



# **Using mathematical models to track phosphorus in a full-scale wastewater treatment plant**

By

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## Abstract

The challenges associated with pollution, declining nutrients and water shortage, resulted in the need for strategies towards cost effective recovery of nutrients from waste types fed to wastewater treatment systems, to forms that are usable and possibly marketable, while ensuring maintenance of good effluent quality from the plant. To address these challenges, the plant wide model (PWM\_SA) of Ikumi *et al.* (2015) was utilized to evaluate and propose operational strategies for Zeekoegat WWTW of the City of Tshwane to help with future design or optimized operation of the system. This goal was achieved by (i) acquisition of all necessary data from Zeekoegat WWTP, (ii) Reconciliation of measured data and subsequent characterization of the influent WW using widely documented protocol to run an excel steady state model which uses explicit mass balanced equations and (iii) setting up Zeekoegat WWTW virtually within the WEST® dynamic simulation environment and ensuring that confidence is achieved in virtual replication of the plant before testing operational scenarios.

The two operational strategies were simulated and evaluated using performance indices (PI's: operational cost index (OCI) and effluent quality index (EQI)) derived from a previous investigation by the International Water Association (IWA) benchmark simulation modelling task group (Copp, 2002, Nopens *et al.*, 2010). These PI's were modified by De Ketele *et al.* (2018) and later extended by Coothen (2021) and they proved to be a useful approach to evaluating the environmental (EQI) and economic (OCI) impact of a WWTP based on any operational strategy implemented i.e., optimizing water resource recovery (WRRFs) and troubleshooting problems to improve our wastewater treatment systems in South Africa.

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## Abbreviations

WWTP	Wastewater treatment plant
WRRFs	Water Resource Recovery Facilities
AS	Activated Sludge
WAS	Waste Activated Sludge
PS	Primary Sludge
AAD	Anoxic-Aerobic Digestion
AD	Anaerobic Digestion
AAD	Anoxic-Aerobic Digestion
DAF	Dissolved Air Floatation
SS	Steady State
BNR	Biological Nutrient Removal
NDBEPR	Nitrification-denitrification (ND) and ND biological excess phosphorus removal (NDBEPR)
EBPR	Biological Excess Phosphorus Removal
OHO	Ordinary Heterotrophic Organism
PAOs	Phosphorus Accumulating Organisms
VFA	Volatile Fatty Acid
PHB	Poly3-Hydroxy-Butyrate (C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> )
PP	Polyphosphate
ADM1	Anaerobic Digestion Model Number 1
ASM1	Activated Sludge Model Number 1
ASM2	Activated Sludge Model Number 2
ASM2d	Activated Sludge Model Number 2d
PWM_SA	Plant Wide Model South Africa (UCT)
MMP	Multiple Mineral Precipitations
PI's	Performance Indices
EQI	Effluent Quality Index
OCI	Operational Cost Index
IWA	International Water Association
BSM2P	Benchmark Simulation Model No.2 Extended to include Phosphorus
AE	Aeration Energy
PE	Pumping Energy
SP	Sludge Production
EC	External Carbon
ME	Mixing Energy
MP	Methane Production
HE	Heating Energy
NR	Nutrient Recovered
WEST®	Wastewater Treatment Plant Engine for Simulation and Training
UCT	University of Cape Town

# **1. Introduction**

## **1.1. Background and motivation to the work**

The challenges associated with pollution, declining nutrients and water shortage, resulted in the need for strategies towards cost effective recovery of nutrients from waste types fed to wastewater treatment systems, to forms that are usable and possibly marketable, while ensuring maintenance of good effluent quality from the plant. Hence, there is currently a paradigm shift, involving the transition of wastewater treatment plants (WWTPs) into water resource recovery facilities (WRRFs), for promotion of environmentally and economically sustainable infrastructure and preservation of water resource quality. Previously developed predictive WWTP models can play a crucial role in these developments, acting as tools to assist players in the sector in management of treatment systems, with a focus on reuse and recovery. These mathematical models contain sets of equations that virtually replicate the real system - hence their potential to generate critical data that could be applied in long term planning and management of recoverable resources.

Various mathematical models have been developed for activated sludge (AS) and anaerobic digestion (AD) in wastewater treatment systems. These models (both steady state and dynamic simulation models) are based on basic principles of mass balanced stoichiometry. The simplicity of steady state models results in their usefulness for design, since the flows and loads are assumed to be constant (Ekama & Wentzel, 2008). Thereby allowing one to determine initial conditions for the system (such as sludge age, reactor volume, recycle and waste flows etc.) needed to run a dynamic simulation model, thus being able to predict system response with changes in time for existing or proposed systems.

For an existing system, dynamic plant wide models can be applied to its operation to minimize energy consumption and reduce operating cost while maximizing nutrient recovery and improving effluent quality (Ikumi *et al.*, 2014).

## **1.2. Problem statement**

There are various problems facing biological nutrient removal (BNR) systems in South Africa, including the impact of sludge return flows and more. Previous collaborative studies between University of Cape Town (UCT) and University of Kwazulu Natal (UKZN) involved the integration of various unit operation models to form integrated plantwide models that could virtually replicate the entire WWTP (Ikumi, 2011). These models included, both a simplified steady state model implemented in MS. Excel and a more complex dynamic simulation model that was implemented in WEST® (i.e., the plant wide model of South Africa -PWM\_SA; Ikumi *et al.* 2015). These models were prepared to offer expert guided evaluations to proposed strategies for design and optimized operation strategies of WWTPs. PWM\_SA model was calibrated using BIOMATH protocol (Vanrolleghem *et al.*, 2003) against laboratory scale WWTP systems, configured for various nutrient removal AS system configurations linked to sludge treatment via

both anaerobic digestion and aerobic digestion (Ikumi *et al.*, 2014; Ikumi, 2020; Ikumi and Harding 2020). The simplified steady state model that was developed in parallel with the dynamic PWM\_SA model is often used together with PWM\_SA for systems that are evaluated at steady state, due to the intuitive checks that can be achieved by virtue of its simple and explicit nature, together with its capability to calculate initial reactor conditions that avoid trial and error simulations that are often required when using dynamic models.

However, there are very few studies that involve the use of plantwide models in prediction of performance for real and full-scale plant wide systems (Ikumi *et al.*, 2015).

To showcase the potential for such models to be used as decision making tools for real systems, it is proposed that the PWM\_SA be used to evaluate design and operational strategies for various full-scale wastewater treatment plants in South Africa. For this study, the model (PWM\_SA) was used to evaluate and propose operational strategies for Zeekoegat WWTW of the City of Tshwane.

### **1.3. Aim and objectives**

The main aim of the study was to showcase the utilization of modelling tools to simulate Zeekoegat full scale WWTW for proposed operational strategies that could be useful in future design or optimized operation of the system. To attain this aim, the following objectives needed to be achieved:

- i. Setting up Zeekoegat WWTW virtually using steady state MS Excel spreadsheet (SS Excel) models and using the plantwide model for South Africa (PWM\_SA; Ikumi *et al.*, 2015) within the experimental environment of the WEST® dynamic simulation software; ensuring that confidence is achieved in the virtual replication of Zeekoegat WWTW.
- ii. To showcase the possibilities of using modelling tools towards evaluation of plant operational scenarios, through simulation of the virtually replicated Zeekoegat WWTW, using both the SS Excel model and the PWM\_SA WEST® model, under different operating strategies and the application of performance indices (PI's: operational cost index (OCI) and effluent quality index (EQI)) derived from a previous investigation by the International Water Association (IWA) benchmark simulation modelling task group (Copp, 2002, Nopens *et al.*, 2010) to compare the outcomes of the different scenarios. The PI formulations were recently extended by De Ketele *et al* to suit South Africa WWTWs. For this project the main scenarios considered involve (a) the plant configuration with no improvements i.e., no fermenters & no VFAs added (b) the configuration with optimized fermenters, to increase VFAs in the Anaerobic zone of the bioreactor, which will improve P removal and (c) the plant configuration including the dosing of external carbon/electron source (VFAs) to improve P removal.

#### **1.4. Scope and limitations**

This project was done as a desk study hence there was no fieldwork and no laboratory experimental campaign performed within the project, the data obtained from literature studies such as Musvoto and Ikumi (2015) was sufficient to provide the required inputs for the modelling tasks involved in this project. The report by Musvoto and Ikumi (2015) contained the wastewater characteristics from the period of 2012 to 2014 for Zeekoegat WWTW.

During simulations, the plant was assumed to operate under ideal conditions, including adequate operation of mechanical and instrumentation equipment in the plant. Furthermore, the plant wide models used were only applied as tools under steady state conditions, for instance no material loads and flows were not changing.

The models applied for this project are mechanistic mass balanced mathematical models which included the University of Cape Town steady state model that is developed in Microsoft Excel and the Plantwide model of South Africa, which was developed in WEST®. These models were developed and calibrated in previous studies. Publications by Ekama et al (2009), Ikumi (2011), Quavauvilliers (2020) and Ekama (2021) can be referred to for the development, calibration and application of the plantwide steady state model. Also, the publications by Ikumi *et al.* (2015), Ikumi and Harding (2020), Ikumi (2020); Ghoor (2021) and Matesun *et al.* (2021) are some of the references that detail the development and calibration of the PWM\_SA model.

The evaluation of outputs generated by the mathematical models was performed according to the Benchmark Simulation Model No. 2P (BSM2P) developed by the International Water Association (IWA) task group performance indices (Jeppsson *et al.*, 2007; Solon *et al.*, 2017) that have been extended by De Ketele *et al.* (2018). Other evaluative methods (e.g., life cycle assessments) were not included in this study.

#### **1.5. Plan of development**

The report starts with an introduction (Chapter one) which provides the background about the project, aim/goal and the objectives. Chapter two contains literature review of the material used to achieve the goal of the study, mainly focusing on plant-wide modelling.

Chapter three contains experimental methods and programmes used during the study. The site layout of Zeekoegat WWTW is briefly described, including some plant performance data such as concentrations and loads to the wastewater treatment plant. Finally, the influent component concentrations to the modelling software, wastewater treatment plant engine for simulation and training (WEST®) were presented.

Chapter 4 provides the comparison between steady state excel model and the predictions from dynamic simulations using the PWM\_SA model in WEST®), followed by sections five and six where conclusions and recommendations are made respectively.

## 2. Literature Review

The purpose of this section is, firstly to provide the general objectives of a typical wastewater treatment plant (WWTP) and to discuss prominent activated sludge (AS) system configurations such as nitrification-denitrification (ND) system and ND biological excess phosphorus removal (NDBEPR) systems. The rest of the literature shall be dedicated to discussion of plant wide model PWM\_SA of Ikumi *et al.* (2014) and other ideas, which were used to accomplish the goal of the study.

### 2.1. Broad objectives of wastewater treatment

In general, a typical WWTP plant is designed, operated and maintained to primarily achieve the following objectives (Ekama and Wentzel, 2008):

- i. Remove organics (C) to avoid deoxygenation in the receiving waters such as lakes/ rivers due to heterotrophic growth of micro-organisms, such as ordinary heterotrophic organisms (OHOs).
- ii. Remove ammonia by nitrification (oxidizing it to nitrate) to avoid deoxygenation of the receiving waters such as lakes/ rivers due to autotrophic growth of micro-organisms. furthermore, ammonia is toxic, and must be removed before discharge, in line with applicable legal requirements.
- iii. Remove nutrients: Nitrogen (N) and Phosphorus (P) to prevent eutrophication in the receiving waters, with P being widely accepted as the limiting nutrient.

Overview of Biological Processes for wastewater treatment in Activated Sludge (AS) systems. The microorganism types that mediate a given set of common bioprocesses, towards WW treatment, in the AS system are lumped together as a "surrogate" organism (Beeharry *et al.*, 2002). For NDBEPR AS systems there are three main categories of these organisms: (i) Ordinary heterotrophic organism's (OHO's), mediating removal of organics and denitrification, (ii) phosphorous accumulating organism's (PAO's), which mediate removal of organics and EBPR and (iii) autotrophic nitrifying organism's (ANO's), mediating nitrification.

