 gives the default values used in the previous section and 0.5 corresponds to an arbitrarily reduction factor of 50%). In the second case, the original anaerobic digester (AD) volume was increased by up to 100% (double volume). Once this was established, the model was consulted with respect to COD recovery as methane. Predictions indicated that (see Fig. 5a) THP can achieve higher recovery efficiencies (≈50%), even with the most pessimistic parameter values, i.e. very low biodegradability after THP and inhibition thresholds. This is applicable to loads up to 64 Tons TSS/d. At higher load values, the system gets overloaded and rapidly collapses, also depending on model parameter values. However, the options with bigger AD volume can deal with higher loads (up to 160 T/d) although the relative recovery is always much lower ($<$ 40%) (see Fig. 5b). Strategies without THP, or double reactor volume, can only deal with a very limited amount of imported sludge. The selection between increasing the AD volumeand / or THP is a complicated balance between future sludge production projections (forecast), CAPEX and OPEX (see point 5.4 in the discussion section)

### *5.2. Effect of the HRT and MLSS on the PN/ANX granular sludge reactor*

The second set of simulations shows the impact of partial nitration/anammox (PN/ANX) on the stream AD. Fig. 4c shows the effect of increasing the imported sludge contribution as described above on the COD recovery. The role of HRT and MLSS on nitrogen removal is presented in Fig. 5d,e. Results show that the lower sludge production by autotrophic denitrifiers in SMS3 (THP+PN/ANX) would allow a higher digestion capacity (for the same range of situations) when compared with the base case scenario SMS1 (THP+AD) (Fig. 5a). As mentioned before, anammox (ANX) bacteria have lower yields compared to OHO i.e. kg VSS produced /kg COD consumed is much lower for ANX bacteria. Fig. 5d shows that mass balances in the PN/ANX reactor may well vary between 50 and 85% High hydraulic retention time (HRT) and mixed liquor suspended solids (MLSS) concentration (also biofilm area) favors N conversion processes. Nevertheless, Fig. 5e reveals again the poor effect of treating reject water on the overall N removal (Fig. 5e). In other words, even though having a high percentage of N removal in the PN/ANX unit, the impact from a plant-wide perspective (and consequently effluent quality) is low. As long as dissolved oxygen in both the aerobic (AER1–8) and re-aeration (reAER1–8) zone are kept to suitable limits and the sludge retention time (SRT) is high enough, the current design of the Cape Flats plant should be able to handle the extra N loads from the sludge line.

### 5.3. Effect of AD pH & Mg and Na load on the struvite reactor

The last set of simulations explores the effect of operational pH on anaerobic digester (AD) + NaOH and MgO addition on the struvite reactor (*SMS4*). pH in the AD is evaluated between pH values from 6.5 to 7.5. The load of Mg is reduced to half the default value and increased to twice the default value. The addition of NaOH was adjusted to set the pH in the struvite reactor (between 8.5 and 9.5). Computer simulation revealed that the potential quantity of P recovered as struvite in Cape Flats depends on the magnesium concentration (See Fig. 5f and g). Even though NaOH and pH in the AD might influence the release of free ions from their paired forms and facilitate the formation of precipitates (Latif et al., 2017), the simulations in this case study indicate that it does not have a big impact.

## 6. Discussion

### 6.1. General applicability of the developed model library

As mentioned in the introduction, there are very few studies, where sludge treatment alternatives are evaluated in a plant-wide context. The model library presented here has required quite a large development effort in order to achieve a good compromise between model complexity and computational efficiency. Indeed, the set of models present an anaerobic digester (Batstone et al., 2002), a physico-chemical approach (Flores-Alsina et al., 2015), a precipitation/struvite tank/separator (Kazadi-Mbamba et al., 2016) an Anammox biofilm-based reactor (Wanner et al., 2006) with mass transfer limitations and microbial competition for space. The latter required quite some rework in order to handle model compatibility and stiffness issues i.e. optimized discretization schemes, interfacing, etc. This implementation (which will be freely distributed) will allow users to develop/simulate different treatment/recovery strategies using the most common configurations and evaluate their performance in a plant-wide context (evaluation criteria are included within the package). The special numerical routines implemented in these models allowed simulating these elements without problems (Flores-Alsina et al., 2015).