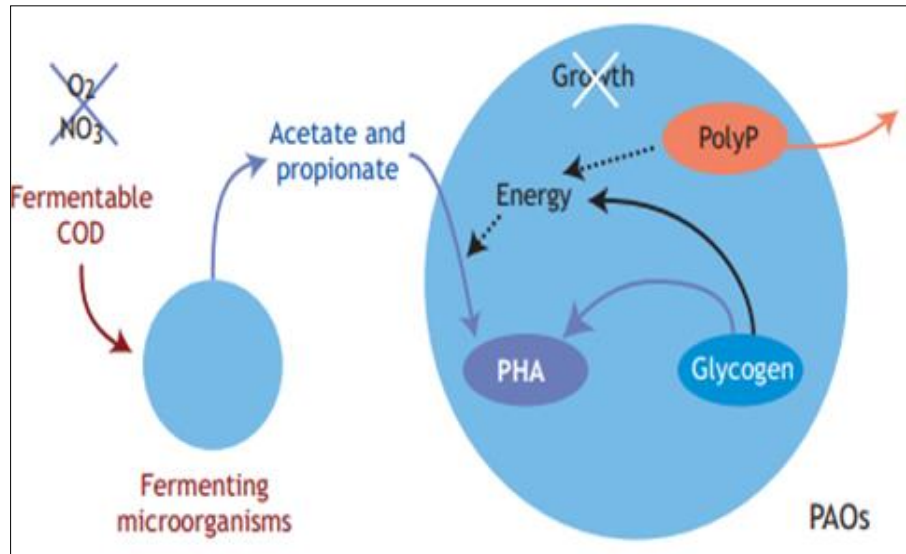
Heterotrophic microorganisms (OHOs) are known to exist in AS systems and work to degrade the organic compounds in wastewater, for their growth and energy generation. They normally require oxygen (i.e., as an electron acceptor for the energy generating process) for their metabolism hence carry out most of their bioprocesses under aerobic environments (Marais and Ekama, 1976). When oxygen is not present, some heterotrophic organisms (facultative OHOs) can use nitrates in place of the oxygen, and the nitrates are reduced to nitrogen gas (i.e., the process of denitrification) (Dold *et al.*, 1980).

Autotrophic nitrifying organisms (ANOs) are known to grow strictly in aerobic conditions. Here they convert ammonia to nitrate (i.e., they carry out nitrification). Hence the ANOs and facultative OHOs are used for the complete N removal process (i.e., from ammonia to nitrogen gas) and

require the alternating aerobic ( for nitrification) and anoxic (for denitrification) conditions (Dold *et al.*, 1980).

PAOs are microorganisms with the capability for internal storage of large quantities of P as polyphosphate chains (PP;  $Mg_cK_dCa_ePO_3$ ) at the expense of carbon in the aerobic conditions and carbon at the expense of PP at the anaerobic zone of the AS system (Daigger *et al.*, 1999; Ikumi and Ekama, 2019). Hence, the PAOs require environments that allow for their subjection to alternating anaerobic and aerobic conditions and a supply of RBCOD in the substrate feed. The PP is a high-energy storage molecule that, when broken down, allows for release of energy for biochemical reactions within the microorganism (Ikumi and Ekama, 2019). The PAOs use this metabolism in anaerobic zones of the AS system to generate the energy required for sequestering of VFAs and synthesis of high-energy internal storage organic compounds known as poly-3-hydroxyalkanoates (PHA). With the anaerobic breakdown of PP, P is released as orthophosphates. During the subsequent aerobic phase of the AS system, the PAOs utilize their stored PHA as a carbon and energy source for growth (anabolism) and energy generation (catabolism), whereby the oxygen available can be used as electron acceptor (in anoxic conditions nitrates could also be used, but is known to result in lower efficiency of P uptake by the new PAOs formed via the growth process; Hu *et al.*, 2000)). Hence as part of the PAO growth (biomass reproduction) the energy (generated via catabolism) is also used towards the manufacture of PP, using the available OP and metal counter ions (Mg, K and Ca) present in the reactor mixed liquor. The aerobic P uptake is usually higher than the anaerobic P release, resulting in achievement of net P removal by harvesting the P rich sludge from the aerobic zone (Liu *et al.*, 1996; Wentzel *et al.*, 1990). To encourage PAO growth, VFAs are often added to the influent feed (e.g via chemical dosage of acetate, propionate, etc. or inclusion of a fermentation stage prior to feeding of the influent to the anaerobic zone). Further, to enhance VFA uptake, a pH in the region of 7.25 could be maintained in the anaerobic zone of the AS system (Liu *et al.*, 1996). The Figure 1 below shows an overview of the PAO metabolism in AS systems.





**Figure 1:** The PAO metabolism, towards EBPR through anaerobic P release and aerobic P uptake (Wentzel *et al.*, 2008)

In nitrification-denitrification (ND) systems, the OHOs and ANOs are commonly present. However, in ND excess biological P removal (NDEBPR) AS systems, all three microorganism groups are present (i.e., mixed cultures or OHO, PAO and ANO are found in the reactor mixed liquors), with the PAO and OHO organism populations known to interact in the anaerobic zone (OHOs ferment readily biodegradable organics into volatile fatty acids (SCFA) that could be taken up by PAOs), but carry out their aerobic bioprocesses independently of each other (Wentzel *et al.*, 1990). The COD substrate allocation is hence divided into the quantity to be utilised by OHOs and that sequestered by PAOs. Where there is a large population of PAOs, the large portion of readily biodegradable COD (RBCOD) is usually used by the PAOs, since they can take up substrate in the anaerobic zone, which is often the first reactor that receives the influent WW requiring biological treatment. The slowly biodegradable COD (SBCOD), which requires slow conversion to RBCOD (via hydrolysis), is usually taken up by the OHOs in the aerobic zone (Ramphao *et al.* 2004).

Although the three common microorganism groups (OHOs, ANOs and PAOs) can only grow under specific conditions, they are capable of death under all reactor conditions (anaerobic, anoxic and aerobic), irrespective of substrate availability in the influent. Microorganism death is known to occur continually, at a rate which is specific to the biomass (e.g.,  $b_H = 0.24/d$  for OHOs and  $b_G = 0.04/d$  for PAOs). With microorganism's death, there is a process commonly referred to as endogenous respiration, whereby the remains of dead biomass being organic are split into biodegradable portion and an unbiodegradable portion. The biodegradable portion is broken down as the BPO (SBCOD) from WW, while the unbiodegradable portion accumulates in the reactor as the UPO from WW. According to the endogenous respiration theory, the utilisation of BPO is a catabolic process that requires the terminal electron acceptor such as oxygen or nitrates for breakdown of BPO towards energy generation. The unbiodegradable portion is commonly referred

to as the endogenous residue fraction ( $f_{EH} = 0.2$  for OHOs and  $f_{EG} = 0.25$  for PAOs; Dold *et al.*, 1980; Wentzel *et al.*, 1990).

Another theory, known as the death regeneration model accounts for the same quantities of active biomass loss, oxygen utilisation and endogenous residue accumulation in a different way. In the death regeneration concept, 62 % of the active biomass die within a day and 0.08% of this active mass accumulates as unbiodegradable matter, while the other 61.2% becomes slowly biodegradable COD (SBCOD). Some of this SBCOD is used for anabolism (for growth of new biomass; 38%), while the remainder is used for energy generation (catabolism). Therefore, the biomass found in the system ends up comprising of newly formed biomass (38%) together with the other 38% that did not participate in the death process – this is a total of 76% biomass, hence 24% lost in a day (Marais and Ekama, 1976; Dold *et al.*, 1980).

### **2.1.1. Organic carbon and nitrogen removal systems (ND system-configurations)**

The ND systems achieve the first two objectives (i & ii stated in 2.1 above) of a WWTP and different configurations exist to remove organic carbon and nitrogen. These configurations were developed depending on the type of electron donor (ED) in the bioprocess. The first configuration is ‘Wuhrmann’ (post-denitrification)-uses endogenously generated organics to denitrify the nitrate, because all the influent organics are consumed in the aerobic reactor, slowing down denitrification rate and often needing external substrate like methanol to be dosed to improve denitrification (Ekama and Wentzel, 2008).

Modified Ludzack-Ettinger (MLE) is a more popular ND system, enabling pre-denitrification in the primary anoxic reactor allowing influent organics to be utilized first for denitrification before organic carbon removal by ordinary heterotrophic organisms (OHOs)- leading to relatively high N removal, with effluent nitrate ( $\text{NO}_3^-$ )  $> 4$  mgN/l, at an a-recycle (from aerobic reactor to primary anoxic reactor) having a limit of  $\approx 5:1$  (Ekama and Wentzel, 2008). The third ND system is the 4 stage Bardenpho, which allow for pre-and post-denitrification, complete denitrification is possible for low TKN/COD ratio and often methanol is dosed to increase denitrification rate, at the secondary anoxic reactor ((Ekama and Wentzel, 2008).

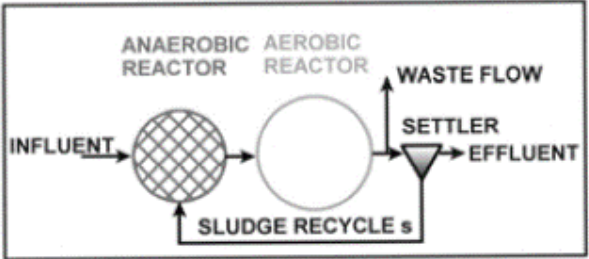
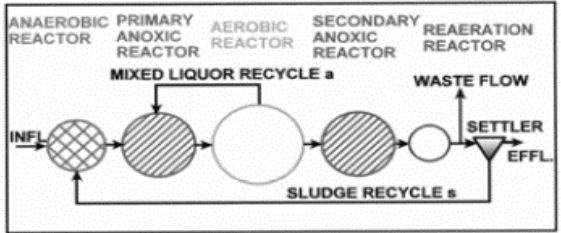
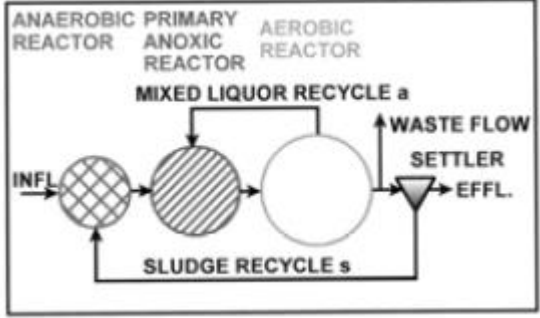
### **2.1.2. Organic carbon, nitrogen and phosphorus removal systems- NDBEPR systems**

Compliance with legal requirements on effluent quality is a key objective of every WWTP, thus the functions of AS systems include biological removal of C, N and P (Ekama and Wentzel, 1997). In an NDBEPR system all the objectives of a typical WWTP are achieved, by the simple incorporation of excess phosphorous removal in nitrification denitrification (ND) system-first developed/discovered by Barnard (1973).

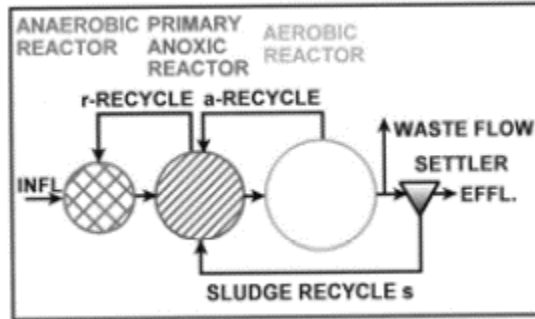
The system configurations (as shown in the Table 1 below) are manipulated to create environmental conditions in the activated sludge system which stimulate optimal growth and

action of micro-organisms which naturally mediate the processes needed to treat wastewater (WW). For example, in the aerated zone autotrophic nitrifying organisms (ANO) or nitrifiers convert free and saline ammonia (FSA) to nitrate, which subsequently gets converted to nitrogen gas (denitrification, mediated by OHOs) in the unaerated/anoxic zone. To further stimulate P removal, the raw WW or settled WW is fed to an anaerobic zone (no dissolved oxygen, no nitrate)- this provides readily biodegradable chemical oxygen demand (RBCOD) to the polyphosphate accumulating organisms (PAOs) which mediate the process of P-removal. Hence the anoxic zone is included in NDEBPR AS systems to allow for denitrification, thus protecting EBPR from the detrimental effect of recycling nitrate to the anaerobic zone. Hence during NDEBPR AS system design, the selection of recycle flows from the aerobic to anoxic zone is regulated to ensure minimum nitrate recycle to the anaerobic zone (Ikumi, 2011).

**Table 1:** Various configurations of a WWTP system (Wentzel et al., 2008)

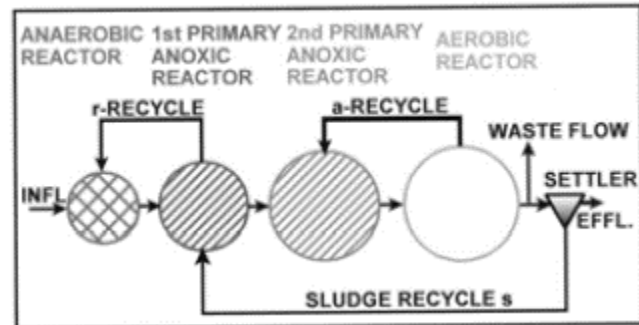
System	Configuration
<p><b>PHOREDOX SYSTEM:</b></p> <ul style="list-style-type: none"> <li>• P removal by PAOs (using readily biodegradable substrate) and C removal by OHOs</li> <li>• No nitrification (short sludge age)</li> <li>• Called AO in US</li> </ul>	
<p><b>5 STAGE BARDENPHO</b></p> <ul style="list-style-type: none"> <li>• Phoredox for P removal into 4 stage Bardenpho for N removal (Barnard, 1975)</li> <li>• Inclusion of secondary anoxic reactor to remove remaining nitrates and secondary aerobic one to further nitrify the ammonia released during endogenous respiration</li> <li>• Possible to obtain no <math>\text{NO}_3^-</math> in the effluent (if TKN not too high)</li> </ul>	
<p><b>3 STAGE BARDENPHO</b></p> <ul style="list-style-type: none"> <li>• No secondary anoxic reactor and re-aeration zone.</li> <li>• Nitrate to Anaerobic reactor through s-recycle and effluent</li> <li>• Anaerobic reactor included to enable PAO growth.</li> </ul> <p>Zeekoegat WWTW at the time of the study was operated as 3-stage Bardenpho system i.e. Anaerobic zone to grow PAOs, then Anoxic to remove <math>\text{NO}_3^-</math> and Aerobic for C removal by OHOs growth and nitrification by ANOs.</p>	
<p><b>UCT SYSTEM (1980)</b></p> <ul style="list-style-type: none"> <li>• Prevents <math>\text{NO}_3^-</math> recycle into the anaerobic zone.</li> </ul>	

- Allows study of BEPR without  $\text{NO}_3^-$  interference.
- High chance of Zero  $\text{NO}_3^-$  going to Anaerobic zone.
- Called VIP in US



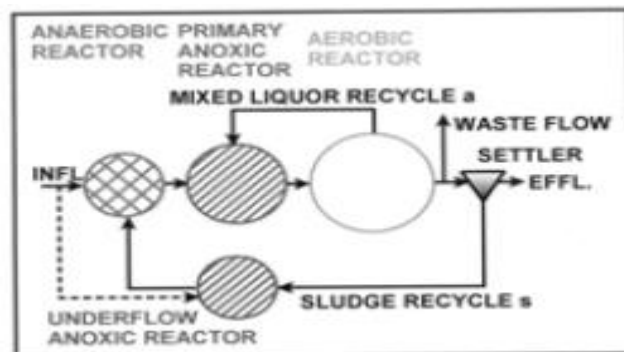
MUCT SYSTEM (1980)  
Modified UCT system

- Allows independent operation of a and s recycles for zero  $\text{NO}_3^-$  to anaerobic reactor compared to the UCT system which loads one anoxic reactor with both a and s recycle streams
- Required maximum TKN/COD $\approx$  0.12



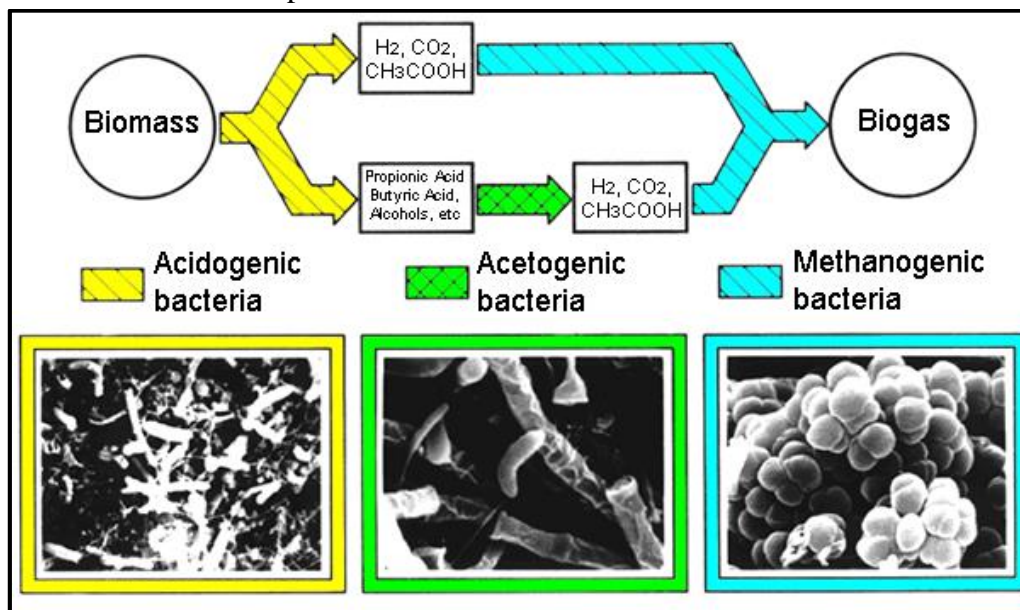
JHB SYSTEM (1976-1986)

- Prevents  $\text{NO}_3^-$  recycle to anaerobic zone in 3 stage Bardenpho
- Denitrifies  $\text{NO}_3^-$  in s-recycle to anaerobic zone
- Smaller anoxic zone cf. UCT system but slower denitrification rate
- Add some influent to increase denitrification rate



### 2.1.3. Sludge Treatment using the Process of Anaerobic Digestion

Anaerobic digestion (AD) is a process commonly used for the treatment of sludge generated in the primary (i.e., primary settling tanks, PST, that produces primary sludge) and secondary treatment (i.e., the AS process that produces WAS) of sewage. In AD treatment processes, the organics found in the sludge are broken down to form methane ( $\text{CH}_4$ ) and carbon dioxide ( $\text{CO}_2$ ). This takes place through four main metabolic processes carried out by multiple microorganism types: (i) sludge hydrolysis, which involves the breakdown of complex organics (e.g., carbohydrates, proteins and lipids) by acidogenic microorganisms (acidogens) to simple products (i.e., sugars, fatty acids and amino acids). The acidogens use extracellular enzymes for this process and the hydrolysed products can be used for the next AD process, i.e (ii) acidogenesis. Acidogenesis involves the fermentation of hydrolysis products to short chain fatty acids (SCFA, e.g. acetic acid or propionic acid; depending on the substrate used and the hydrogen partial pressure of the system) (Van Rensburg *et al.*, 2001). The third process (iii) acetogenesis involves the conversion of SCFAs with more than two carbon atoms (e.g., propionic and butyric acids) into acetic acid ( $\text{CH}_3\text{COOH}$ , also given as HAc),  $\text{CO}_2$  and  $\text{H}_2$ . This process is carried out by microorganism collectively known as acetogens (McInerney *et al.*, 1979; Batstone *et al.*, 2001). The final process is (iv) methanogenesis, which involves the conversion of HAc to  $\text{CO}_2$  and  $\text{CH}_4$  by acetoclastic methanogens and subsequent conversion of  $\text{H}_2$  to  $\text{CH}_4$  and water ( $\text{H}_2\text{O}$ ) by hydrogenotrophic methanogens (in this  $\text{CO}_2$  is used as the internally generated electron acceptor that reduces  $\text{H}_2$ ). The Figure 2 below shows an overview of the AD processes.



**Figure 2:** Anaerobic digestion bioprocesses and microbial species (Abstracted from Quavauvilliers, 2021)

The methanogens are known to be pH – sensitive, hence for healthy AD operations, the acetogens and acetoclastic methanogens must utilize the SCFAs as soon as they are generated, for the maintenance of a near neutral pH.

Increased net production of SCFA would result in the pH dropping and subsequent inhibition of the hydrogenotrophic methanogenesis process, which stalls the generation of CH<sub>4</sub>. This would then result in an increased hydrogen partial pressure, which causes the bio-metabolic pathways for acetogenesis tending towards the further production of propionic and butyric acids (Veeken *et al.*, 2000; Batstone *et al.*, 2001). Therefore optimal operation of AD such that the biodegradable organics are converted to end products (such as CH<sub>4</sub>, CO<sub>2</sub> and H<sub>2</sub>O) requires for minimal build-up of intermediate products (all products generated at a previous AD process getting converted into the next one, through low inhibition of the mediating biomass) (McCarty, 1974). For this to be possible the system alkalinity and pH are monitored together with other inhibitors (e.g., alternative external electron acceptors such nitrates & sulphates that result in growth of sulphate and nitrate reducing bacteria respectively, which can outcompete methanogens for the available substrates in the AD) (Pohland, 1992).

The sludge found in the AD effluent is usually stable, with a very low biodegradable organics present, allowing for it to be dried and used as part of organic fertiliser or as a soil conditioner. In some instances, the sludge contains significant portions of undesirable constituents, such as heavy metals, hence requires disposal (Pohland, 1992). The microorganisms involved in AD are known to have a relatively much lower yield than the OHOs found in AS systems, hence a small portion of the waste sludge COD is converted to new biomass and a large portion is converted to methane which mostly gets evolved into the gaseous phase (CH<sub>4</sub> is about 65 to 75% of the gas generated in AD, with CO<sub>2</sub> about 25 to 40% and smaller volumes of between 1 and 5% for N<sub>2</sub>, hydrogen (H<sub>2</sub>) and hydrogen sulphide). The methane production can be directly correlated to the quantity of waste COD reduction (McCarty, 1974; Ross *et al.*, 1992; Ikumi, 2011). The methane is a utilisable resource, as a fuel for digester heating and/or electricity co-generation. Apart from the stable organics, the AD effluent contains high concentrations of nutrients (N as ammonia and P in the form of OP), which had been released during breakdown of organics (i.e., the nutrients bound in the sewage sludge organics). After the AD sludge is thickened and dried, the nutrients generated as AD dewatering liquor are often recycled upstream to the AS system for their biological (or chemical removal). In some cases, there are side-stream treatment technologies employed for the removal or recovery of these nutrients (e.g., formation of struvite, MgNH<sub>4</sub>PO<sub>4</sub>, via precipitation and crystallisation process reactors – the struvite is later usable as a slow-release inorganic fertiliser).

During AD of WAS from NDEBPR AS systems (i.e., containing PAOs and their stored PP) it has been noted that PP degradation into OP and counter ions (Mg<sup>2+</sup>, K<sup>+</sup> and Ca<sup>2+</sup>) is largely similar to the P release in the anaerobic zone of the AS system (Ikumi and Ekama, 2019). This usually happens quicker than the BPO breakdown rate (which also results in nutrient release – the organically bound N and P release as NH<sub>4</sub> and OP respectively). When the molar product of Mg<sup>2+</sup>, NH<sub>4</sub><sup>+</sup> and PO<sub>4</sub><sup>3-</sup> generated exceeds the solubility product, (K<sub>sp</sub>, in mols/l) of struvite (MgNH<sub>4</sub>PO<sub>4</sub>), the result is formation of struvite precipitates (which are noticeable as hard crystalline deposits) in the AD reactor (or pipes and pumps). Hence AD system operation requires careful control of such processes to avoid unwanted blockages in the sludge treatment facilities.

## 2.2. Model development and mathematical models in general

A purposeful representation or description of a system of interest can be regarded as a model (Ekama and Wentzel, 2008). Therefore, in a wastewater treatment (WWT) system, a model would be a set of simultaneous, stoichiometric and kinetic rate equations describing the various processes, with some weak acid-base chemistry running in the background-influencing the alkalinity in the system, also represented by a set of equations (speciation routines). The ambition is generally to develop a model which reasonably replicates the system under study, to allow for better outcome prediction during simulation of a chosen WWT system.