### 6.2. Suitability of THP for centralized bio-solids management

Sludge management analysis reveals that process flowsheets with thermal hydrolysis pre-treatment (THP) could handle a higher loading capacity due to the expected change in viscosity, which would allow an effective feed at 9% TS as compared to the normal feed concentrations of 6% TS (see Table 3). In addition, THP resulted in: i) a better energy balance in spite of having higher heat demands (see Table 4); ii) increased biodegradability/solubility (see Fig. 4); iii) changes in the methanogenic microbial population due to high $NH_X$ presence (see Figure S5 in Supplementary Information); and, iv) generation of lower solid volumes for disposal (see Table 4) by improving sludge dewaterability. High temperature and pressure ensure sludge pasteurization, such that the treated sludge could be used for agricultural purposes (better quality) instead of being disposed to landfill. This also depends on the concentrations of heavy metals, which are not predicted by the model. It is important to highlight though that the changes in sludge quality and properties by THP strongly affect the composition of the reject water streams, i.e. through formation of dissolved organic non-biodegradable nitrogen (DON) and phosphorus (DOP) compounds (Barber 2016). Nevertheless, the results in Section 4.1 already indicated that their effect on overall process performance was negligible for this particular system. The SPH system was necessary independently of the chosen stabilization strategy (conventional AD or THP+AD). THP is capital-intensive though, and this capital can be more effectively leveraged by centralizing biosolids treatment with the sludge from Athlone, Mitchells Plain and Wildevoelvlei, which are currently not receiving any sludge treatment.

### 6.3. Study assumptions and the need for additional experiments

The figures displayed in sections 4.2.1 and 4.2.2 revealed that the results of this project strongly depend on the assumptions upon which the models are constructed. An important aspect not accounted in the study is uncontrolled struvite precipitation in different parts of the flow diagram i.e. flotation/dewatering. This may have an important effect on the overall mass balance as well as the performance of the different units (Sanchez-Ramirez et al., 2019). Another challenge we had when run this project was lack of reliable data on influent biodegradability brought the authors to consider literature values (Henze et al., 2000). This will affect the energy recovery potential (Jeppsson et al., 2007), the capacity to denitrify all the nitrate produced in the aerobic zone (Yuan et al., 2002) and the competition between OHO and PAO (Lopez-Vazquez et al., 2009) amongst other factors. The same applies for the THP (Wett et al., 2014; Aichinger et al., 2019). Additional laboratory experiments should be carried out in order to better determine the temperature / pressure effect on pasteurization, solubilization and viability of sludge streams (Carrere et al., 2010). The effect of $NH_3$ inhibition should be better addressed too (default parameter values have been used as reported in Batstone et al., 2012 and Wett et al., 2014). The latter has a strong effect on methanogenesis but also acetate oxidation (Arnell et al., 2016; Astals et al., 2018; Batstone et al., 2020). In the baseline simulations, the model did not indicate an important $NH_3$ inhibition. In case this was a problem, the proposed approach allows the addition of different mitigation strategies (dilution, stripping) in order to reduce the undesirable inhibitory effects. Finally the effect that derived THP compounds may have on the subsequent PN/ANX should be mentioned (Zhang et al., 2018). Recent investigations reported potential mass transfer problems in aerobic granules due to the formation of colloidal compounds during THP. These effects have not been accounted for by the model presented here, since additional organic characterization is necessary, but also easily accountable within the proposed approach. Again, all these elements can be evaluated in a plant-wide context with the models presented here, which has not been possible until now.

### 6.4. Plant-wide optimization procedures

The set of models proposed here allows plant-wide optimization approaches. For example, it has been demonstrated that the effect of sludge retention time (SRT), Fe addition and the addition of a re-dissolution tank may affect potential struvite recovery (Lizarralde et al., 2019). This study adds the possibility of including different strategies to decrease N rich anaerobic digester supernatants using granular/biofilm based technologies. Until now, these units had to be simulated separately due to software incompatibility problems (Reichert, 2001; Jia et al., 2020). Another important factor not further explored in this study is the primary clarifier efficiency, energy recovery in the AD and autotrophic N removal + chemical P removal (Batstone et al., 2015a). The implementation also allows the addition of sophisticated control mechanisms in both reject water treatment units as shown in the scenario analysis. For example, it has been possible to simulate control of pH in AD and the struvite reactor to see the effect on P availability. pH in the PN/ANX was not controlled but it could be included and hence allowing assessment of removal efficiency versus risk of intra-granule precipitation (Feldman et al., 2019).