The summary of important tasks involved during model development is provided in the figure below. Suffice to note that, the tasks provided cannot be implemented sequentially, some may need to be carried out concurrently (Ekama and Wentzel, 2008):

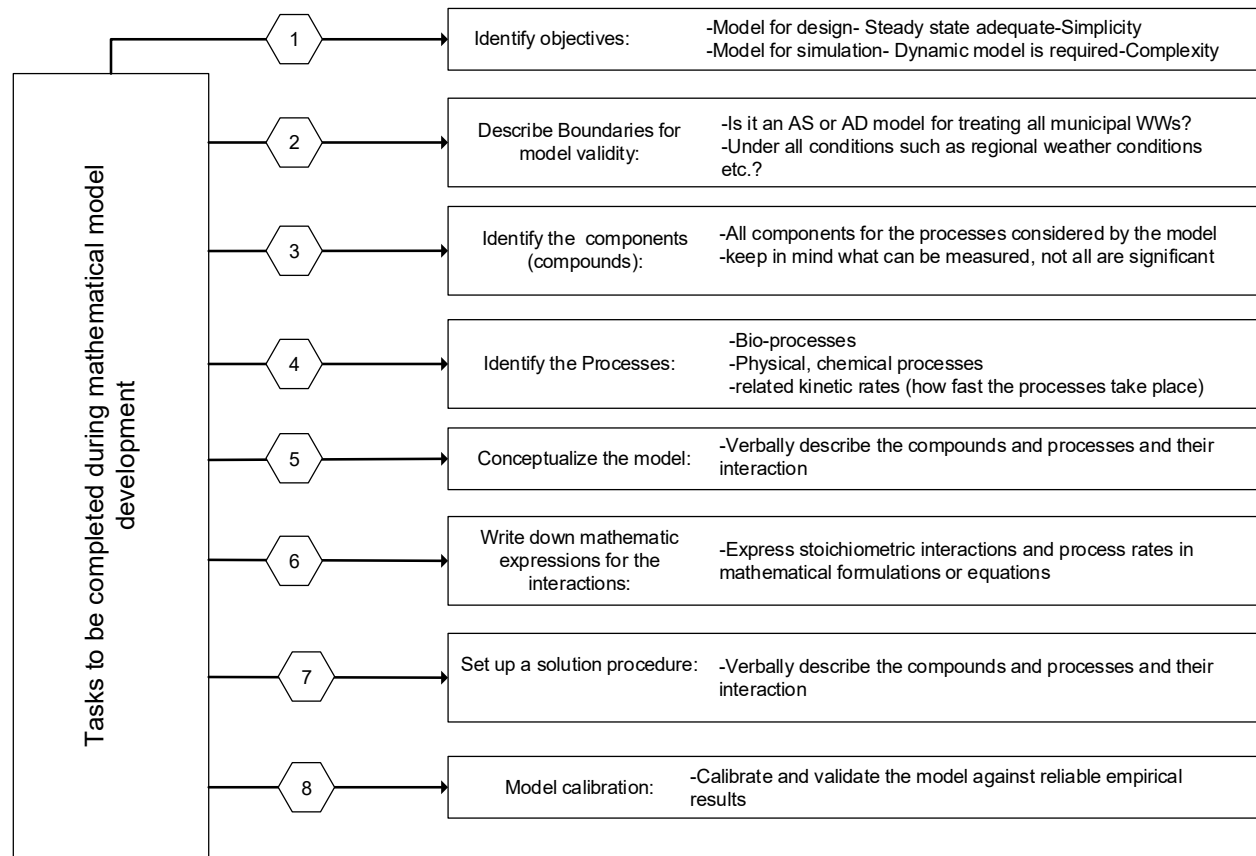


Figure 3: Steps for developing a mechanistically based mathematical model for wastewater treatment



### 2.2.1. Steady-State Models

Steady-state models are simple WWTP models developed, based on the stoichiometry and rate-limiting kinetics of the system processes. They are known to connect the given influent characteristics to system performance criteria (e.g., effluent quality) via explicit equations that allow for calculation of reactor sizes, interconnecting flows, and other WWTP design parameters (e.g. sludge age, reactor mass fractions and oxygen demand) (Wentzel, *et al.*, 2006; Ikumi, 2011). For these calculations to be possible, the SS models often assume that the system is at a stable steady state. In contrast, the dynamic simulation models are more complex, containing simultaneous algebraic equations running and different kinetic rates, and can be used after the sizing of a system towards refinement of design and for decision support in optimized system operation for changing flows and material loads. Wentzel, *et al* (2006) summarises the main uses of steady-state models as for:

- Rapid, simple and easy estimation of system design and operational parameters such as reactor volume, sludge age, recycle ratios, and oxygen utilisation for a specific design standard,
- Investigating how sensitive the performance of the system is to the operational and design parameters,
- Estimating the upstream products which are used as inputs for downstream processes, and
- Provide a reference for cross-checking validated plant-wide model of South Africa (PWM\_SA) simulation output results.

The processes deemed not to have reached completion are then either simplified or retained as rate limiting (when the processes are slowest and dictate the sizing requirements of the system, e.g. sludge hydrolysis in AD and nitrification in AS systems). Although this makes steady state models much simpler than dynamic simulations ones (which contain sets of simultaneous equations that run at different rates), the steady state models have been noted to provide similar results to the complex dynamic models, when simulated at steady state. Steady-state models are therefore known to be complementary to dynamic simulation models for enhancement and reliability of their use through pre-processing the inputs needed for dynamic simulation models. Apart from being simpler than dynamic models, the steady state models can be programmed into spreadsheets which are widely accessible.

### 2.2.2. The Primary Settling Tank Simplified Steady State Model

A simplified approach for modelling the PST in the steady state (SS) UCT spreadsheet model is adopted, such that removals of UPO, BPO and ISS settleable particles is achieved in observed fractions (Wentzel *et al.*, 2006; Ikumi *et al.*, 2014), which yield the observed PS, so that the settled WW characteristics can be predicted from the raw wastewater (raw WW) characteristics and the PST performance. The characterised raw wastewater (comprising the COD of VFAs, FBSO, Unbiodegradable soluble organics (USO), BPO and UPO, together with FSA, OP and ISS) is taken as input to the PST model. The particulates (UPO, BPO and ISS) are then divided into settleable and non-settleable fractions (parameterized value but settleable portions initially taken to be in the range of 84% UPO, 47% BPO and 80% ISS, as observed in Wentzel *et al.* (2006)). Together the settleable BPO, UPO and ISS, make up the TSS of PS (PST underflow) generated via the settling process. The soluble components are taken to be the same for raw WW, settled WW (PST overflow) and PS. Hence, the PST is deemed to remove 100% of settleable solids, while ensuring a 100% water, COD, N, P and ISS material mass balance (i.e., the % UPO, BPO and ISS settled out in the PST are set, depending on the PST performance).

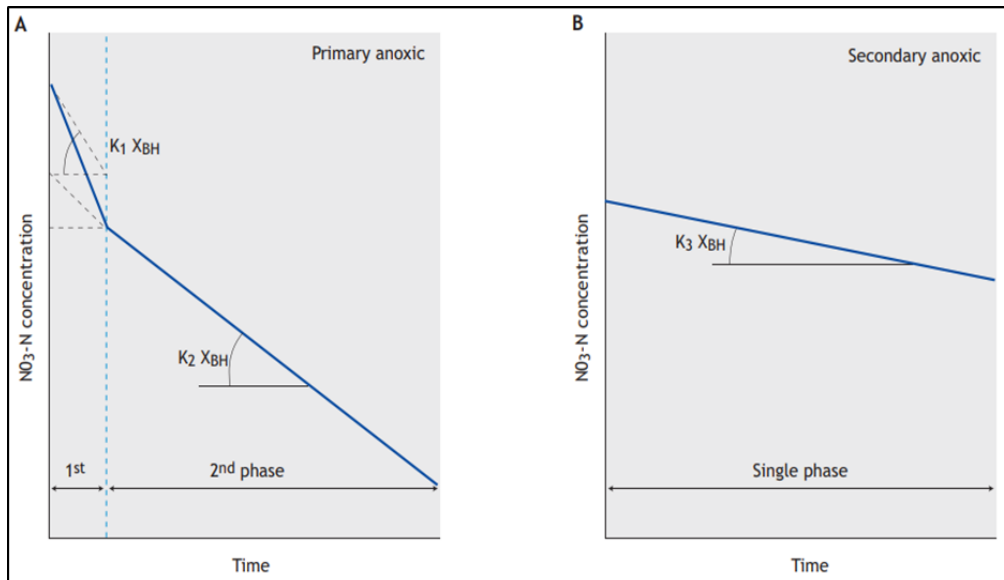
Polorigni *et al.* (2020) extended this PST model by assigning different settling velocities to the UPO, BPO and ISS, each divided in settling proportions (modelled as percentages) and grouped into 5 different settling velocity groups, then calculating the different fractions of UPO, BPO and ISS, removed by PSTs. For these calculated removals, the upflow velocity in the PST is compared to the settling velocity assigned to each settling velocity group, which contains different settling proportions of UPO, BPO and ISS. If the upflow velocity in the PST is slower than the settling velocity of a settling velocity group, then the UPO, BPO and ISS settling proportions of that group are completely removed from the water flow and become part of the primary sludge. On the other hand, if the upflow velocity in the PST is faster than the settling velocity of that settling velocity group, then none of the UPO, BPO or ISS are removed from the water flow, and remain part of the settled WW exiting the PST. The settling velocity groups are assigned decreasing settling velocities to mimic velocity patterns in a settleometer experiment and in such a way that they allow realistic removals that are in accordance with the maximum overflow rates for PSTs operations at peak wet weather flow (PWPF) and ADWF, (Polorigni *et al.*, 2020).

### 2.2.3. University of Cape Town (UCT) activated sludge (AS) steady state model

The University of Cape Town-based research group developed a steady-state (AS) model which uses the principle of strict material mass balances to track influent biodegradable and unbiodegradable organics, nitrogen and phosphorus through various AS bioprocesses. In this SS model, the virtual AS system is assumed to be at steady state, and as long as the sludge age is greater than 3 days, it is assumed that biodegradable organics are completely utilised for biomass growth (i.e., generation of OHOs) and energy generation. However, despite the biomass growth process being assumed as complete, with utilisation of biodegradable organics, the death process is deemed slow (i.e., does not reach completion, even at long sludge ages), therefore, the kinetics of biomass death (via the endogenous respiration model of Dold *et al.*, 1980) are incorporated into the steady-state model (Marais and Ekama, 1976; Wentzel *et al.*, 1990; Ekama and Wentzel, 2008).

To replicate the nitrification process, the steady-state model assumes (i) ANOs largely utilise  $\text{NH}_4$  and nitrite ( $\text{NO}_2$ ) for energy requirements (catabolism) - i.e., the synthesis of nitrogen is small enough to be neglected and (ii) ANOs convert ammonia directly into nitrate - the rate of conversion of ammonia to nitrite much slower, hence any nitrite that is available will be directly converted to nitrate (Ekama & Wentzel, 2008). Consequently, in this steady state model, only the kinetics of ANOs are considered and the rate of ammonia conversion can be equated to the rate of nitrate formation.

The denitrification process is modelled based on the kinetics of the conversion of nitrate to nitrogen gas using the available substrate. The kinetic rate varies based on the substrate used as shown in Figure 4 below: i.e., the influent RBCOD with a faster rate ( $K_1$ ), SBCOD with slower rate ( $K_2$ ) and SBCOD generated by biomass through endogenous respiration with slower rate ( $K_3 = 2/3 K_2$ ), as shown in the Figure 4 below. The growth of OHOs by utilising the incoming substrate as shown in figure 4 provided the basis to integrate denitrification into activated sludge kinetic simulation models.



**Figure 4:** Denitrification rates in the primary and secondary anoxic plug flow reactors (Ekama and Wentzel, 2008b)

AS noted in the Section 2.1 above, the EBPR model is based on principles of substrate allocation between PAOs and OHOs, which determines their growth and mass generated in the system (i.e., using their yield ( $Y_H = Y_G = 0.45 \text{ mgVSS/mgCOD}$  substrate) within the growth stoichiometry given in the Table 2 below and the death stoichiometry and kinetics). The P removal can then be calculated based on the quantity of PP accumulated by the PAOs (the maximum is  $0.35 \text{ mgP/mgPAOVSS}$  as noted in Section 2.1 above) and that used as nutrient for biomass (OHO and PAO) growth. The Table 2 below provides the set of Equations that are integrated to replicate the steady state AS system model.

#### 2.2.4. Anaerobic Digestion (AD) Model

The original UCT AD SS model was developed by Sötemann *et al.* (2005) based on COD, C, H, O, N mass balances in the breakdown of sludge organics (given an empirical composition of  $C_xH_yO_zN_a$ ) from sewage treatment plants. Since the process of hydrolysis is slowest it was deemed to be the rate limiting process in the AD system and the stoichiometric process for acidogens, acetogens and methanogens (mentioned in Section 2.1.3 above) were assumed to occur instantaneously following the completion of sludge hydrolysis. The generalized reaction stoichiometry adopted by Sötemann *et al.* (2005) is an extension of the one developed by McCarty (1974), that caters for AD of complex organics from COD and N removal systems. Into this stoichiometry the products of sludge hydrolysis are used to form the products of AD biomass (given an empirical composition of  $C_kH_lO_mN_n$ ),  $CH_4$ ,  $HCO_3^-$ ,  $CO_2$  and  $H_2O$  together with the released nutrients of  $NH_4^+$ . The stoichiometric products ( $NH_4^+$ ,  $HCO_3^-$ , and  $CO_2$ ) are used to predict the weak acid/base chemistry of the system; whereby  $CH_4$  and  $CO_2$  set the partial pressure of  $CO_2$  ( $p_{CO_2}$ ) and together with  $HCO_3^-$ , they establish the AD pH. Also, since the acidogens are the highest population of biomass in the AD, their yield value is accepted to represent that of the AD biomass. The acidogen ( $Z_{AD}$ ) yield coefficient ( $Y_{AD}$ ) is 0.089, while that of acetoclastic methanogen ( $Z_{AM}$ ) and hydrogenotrophic methanogen ( $Z_{HM}$ ) biomass is lower ( $Y_{AM} = 0.04$ ,  $Y_{HM} = 0.01$ ). The  $Y_{AD}$  was deemed to be the main overall biomass concentration in this SS AD model and since acidogenesis produces 67% acetic acid for  $Z_{AM}$  growth (and 33% hydrogen), 67% of the  $Y_{AM}$  value was added to this  $Y_{AD}$ , which increased the  $Y_{AD}$  (now taken as overall AD biomass yield) value to 0.113 (mgCOD organism/mgCOD substrate) to account  $Z_{AM}$  and  $Z_{HM}$  biomass growth in AD.

Thus, the SS AD model of Sötemann *et al.* (2005) consists of three parts: (i) the kinetic model which aims at determining the rate of biodegradable COD utilisation and methane gas (CH<sub>4</sub>) production for a given sludge age; (ii) the stoichiometric model which predicts the products (including HCO<sub>3</sub><sup>-</sup> that establishes alkalinity for systems that do not contain excess P) of AD bioprocesses and (iii) a weak acid/base chemistry model, from which the pH of the anaerobic digester is established based on the partial pressure of CO<sub>2</sub> and alkalinity generated. The sets of equations used towards the AD stoichiometry and weak acid/base chemistry are provided in Table 2 below.

### 2.2.5. Activated sludge and anaerobic digestion stoichiometry

Stoichiometric equations for steady state models of the AS and AD biological processes described above can be found in the Table 2 below (Henze *et al.*, 2008; Ekama *et al.*, 2011).

**Table 2:** Table...: The Steady State AS and AD model stoichiometry (Abstracted from Fotso Simo, 2020; all terms are defined in the C: Table C2

Equation	Equation Number	Reference
<b>Organic Removal Stoichiometry</b>		
$FS_{ti} = Q_i S_{ti}$	(1)	Ekama and Wentzel (2008a)
$FS_{bi} = FS_{ti}(1 - f_{Srus} - f_{Srup})$	(2)	
$FX_{li} = \frac{FS_{ti} f_{Srup}}{f_{cv}}$	(3)	
$FX_{IOi} = Q_i X_{IOi}$	(4)	
$MX_{BH} = FS_{bi} \frac{Y_H R_s}{(1 + b_H R_s)}$	(5)	
$MX_{EH} = f_H b_H MX_{BH} R_s$	(6)	
$MX_I = R_s \frac{FX_{li}}{f_{cv}}$	(7)	
$MX_V = MX_{BH} + MX_{EH} + MX_I$	(8)	
$MX_{IO} = FX_{IOi} R_s + f_{iOHO} MX_{BH}$	(9)	
$MX_t = MX_V + MX_{IO}$	(10)	
$FO_c = FS_{bi} [(1 - f_{cv} Y_H) + (1 - f_H) b_H \frac{Y_H f_{cv} R_s}{(1 + b_H R_s)}]$	(11)	
$FX_t = \frac{MX_t}{R_s}$	(12)	
$S_{te} = S_{use} + f_{cv} X_v$	(13)	
<b>Nitrogen Removal Stoichiometry</b>		
$N_a = N_{ae} = \frac{K_{nT}(b_{AT} + \frac{1}{R_s})}{\mu_{AmT} - (b_{AT} + \frac{1}{R_s})}$	(14)	Ekama and Wentzel (2008b)

$N_{ae} = \frac{K_{nT}(b_{AT} + \frac{1}{R_s})}{\mu_{AmT}(1 - f_{xt}) - (b_{AT} + \frac{1}{R_s})}$	(15)	
$N_{ae} = \frac{K_{nT}}{(S_f - 1)}$	(16)	
$N_{ae} = N_{ai} + N_{obsi} + N_{obpi} - (N_s - N_{oupi})$	(17)	
$N_{te} = N_{ouse} + N_{ae}$	(18)	
$N_s = f_n \frac{MX_v}{Q_i R_s}$	(19)	
$N_{te} = N_{ti} - N_s$	(20)	
$N_{ne} = N_c = N_{ti} - N_{te} - N_s$	(21)	
$D_{p1RBCOD} = \frac{f_{sb's} S_{bi}(1 - f_{cv} Y_H)}{2.86}$	(22)	
$D_{p1SBCOD} = \frac{K_2 f_{x1} S_{bi} Y_H R_s}{(1 + b_h R_s)}$	(23)	
$D_{p1} = D_{p1RBCOD} + D_{p1SBCOD}$	(24)	
$D_{p3SBCOD} = \frac{K_3 f_{x3} S_{bi} Y_H R_s}{(1 + b_h R_s)}$	(25)	
$D_{p3} = 0 + D_{p3SBCOD}$	(26)	
$FO_n = 4.57 N_c Q_i$	(27)	
$FO_d = 2.86(N_c - N_{ne}) Q_i$	(28)	
$FO_t = FO_c + FO_n - FO_d$	(29)	
<b>Phosphorus Removal Stoichiometry</b>		
$MX_{PAO} = \frac{Y_{PAO}}{(1 + b_{PAO,T} R_s)} FS_{bs,PAO} R_s$	(30)	
$MX_{E,PAO} = f_{XE,PAO} * b_{PAO,T} * MX_{PAO} * R_s$	(31)	
$MX_{OHO} = \frac{Y_{OHO}}{(1 + b_{OHO,T} R_s)} FS_{b,OHO} R_s$	(32)	
$MX_{E,OHO} = f_{XE,OHO} * b_{OHO,T} * MX_{OHO} * R_s$	(33)	
$MX_I = \frac{f_{XI,COD,i} FS_{ti} R_s}{f_{cv}}$	(34)	
$S_{bsf,i,conv} = S_{bsf,i} - 8.6(sS_{NO3,s} + S_{NO3,i}) - 3.0(sS_{O2,s} + S_{O2,i})$	(35)	
$S_{bsf,ANn} = \frac{S_{bsf,i,conv}}{(1 + s)} \frac{1}{[1 + k_{F,T} \frac{MX_{OHO}}{Q_i(1 + s)} \frac{f_{AN}}{N}]^n}$	(36)	
$FS_{bs,PAO} = Q_i [S_{bsf,i,conv} - (1 + s) S_{bsf,ANn}] + Q_i S_{bsai}$	(37)	
$\Delta P_{PAO} = f_{P,PAO} \frac{MX_{PAO}}{R_s} \frac{1}{Q_i}$	(38)	

Henze et al. (2008)

$\Delta P_{OHO} = f_{P,OHO} \frac{MX_{OHO}}{R_s} \frac{1}{Q_i}$	(39)	
$\Delta P_{XE} = f_{P,XE} \frac{(MX_{E,PAO} + MX_{E,OHO})}{R_s} \frac{1}{Q_i}$	(40)	
$\Delta P_{XI} = f_{P,XI} \frac{MX_{I,i}}{R_s} \frac{1}{Q_i}$	(41)	
$\Delta P_{SYS,POT} = \Delta P_{PAO} + \Delta P_{OHO} + \Delta P_{XE} + \Delta P_{XI}$	(42)	
$\Delta P_{SYS,ACT} = \min(\Delta P_{SYS,POT}; T_{P,i})$	(43)	
$MX_{VSS} = MX_{PAO} + MX_{OHO} + MX_{E,PAO} + MX_{E,OHO} + MX_I$	(44)	
$MX_{FSS} = f_{FSS,OHO}MX_{OHO} + f_{FSS,PAO}MX_{PAO} + FX_{ISS,i}R_s$	(45)	
$MX_{TSS} = MX_{VSS} + MX_{ISS}$	(46)	
$f_{p,TSS} = \frac{f_{P,OHO}MX_{OHO}}{MX_{TSS} f_{VT}} + \frac{f_{P,XE}(MX_{E,OHO} + MX_{E,PAO})}{MX_{TSS} f_{VT}} + \frac{f_{P,XI}MX_{I,i}}{MX_{TSS} f_{VT}} + \frac{f_{P,PAO}MX_{PAO}}{MX_{TSS} f_{VT,PAO}} + \frac{f_{P,FSS,i}MX_{FSS}}{MX_{TSS}}$	(47)	
$X_{P,e} = f_{P,TSS}TSS_e$	(48)	
$T_{P,e} = T_{P,i} - \Delta P_{SYS,ACT} + X_{P,e}$	(49)	
$FO_{2,PAO} = (1 - f_{CV}Y_{PAO})FS_{bs,PAO} + f_{CV}(1 - f_{E,PAO})b_{PAO,T}MX_{PAO}$	(50)	
$FO_{2,OHO} = (1 - f_{CV}Y_{OHO})FS_{b,OHO} + f_{CV}(1 - f_{E,OHO})b_{OHO,T}MX_{OHO}$	(51)	
$FO_C = FO_{2,OHO} + FO_{2,PAO}$	(52)	
<b>Anaerobic Digestion Stoichiometry</b>		
$R = \frac{V}{Q}$	(53)	
$S_{bpi} = (1 - f_{PS'up})S_{ti} - S_{bsai}$	(54)	
$S_{upi} = f_{PS'up}S_{ti}$	(55)	
$S_{bp} = \frac{K_s(\frac{1}{R} + b_{AD})}{Y_{AD}K_m - (\frac{1}{R} + b_{AD})}$	(56)	
$S_{bp \text{ hydrolysed}} = S_{bpi} - S_{bp}$	(57)	
$Z_{AD} = \frac{Y_{AD}(S_{bpi} - S_{bp})}{[1 + b_{AD}R(1 - Y_{AD}\{1 - f_{AD}\})]}$	(58)	
$Z_E = f_{AD} * b_{AD} * Z_{AD} * R_s$	(59)	
$r_h = \frac{K_m S_{bp}}{[Z_{AD}(K_s + S_{bp})]}$	(60)	
$S_m = (1 - Y_{AD})Rr_h + S_{bsai}$	(61)	
$Q_m = [(1 - Y_{AD})Rr_h + S_{bsai}] \frac{24}{64}$	(62)	
$S_{te} = S_{up} + Z_{AD} + S_{bp} + Z_E + S_m$	(63)	

Söttemann et al. (2005)

$C_xH_yO_zN_a + \left( 2x + a - z - \frac{ED_S}{D_B}(n + 2k - m) - \frac{(1 - E)D_S}{4} \right) H_2O$ $\rightarrow \left( x - a - \frac{ED_S}{D_B}(n - k) - \frac{(1 - E)D_S}{8} \right) CO_2$ $+ \left( \frac{(1 - E)D_S}{8} \right) CH_4 + \left( \frac{ED_S}{D_B} \right) C_kH_lO_mN_n$ $+ \left( a - \frac{nED_S}{D_B} \right) NH_4^+ + \left( a - n \frac{ED_S}{D_B} \right) HCO_3^-$	(64)	
$CH_3COOH \rightarrow CH_4 + CO_2$ and	(65)	
$CH_3COO^- + H_2O \rightarrow CH_4 + HCO_3^-$	(66)	
$S_{bsHAc} = \frac{S_{bsai}}{(1 + 10^{pH_i - pK'_a})}$	(67)	
$S_{bsAc} = \frac{S_{bsai}}{(1 + 10^{pK'_a - pH_i})}$	(68)	
$p_{CO_2} = \frac{[HCO_3^-](1 + 10^{pK'_{c1} - pH} + 10^{pH - pK'_{c2}})}{10^{-pK'_{HCO_2}}(1 + 10^{pH - pK'_{c1}} + 10^{2pH - pK'_{c1} - pK'_{c2}})}$	(69)	

In the Table 2 above, Equations 1-13 represent the stoichiometric equations for organic removal (as provided by Ekama and Wentzel, 2008), where excess P is not removed (i.e., no PAOs present in the AS reactors), Equations 14-29 represent N removal (as given by Dold et al., 1980; Ekama and Wentzel, 2008), Equations 30-52 represent P-removal (as given by Wentzel, 1989; Wentzel *et al.*, 1990) and Equations 53-69 represent the processes taking place in the AD (as given by Sötemann *et al.*, 2005).