### *6.5. Future research: economics and sustainability of the evaluated alternatives*

The results of this study are part of a project financed by the DANIDA fellowship center, which collaborates closely with the Danish Ministry of Foreign Affairs. Additional investigations will be carried out to complement the presented study. For example, the study will be complemented with additional economic and sustainability assessment methods. Hence, Table 4 could be extended with CAPEX and then use OPEX to calculate the THP return period of investment. Another interesting aspect deserving a more detailed investigation is the PN/ANX reduced sludge production and how this might affect the BFF plant capacity to accept extra sludge. In this situation, the charging cost of treating the imported sludge and the cost for disposal must be included. The latter can change dramatically depending on the quality of the sludge. The current practice is only sending primary sludge to landfill, and secondary sludge is used for agricultural purposes (for fodder crops only). The highest quality digested sludge would then allow to dispose the combined (primary and secondary) digested sludge to any agricultural application (not just for fodder crops) as long as heavy metals are kept at an acceptable level. Along the same line, Life cycle assessment (LCA) and Life cycle costing (LCC) would be a good addition and in fact a future line of research (Arnell et al., 2017; Roldan et al., 2020). Some interesting facts related to the concept of BBF per se (centralized versus decentralized sludge treatment), the effect of THP in terms of energy usage, and location of struvite recovery (before, within or after the anaerobic digestion) could be balanced with potential global warming impacts and the other categories included in life cycle assessment methodologies (Corominas et al., 2013).

## 7. Conclusion

The main findings of this study can be summarized by the following points:

1) A plant-wide model has been extended and calibrated to mathematically describe the CF wastewater treatment works performance. The proposed approach accounts for the transformations of COD, N and P in both water and sludge line. Predictions for TSS, VSS/TSS ratio, TN, TP, $NH_4^+/NH_3$, $H_xPO4^{3\text{-}x}$, $NO_x$ alkalinity and pH at different plant locations are included within the interquartile range of the influent / effluent / process database collected from 2014 to 2019. 80% of all dynamically simulated values (influent characteristics and Bio P efficiency) are included within the plant measurementś 50% uncertainty range.
2) The mass balance methodology developed in this paper revealed that the current design/operational mode allows for the conversion of 36.5% of the incoming COD into methane in the digester (390 ($Nm^3$ $CH_4$/ton COD converted). N is removed via stripping (36%) while both N and P can be accumulated in the sludge (41% and 65% respectively). The current sludge disposal practice is landfill.
3) The analyses of sludge management strategies for the future BBF with the library developed in this study indicate that THP may achieve higher COD recovery, reduce sludge production, modify the methanogenic population and increase capacity for a wide range of sludge biodegradability assumptions. Model predictions do not indicate an effect on i) ammonia inhibition and ii) formation of non-biodegradable N and P compounds. Doubling the AD volume ensures higher loadings (capacity), but the percentage of COD recovery from the influent would be much lower as compared to using THP.
4) PN/ANX seems to have a marginal benefit when it comes to the overall N removal (even though it can remove up to 80% of the $NH_4^+/NH_3$ in the reject water stream). The model indicated that the design activated sludge volume is enough to deal with the expected increase in nitrogen load as long as the sludge retention time and aeration are maintained at suitable values. The lower sludge production of ANX microorganisms compared to OHO reduces bio-solids production and slightly increases AD capacity
5) The study also revealed that the only way to decrease phosphorus in the effluent to 90% is to promote the formation of inorganic precipitates in a SPH reactor. Presence of magnesium seems to be the limiting factor when it comes to struvite formation, since the pH in the AD and NaOH addition have a limited effect on recovery (for this case study).
6) The set of models presented herein (process models, evaluation criteria) will allow process engineers in water utilities to evaluate different technological solutions for sludge treatment in a plant-wide context. The models should be complemented with additional experiments to determine important model parameters in order to achieve more accurate predictions in the scenario analysis.

## Software availability

The Matlab/Simulink implementation of the BSM2 implementation + influent generator is available on request. To express an interest for obtaining the code, please contact Dr. Xavier Flores-Alsina (xfa@kt.dtu.dk) or Prof. Krist V. Gernaey (kvg@kt.dtu.dk) at the Department of Chemical and Biochemical Engineering at the Technical University of Denmark.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.


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## Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.watres.2020.116714.

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