### 2.2.6. Integrated AS and AD plantwide steady state model

Ekama (2009) presents the plantwide steady state model that uses mass balanced steady state stoichiometry to track the COD, C, H, O, N, P masses and charge along the activated sludge (AS) organics degradation, nitrification and denitrification (ND) and anaerobic (AD) and aerobic (AerD) digestion of wastewater sludge of the entire WWTP. This was done by assigning a stoichiometric composition ( $x, y, z,$  and  $a$  in  $C_xH_yO_zN_a$ ) to each of the five main influent wastewater organic fractions, i.e. (i) influent volatile fatty acids (VFA, assumed to be acetic acid), (ii) fermentable readily biodegradable soluble organics (F-BSO), (iii) unbiodegradable soluble organics (USO), (iv) slowly biodegradable particulate organics (BPO) and (v) unbiodegradable particulate organics (UPO), the influent free and saline ammonia (FSA) and the activated sludge (AS) and anaerobic digester (AD) biomass, and determining the products formed from them using the mass balanced stoichiometries. Contrary to complex dynamic simulation models, simple steady state models assume most of the processes at steady state to have achieved completion. The processes deemed not to have reached completion are then either simplified or retained as rate limiting (when the processes are slowest and dictate the sizing requirements of the system, e.g. sludge hydrolysis in AD and nitrification in AS systems). Although this makes steady state models much simpler than dynamic simulations ones (which contain sets of simultaneous equations that run at different rates), the steady state models have been noted to provide similar results to the complex dynamic models, when simulated at steady state. Steady-state models are therefore known to be complementary to dynamic simulation models for enhancement and reliability of their use through pre-processing the inputs needed for dynamic simulation models. Apart from being simpler than dynamic models, the steady state models can be programmed into spreadsheets which are widely accessible.

Ekama (2009) utilizes the approach of a C, H, O, N, P and charge balance, to develop the stoichiometry for anoxic-aerobic processes (including organic breakdown, nitrification and denitrification; Henze *et al.*,

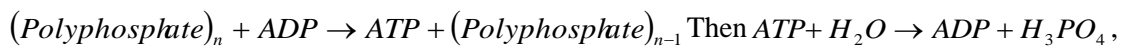
2008) of the activated sludge (AS) system, aerobic digestion (AerD) of waste activated sludge (WAS) and AD of PS and WAS. In this plantwide model, the AS anoxic-aerobic processes are broken down into three parts, the same way as was done for the AD mode by Sötemann *et al.* (2005), i.e., (i) A COD mass balanced based kinetic part (Part 1), which links the biodegradable organics (COD) concentration removed to the sludge production and oxygen demand via the system sludge age (these Parts 1 were developed previously, Marais and Ekama, 1976; WRC, 1984; Ekama *et al.*, 2006a; Henze *et al.*, 2008); (ii) a COD, C, H, O, N, (P) and charge balanced stoichiometry part (Part 2; Ekama, 2009) which transforms the biodegradable COD removed and its C, H, O, N and P composition (reactants) to sludge mass, oxygen demand, gaseous CO<sub>2</sub>, ammonia, nitrate, nitrogen gas, orthophosphate and dissolved CO<sub>2</sub> (H<sub>2</sub>CO<sub>3</sub> Alkalinity) (products); and (iii) an inorganic carbon (and phosphate if significant) weak acid/base chemistry part (Part 3), from which the alkalinity consumption can be calculated to determine whether or not chemical dosing is required to maintain the activated sludge (AS) and aerobic digester (AerD) reactors pH above 7 (this is possible with the alkalinity changes from the influent, due to nitrification and denitrification calculatable from the proton gain/ loss according to bioprocess stoichiometry). Unlike for AD steady state models, the AS model cannot use the weak acid/ base chemistry speciation calculations to determine reactor pH calculation, since with aeration the because the partial pressure of CO<sub>2</sub> in the liquid phase is not in equilibrium with the reactor headspace.

The plantwide steady state model of Ekama *et al.* (2009) has been getting refined as new information on the wastewater treatment process modelling becomes available. Further, the plantwide steady state model is being continuously structured into engineering tools that would be applicable by various stakeholder levels for decision making on design and operation of wastewater treatment systems.

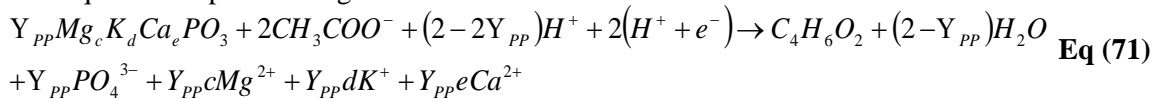
### 2.2.7. Adjustment of the SS AD model to include AD of P-rich sludge

Ikumi *et al.* (2015) extended the steady state AD model to include AD of WAS from EBPR AS systems. There was significant increase in complexity of the AD model to cater for the PP breakdown in AD and its impact on AD performance in terms of mineral precipitation and system alkalinity and pH changes. Ikumi and Ekama (2019) noted that the PAOs behaviour in the anaerobic zone of the AS system (i.e., the formation of energy-rich poly3-hydroxybutyrate (PHB) at the expense of their aerobically generated PP) would potentially occur when the PAOs containing PP are sent into an AD with volatile fatty acids (VFAs) present. However, due to lack of an alternating aerobic environment in AD, the PAOs ultimately experience lysis (not growth), with all their stored products (PHB and PP) getting released in the process. Since it has been established the PP release in the AD occurs much faster than the PAO biomass hydrolysis rate, Ikumi and Ekama (2019) modelled it as a separate process, using the steps shown below:

- (i) The use of enzymes to degrade PP (via hydrolysis), in the presence of adenosine diphosphate (ADP), for the release of phosphate and production of adenosine triphosphate (ATP, formed as an intermediate for utilization in energy consuming processes and to drive some enzyme-controlled reactions) (Cole and Hughes, 1964; Smolders *et al.*, 1995).



- (ii) Anaerobic uptake of acetate and its conversion to Acetyl-CoA, which is subsequently converted to PHB with the use of NADH<sub>2</sub> (formed as NADH-H<sup>+</sup>, when NAD<sup>+</sup> molecules take up two electrons and two H<sup>+</sup> atoms), as reported by Smolders *et al.* (1995) and also confirmed by Mino *et al.* (1994). The Equation 71 provides a general reaction for anaerobic PP release:

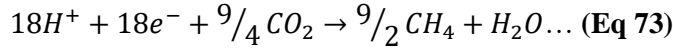
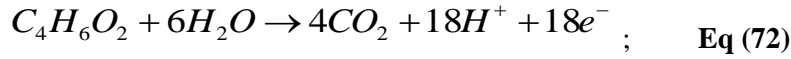


Where Y<sub>pp</sub> is the mols of P released per mol of PHB formed.

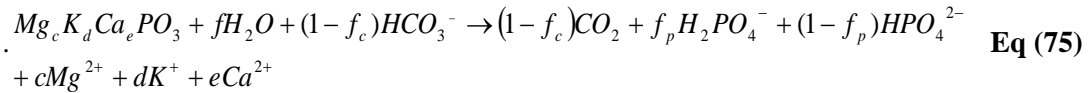
- (iii) In the AD environment, the PAOs are not modelled to compete with the AD biomass for the acetate, but after an initial rapid uptake of acetate and release of PP, leave the remaining acetate to



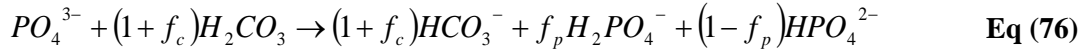
be degraded by AD biomass and give up the PHB with their hydrolysis. Thus, the PHB produced from the reaction of Equation (71) is later broken down in AD, to form CO<sub>2</sub> together with some H<sup>+</sup> and e<sup>-</sup>, as shown (Equation 73). The products of this breakdown contribute (as with other biodegradable organics) towards AD biomass growth and energy (methane) generation:



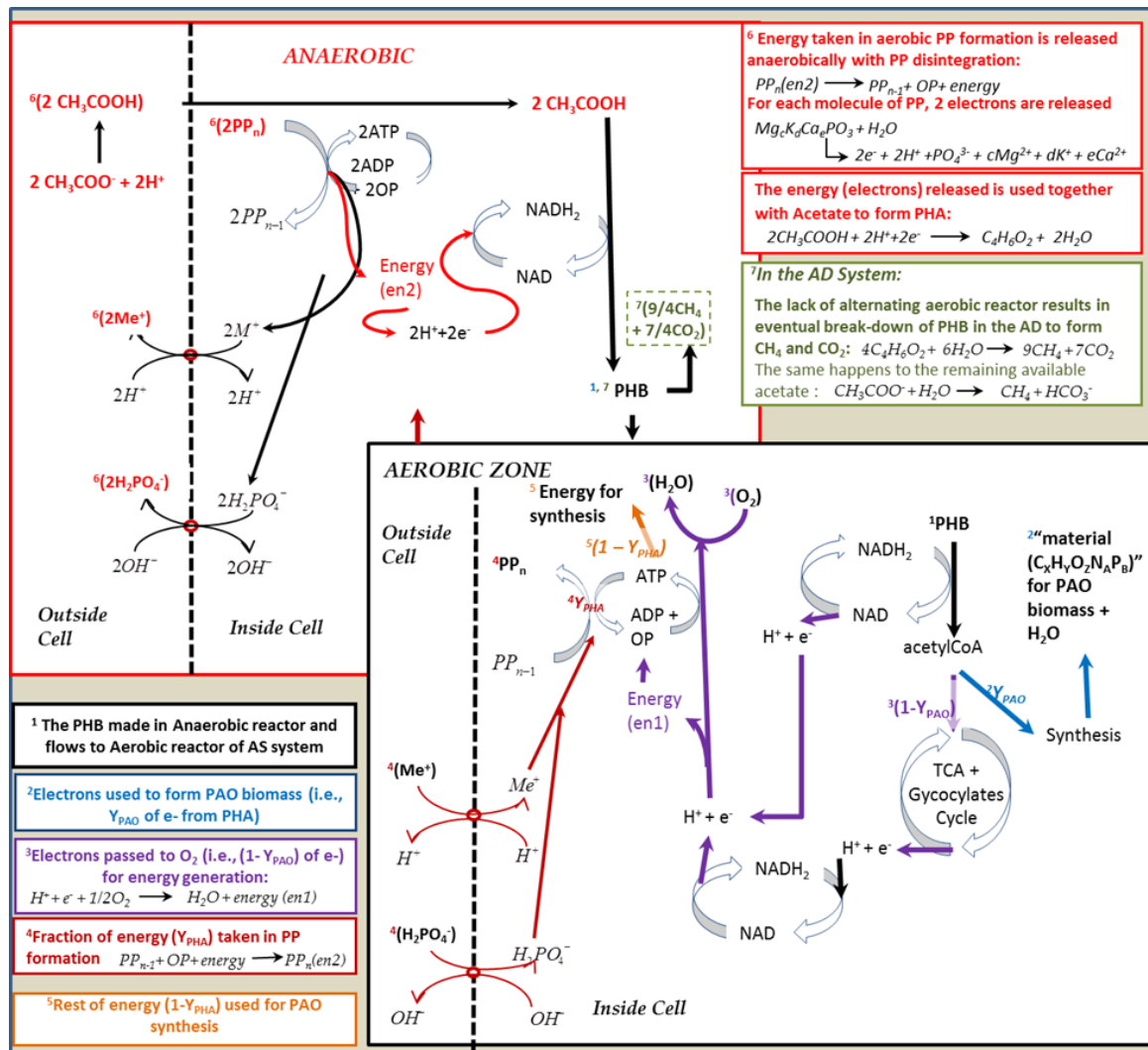
(iv) In the AD, the remaining PP that doesn't get released initially with PHB formation also eventually gets hydrolysed (as shown in Equation 75), since the dead PAO biomass cannot hold on to it further.



Where the f value fractionates the total phosphates to HPO<sub>4</sub><sup>2-</sup> and H<sub>2</sub>PO<sub>4</sub><sup>-</sup>, according to pH, as shown by Harding *et al.*, (2010), i.e.:



It was decided that both the PP release mechanisms in AD, i.e., with PHB formation and with PAO death, together with PHB disintegration be entered into the AD model because all have a possibility of occurrence.



**Figure 5:** Schematic representation of the aerobic PHB utilisation and anaerobic PP release for a AS-AD linked WWTP (Ikumi and Ekama, 2019).

Ikumi (2011) accounts that the final outcome, for an AD system operated at steady state, is equivalent to the PP hydrolysis occurring with the death of PAOs, as was reported by Harding *et al.* (2010) (see Eqs 4a and 4b). This is because in the AD model, the PHB formed eventually gets completely degraded, hence all the COD removed in AD is ultimately destined for conversion to an inevitable quantity of AD biomass and biogas (some electrons go towards  $\text{CH}_4$ ), irrespective of the defined form of the biomass (i.e., the active PAOs are modelled with or without inclusion of glycogen). The discrepancies observed during the calibration raised a few questions regarding the current stoichiometric model: Mainly (i) why is less glycogen produced than consumed? And (ii) is the energy in PP all represented by glycogen (organic material that is measurable as COD) or is there a possibility of it not being measurable as COD in the anaerobic reactor (i.e.,  $\text{NADH}_2$  formed aerobically from PHB degradation). The breakdown of an organic component such as glycogen or acetate, to act as the reducing agent in the anaerobic phase results in  $\text{CO}_2$  production. With the partial pressure of  $\text{CO}_2$  maintained according to Henry's law expression (Loewenthal *et al.*, 1994),  $\text{CO}_2$  gets dissolved into the aqueous phase resulting in a lower pH prediction. Ikumi and Ekama (2019) noticed that better predictions are obtained with acetate uptake for PHB formation than when modelling the AD PP release to occur with PAO death and hydrolysis.

Quavauvilliers (2020) initiated further investigations to determine which of Ikumi and Ekama's (2019) stoichiometry best models PAO behaviour in AD. From this investigation, an AD steady state model was generated that achieved a high degree of correlation with experimental data through including a parameter that allows for the calibration of the model when distinguishing the quantity of P released with PHB uptake and that with PAO lysis. The processes of multiple mineral precipitation (struvite, amorphous calcium phosphate and calcium carbonate) were also included to this model. To avoid spreadsheet errors due to algebraic loops when coding PP breakdown and multiple mineral precipitation, solvers were coded into the spreadsheet to break the algebraic loops when calculating system pH, and its adjustment with PP breakdown and mineral precipitation.

### **2.2.8. Dynamic Models**

Evaluative mathematical models for water and resource recovery facilities (WRRFs) unit operations are useful in contributing towards defining operational strategies that shall promote minimum cost and optimum production targets required for future systems. These mathematical models are used to virtually replicate the real system, in order to generate critical data that could be applied in long term planning and management of recoverable resources.

Dynamic models are complex models that use varying flows and loads to evaluate the time-dependent response of the plant due to dynamic loading conditions (Ekama and Wentzel, 2008a). Ikumi (2011) further summarises the use of these models as:

- For sensitivity analysis of the model application and assessment of various operation strategies.
- Enabling accurate sizing of the different unit processes and the selection of the best design alternative for the optimum plant performance criteria i.e., effluent quality and operation cost.
- Dynamic model tools can be used to provide training to plant operators with respect to the implication of operating conditions on the overall plant performance.

The plantwide wastewater treatment model of UCT and UKZN (PWM\_SA; Ikumi *et al.*, 2015) that can be used to replicate the processes in wastewater treatment plants, shall be extended to include micropollutants of concern, as components to be tracked through the system.

### **The Current UCT Plantwide Dynamic Simulation Model**

The carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P) and chemical oxygen demand (COD) mass balanced three-phase plant-wide model (PWM\_SA, Ikumi *et al.*, 2015) combines biological N and P removal activated sludge based on ASM2d (Henze *et al.*, 1995), AD of primary sludge and AD or anoxic-aerobic digestion (AAD) of WAS with interlinking non-reactive physical thickening unit operations. The properties of the model include: (i) It defines influent wastewater organics concentrations in the same seven types as in municipal wastewater [volatile fatty acids (VFA), biodegradable soluble (BSO) and particulate (BPO) organics, unbiodegradable soluble (USO) and particulate (UPO) organics, where the particulate organics are subdivided into settleable and non-settleable, in the generic form  $C_xH_yO_zN_aP_bS_c$ . Further, it uses the routinely measured parameters COD, VSS, OrgN (which equals total Kjeldahl nitrogen (TKN) – free and saline ammonia (FSA)) and OrgP (which equals Total P (TP) – Ortho P (OP)) to quantify the x, y, z a, b, c values, but because the TOC is not routinely measured, the C composition of the organics is obtained from assumed C/VSS mass ratios ( $f_C$ ). (ii) It is full element (C, H, O, N, P and S) mass balanced. (iii) It has an external algebraic equation equilibrium speciation sub-routine which separates the slow (biological and physico-chemical) and fast (aqueous) processes, (iv) It includes non-ideal aqueous solution

effects (ionic strength correction of dissociation constant (pK) values and ion pairing) to calculate the pH and relevant gas partial pressures, (v) It includes the interaction of mineral precipitation on the pH of the aqueous phase due to the release of phosphates, ammonia and inorganic carbon species in the AD or AAD systems. These features of the PWM\_SA model are global (plant-wide) and so are also included in its primary sedimentation tank (PST; with the UCTPSU submodel of Polorigni *et al.*, 2020), activated sludge (AS; with the ASM2-3P submodel of Ikumi *et al.*, 2020), anoxic-aerobic digester (AAD; also using UCT ASM2-3P) and anaerobic digestion (AD; using UCT SDM3P of Ikumi *et al.*, 2014) sub-models. A brief overview of the sub models that form PWM\_SA model is given below.

- The UCTPSU dynamic model was developed as an extension of a current TSS-based model (Bachis *et al.*, 2015), within PWM\_SA. This is a data-driven model that includes the particle settling velocity distribution (PSVD) concept of Maruejols *et al.* (2012) and fractionates the settling solids into correct portions of UPO, BPO and ISS (Wentzel *et al.*, 2006; Ikumi *et al.*, 2014). Matesun *et al.* (2021) provides that detail towards the data driven approach to application of the UCTPSU model.
- A three phase activated sludge dynamic model (ASM2-3P) was developed by adding full element (carbon (C), hydrogen (H), oxygen (O), nitrogen (N), phosphorus (P) and metals (Me)) mass balanced stoichiometry to extending the existing nitrification- denitrification (ND) excess biological P removal (EBPR) activated sludge (AS) model ASM2 (Henze *et al.*, 1995) and ensuring (i) its compatibility with the three-phase anaerobic digestion dynamic model and (ii) its equivalence to the full element mass balanced stoichiometry ASM dynamic model (without P) of Söttemann *et al.* (2005c). This three-phase activated sludge model with EBPR was applied to plant-wide simulation of NDEBPR activated sludge with anoxic-aerobic digestion of concentrated P-rich waste activated sludge with mineral precipitation to produce dewatering liquor with low nitrogen and phosphorus. As an extension of this ASM2-3P, the model sludge (ISS) production and P removal [(FeOH)<sub>3</sub> and FePO<sub>4</sub>] model (Figure 2.6 shows schematic diagram of process reactions) of Solon (2017) was included using WEST®. The model was essentially the same as for Solon (2017), with appropriate unit conversions (from molar to mass) in the stoichiometry as was done by Ikumi (2011) in order to ensure its compatibility with the PWM\_SA model. Water and protons (H<sup>+</sup>) were also included in the stoichiometry to allow for checking the mass balances of hydrogen (H) and oxygen (O) together with that of iron (Fe) and phosphorus (P). This extended ASM2-3P model was calibrated against de Haas (1990) full-scale observations.
- The dynamic anaerobic digestion model (SDM-3P) was developed by extending the two-phase (aqueous-gas) dynamic anaerobic digestion model for PS and ND activated sludge system WAS by Söttemann *et al.* (2005b), to include phosphorus from NDEBPR WAS, multiple organic types and three-phase (aqueous-gas-solid) mixed weak acid/base chemistry for multiple mineral precipitation. Ghoor (2020) then adjusted the SDM3P model kinetics to ensure predictive capacity for simulating AD failure, AD start-up conditions and upflow anaerobic sludge bed (UASB) reactors (which have temporary failure conditions at the bottom of the bed). This was accomplished by means of calibrating the AD model to an UASB dataset wherein temporary failure conditions are present in the bottom of the reactor, evident by the presence of the intermediate AD reaction products. The calibrated parameters included the maximum specific growth rates and the half saturation coefficients for the four AD biomass groups. Further, the CO<sub>2</sub> evolution kinetics were adjusted from being always at equilibrium (for steady state scenarios) to rate-controlled (with a better representation of system dynamics).

The SDM-3P model was extended further by Ghoor (2020) and Harding (2021) to include biological

sulphate reduction (BSR) processes as described further in sections below.

Due to the significant increase in size and complexity to model wastewater treatment plants, as plant-wide configurations, in three phases, the PWM\_SA model was coded in WEST®, which is a program capable of simulating many bioprocesses in various unit operations assembled into a WRRF. As noted above, the various submodels (UCTPSU, ASM2-3P and SDM3P) share the same set of components- i.e. the supermodel approach of Volcke *et al.*, 2006 was adopted. This has the advantage of (i) placing the physico-chemical states globally and linking the biological components between the AS, AAD and AD parts of the model, (ii) including parameterized stoichiometry (the x,y,z,a,b,c values of the influent organics groups and biomass species), for the bioprocesses and share the same ionic speciation, and as a result (iii) the output components of the PST and AS part become directly the input components for the AAD or AD parts without the need for transformation equations. In general, the simulations of the different chemical and biochemical processes in PWM\_SA are based on determining the materials present at a particular location and time (mass balancing) and determining the physical state that it will take on at that point (speciation) (Brouckaert *et al.*, 2010, 2016). Table 3 below provides an example of the equilibrium and mass balance equations contained in the speciation subroutine. In order to perform these calculations, the PWM\_SA adopts a general physico-chemical modelling framework (Brouckaert *et al.*, 2016). The components and species considered in the model and their interrelationships are given in Table 4 and 5

**Table 3:** Example for equilibrium and mass balance equations for ionic speciation

Weak Acid Sub-System	*Aqueous Equations	Phase	Equilibrium	Mass Balance Equation
			$[NH_3] = \frac{K_{NH_4} \cdot [NH_4^+]}{(H^+)}$	
			$[NH_4SO_4^-] = \frac{[SO_4^{2-}] [NH_4^+]}{K_{NH_4SO_4}}$	
Ammonia				$NH_x = [NH_4^+] + [NH_3] + [NH_4SO_4^-]$
*Where (H <sup>+</sup> ) is the hydrogen ion activity, [X] the molar concentrations of species X and K <sub>X</sub> is the thermodynamic equilibrium constant for species X, adjusted for ionic strength with the Davies equation to account for the activity of ions in non ideal solutions (Stumm and Morgan, 1996).				

**Table 4:** The Universally Selected Model Components

	Component Name	Empirical formula	Notation
Ionic	Water	H <sub>2</sub> O	H <sub>2</sub> O
	Hydrogen ion	H <sup>+</sup>	H
Dissolved Concentrations	Sodium	Na <sup>+</sup>	Na
	Potassium	K <sup>+</sup>	K
	Calcium	Ca <sup>2+</sup>	Ca
	Magnesium	Mg <sup>2+</sup>	Mg
Total Concentrations	Ammonium	NH <sub>4</sub> <sup>+</sup>	NH <sub>4</sub>
	Chloride	Cl <sup>-</sup>	Cl

Soluble Organics	Acetate	$\text{CH}_3\text{COO}^-$	Ac
	Propionate	$\text{CH}_3\text{CH}_2\text{COO}^-$	Pr
	Carbonate	$\text{CO}_3^{2-}$	$\text{CO}_3$
	Sulphate	$\text{SO}_4^{2-}$	$\text{SO}_4$
	Phosphate	$\text{PO}_4^{3-}$	$\text{PO}_4$
	Nitrate	$\text{NO}_3^-$	$\text{NO}_3$
	Dissolved hydrogen	$\text{H}_2$	$\text{H}_2$
	Dissolved oxygen	$\text{O}_2$	$\text{O}_2$
	Unbiodegradable Soluble Organics	$\text{CH}_{Y_u}\text{O}_{Z_u}\text{N}_{A_u}\text{P}_{B_u}$	USO
	Fermentable Biodegradable Soluble Organics	$\text{CH}_{Y_f}\text{O}_{Z_f}\text{N}_{A_f}\text{P}_{B_f}$	FBSO
Glucose	$\text{C}_6\text{H}_{12}\text{O}_6$	GLU	
Particulates	Unbiodegradable particulate organics	$\text{CH}_{Y_{up}}\text{O}_{Z_{up}}\text{N}_{A_{up}}\text{P}_{B_{up}}$	UPO
	Biodegradable particulate organics	$\text{CH}_{Y_{bp}}\text{O}_{Z_{bp}}\text{N}_{A_{bp}}\text{P}_{B_{bp}}$	BPO
	Primary sludge biodegradable particulate organics	$\text{CH}_{Y_{bps}}\text{O}_{Z_{bps}}\text{N}_{A_{bps}}\text{P}_{B_{bps}}$	$\text{BPO}_{PS}$
	Polyphosphate	$\text{K}_{kp}\text{Mg}_{mp}\text{Ca}_{cp}\text{PO}_3$	PP
	Poly-hydroxy-alkanoate	$\text{C}_4\text{H}_6\text{O}_2$	PHA
	Struvite	$\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$	Struv
	Calcium Phosphate	$\text{Ca}_3(\text{PO}_4)_2$	ACP
	K-struvite	$\text{MgKPO}_4 \cdot 6\text{H}_2\text{O}$	MgKP
Inorganic settleable solids		ISS	
Microorganism Biomass	Ordinary heterotrophic organisms	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	OHO
	Phosphate accumulating organisms	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	PAO
	Autotrophic nitrifying organisms	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	ANO
	Acidogens	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	$Z_{AD}$
	Acetogens	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	$Z_{AC}$
	Acetoclastic Methanogens	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	$Z_{AM}$
	Hydrogenotrophic methanogens	$\text{CH}_{Y_o}\text{O}_{Z_o}\text{N}_{A_o}\text{P}_{B_o}$	$Z_{HM}$
	Endogenous residue	$\text{CH}_{Y_e}\text{O}_{Z_e}\text{N}_{A_e}\text{P}_{B_e}$	ER
Gases	Carbon dioxide	$\text{CO}_2$	$\text{CO}_2$
	Methane	$\text{CH}_4$	$\text{CH}_4$
	Hydrogen	$\text{H}_2$	$\text{H}_2$
	Ammonia	$\text{NH}_3$	$\text{NH}_3$

**Table 5:** Ionic Species Selected for the Three Phase Modelling: 1-17 Ions; 23 - 44 Ion pairs

1	H <sup>+</sup>	Hydrogen ion	23	NH <sub>4</sub> SO <sub>4</sub> <sup>-</sup>	Ammonium sulphate
2	Na <sup>+</sup>	Sodium	24	MgPO <sub>4</sub> <sup>-</sup>	Magnesium phosphate
3	K <sup>+</sup>	Potassium	25	CaCH <sub>3</sub> COO <sup>+</sup>	Calcium acetate
4	Ca <sup>2+</sup>	Calcium	26	CaCH <sub>3</sub> CH <sub>2</sub> COO <sup>+</sup>	Calcium propionate
5	Mg <sup>2+</sup>	Magnesium	27	CaHCO <sub>3</sub> <sup>+</sup>	Calcium bi-carbonate
6	NH <sub>4</sub> <sup>+</sup>	Ammonium	28	NaSO <sub>4</sub> <sup>-</sup>	Sodium sulphate
7	Cl <sup>-</sup>	Chloride	29	MgHPO <sub>4</sub>	Magnesium hydrogen phosphate
8	CH <sub>3</sub> COO <sup>-</sup>	Acetate	30	CH <sub>3</sub> COONa	Sodium Acetate
9	CH <sub>3</sub> CH <sub>2</sub> COO <sup>-</sup>	Propionate	31	H <sub>2</sub> CO <sub>3</sub>	Di-hydrogen carbonate
10	CO <sub>3</sub> <sup>2-</sup>	Carbonate	32	MgSO <sub>4</sub>	Magnesium sulphate
11	SO <sub>4</sub> <sup>2-</sup>	Sulphate	33	HPO <sub>4</sub> <sup>2-</sup>	Hydrogen phosphate
12	PO <sub>4</sub> <sup>3-</sup>	Phosphate	34	NH <sub>3</sub>	Ammonia
13	NO <sub>3</sub> <sup>-</sup>	Nitrate	35	MgCO <sub>3</sub>	Magnesium carbonate
14	OH <sup>-</sup>	Hydroxide ion	36	ACPO <sub>4</sub> <sup>-</sup>	Calcium Phosphate Magnesium hydrogen carbonate
15	CH <sub>3</sub> COOH	Acetic acid	37	MgHCO <sub>3</sub> <sup>+</sup>	Calcium hydrogen phosphate
16	CH <sub>3</sub> CH <sub>2</sub> COOH	Propionic acid	38	CaHPO <sub>4</sub> <sup>-</sup>	Sodium carbonate Magnesium di-hydrogen phosphate
17	HCO <sub>3</sub> <sup>-</sup>	Bi-carbonate	39	NaCO <sub>3</sub> <sup>-</sup>	Sodium hydrogen carbonate
18	CaSO <sub>4</sub>	Calcium sulphate	40	MgH <sub>2</sub> PO <sub>4</sub> <sup>+</sup>	Sodium hydrogen phosphate
19	H <sub>2</sub> PO <sub>4</sub> <sup>-</sup>	Di-hydrogen phosphate	41	NaHCO <sub>3</sub>	Sodium hydrogen phosphate
20	MgCH <sub>3</sub> COO <sup>+</sup>	Magnesium acetate	42	NaHPO <sub>4</sub> <sup>-</sup>	Calcium hydroxide
21	MgCH <sub>3</sub> CH <sub>2</sub> COO <sup>+</sup>	Magnesium propionate	43	CaOH <sup>+</sup>	Magnesium hydroxide
22	CaCO <sub>3</sub>	Calcium carbonate	44	MgOH <sup>+</sup>	

## Model Evaluation protocol adopted for Extended PWM\_SA model

To ensure that the extended model goes through rigorous evaluation process, the BIOMATH protocol of Vanrolleghem *et al.*(2003), was applied by Ikumi (2020). This procedure involved (i) the systematic model verification method proposed by Hauduc *et al.* (2010) to check material (COD, C, H, O N, P, Mg, K, Ca) mass balances (ii) preparation of initial parameter values (determined experimentally or obtained from literature) and given their typical range using the method proposed by Brun *et al.* (2002); (iii) evaluation of parameters using (a) the Standardised Regression Coefficients (SRC) and (b) Morris Screening methods. Hence the application of multiple sensitivity analysis methods with multiple objectives was done as recommended by Neumann (2012), to provide more robust conclusions in the identification of (i) important parameters that would cause a significant change in model outputs, and hence need to be known well, (ii) non-influential parameters (those that can be set to any value within their range without much change in outputs) and (iii) interacting parameters (Neumann, 2012). An overview of these methods is given below:

### (1) Standard regression coefficient method

The standard regression coefficients (SRC<sub>ij</sub>) due to each parameter quantify the effect on variable  $j$  when parameter  $i$  is changed (hence allows prioritisation of important parameters). The SRC method involves the fitting of a multivariate linear model to the output of the MC simulation (Martin *et al.*, 2010; Neumann *et al.*, 2012). The SRC's multivariate linear regressions relate each output variable ( $y_j$ ) to all uncertainty parameters ( $\theta_j$ ), to get an equation of the form:  $y_j(\theta) = b_{j0} + \sum_{i=1}^r b_{ij} \cdot \theta_i$ . The standard regression coefficient is defined as  $SRC_{ij} = \beta_{ij} = b_{ij} \cdot \frac{\sigma_{y_j}}{\sigma_{\theta_i}}$ , where  $b_i$  is the slope obtained from linear regression;  $\sigma_{\theta_{ij}}$  is the standard deviation of the 1 000 parameter values generated for parameter  $I$ , and  $\sigma_{y_j}$  is the resulting standard deviation of output variable  $y_j$ . Finally, the coefficient of determination ( $R^2$ ), that indicates how well the multilinear regression model fits the variable's responses, was also calculated using the R program (R Development Core Team, 2011). This indicates how much confidence can be placed in using the calculated values in predicting future results. For variables with  $R^2 > 0.7$ , the SRCs ( $\beta_i$ ) are a valid measure of sensitivity (Saltelli *et al.*, 2004).

### (2) Morris screening method

Morris's screening method (Morris, 1992) is a method used to determine elementary effects for each parameter, to identify which parameters affect the model output variables significantly, and to eliminate non-influential parameters. The computation of these elementary effects requires the variation of one parameter at a time (OAT) across a select number of  $k$  levels (in this case 10), requiring  $k \cdot r$  simulations (where  $r$  is the number of parameters). In this design, each model parameter is varied within a selected uncertainty range of  $p$ , which is also determined using the method proposed by Brun *et al.* (2002). While a particular parameter was varied, all others were assigned their mid-range values. The elementary effect of parameter  $\theta_i$  on variable  $y_j$  is calculated



as:  $d_{ij}(\theta_i) = \frac{[y_j(\theta_1, \dots, \theta_{i-1}, \theta, \theta_i + \Delta, \theta_{i+1}, \dots, \theta_r) - y_j(\theta)]}{\Delta}$ , where  $y(\theta)$  is the output variable obtained when all parameters are set to their prior values, i.e.,  $y(\theta_1, \theta_2 \dots \theta_r)$ .

The mean ( $\mu_{ij}$ ) and standard deviation ( $\sigma_{ij}$ ) of the calculated  $k$  elementary effects are determined for each parameter as measures of the parameter importance.  $\mu_{ij}$  is used to detect parameters with an important overall influence on the output, while  $\sigma_{ij}$  is used to detect parameters involved in interaction with other parameters or whose effect is non-linear (Neumann, 2012; Campolongo *et al.*, 2007).

### **Simulations against experimental data**

With the prioritised model parameters (the ones with greatest effects) and non-influential parameters (those that can be fixed at any value in the range without influencing model variable outputs) determined the final model evaluation steps can be implemented, which involved (i) setting the non-influential parameters at their default values and (ii) random sampling of the remaining influential parameter sets (within their classified ranges) while conducting simulations to compare predicted model outputs with observed outputs. In this case the observed outputs were obtained from the data generated by the laboratory scale experimental systems of Ikumi (2011), towards model calibration (Ikumi, 2020).

### 2.3. Evaluation of Design/Control Strategies using Performance Indices (PI's) in Plantwide Models

The vision of wastewater treatment plants is to keep a healthy environment by discharging good effluent quality to a receiving environment, such as lakes and rivers. Furthermore, WWTPs demand significant energy (power/electricity from the Eskom's power grid), and yet there's an opportunity to make the WWTPs more energy self-sufficient. So, plant wide models allow for different operational control strategies to be simulated to reduce operating cost (OC) for the plant and maximize nutrient and energy recovery while maintaining good/improving effluent quality which complies with legal effluent quality requirements stipulated by the national government or relevant local government department.

These objectives are a paradigm shift from the traditional view of the wastewater treatment infrastructure, currently thought as wastewater treatment plants (WWTPs) to Water Resource Recovery Facilities (WRRFs) (Ikumi *et al.*, 2014).

Operational control strategies considered in this study were simulated using the performance evaluation method adopted by De Ketele *et al.* (2017). This evaluation method involves the use of performance indices (PI's) i.e. Effluent Quality Index (EQI) and Operational Cost Index (OCI). It was emphasized by Ketele *et al.* (2017) that regardless of the operational strategy chosen, effluent quality needs to be maintained in line with legal requirements (DWA, 1984) administered by the department of Water and Sanitation (DWS).

The PI's can be expressed mathematically, and therefore can be implemented on a simulated virtual plant.

#### I. Effluent Quality Index (EQI)

$$EQI = \frac{1}{T \times 1000} \int_{t_0}^{t_0 + 7 \text{ days}} [PU_{TSS}(t) + PU_{COD}(t) + PU_{BOD}(t) + PU_{TKN}(t) + PU_{NO}(t)] \cdot Q_e(t)$$

(Eq 77)

Where,

EQI, is Effluent quality index: kg pollution per day

T, is time horizon (final 7 days): days

Q<sub>e</sub>, is effluent flowrate: m<sup>3</sup>/day

PU<sub>x</sub>, this term contains the concentration of the pollutant considered

#### II. Operational Cost Index (OCI)

Operational cost index (OCI) is about inclusion of operating cost factors and indicates potential savings which could be achieved by implementing different strategies for design or control operations (De Ketele *et al.*, 2017).

The Benchmark simulation model 2 (BSM 2) of Nopens *et al.* (2010) had the following equation for calculating OCI:

$$OCI = AE + PE + 3 \times SP + 3 \times EC + ME - 6 \times MP + HE^{net} \dots\dots\dots (Eq 78)$$

Where,

AE is Aeration Energy: kWh/d

PE is pumping energy: kWh/d

SP is sludge production for disposal: Average kgTSS/d

EC is external carbon addition: Average kgCOD/d

ME is mixing energy: kWh/d

MP is methane production: Average kg CH<sub>4</sub>/d

HE is net heat needed to heat the sludge in AD (heat produced by methane accounted for): kWh/d

Clearly, the terms in Eq 78 above have different units, to normalize this, Volcke *et al.* (2006) modified it so that all the units can be in South African Rand per day i.e. ZAR/d as follows:

$$OCI = ((AE + PE - MP + ME + HE) + SP \times Energy\ cost) + SP \times Disposal\ cost + EC * Carbon\ cost \dots\dots\dots$$

(Eq 79)

Where,

Energy cost in ZAR/kWh

Disposal cost in ZAR/kgTSS

Carbon cost in ZAR/kgCOD

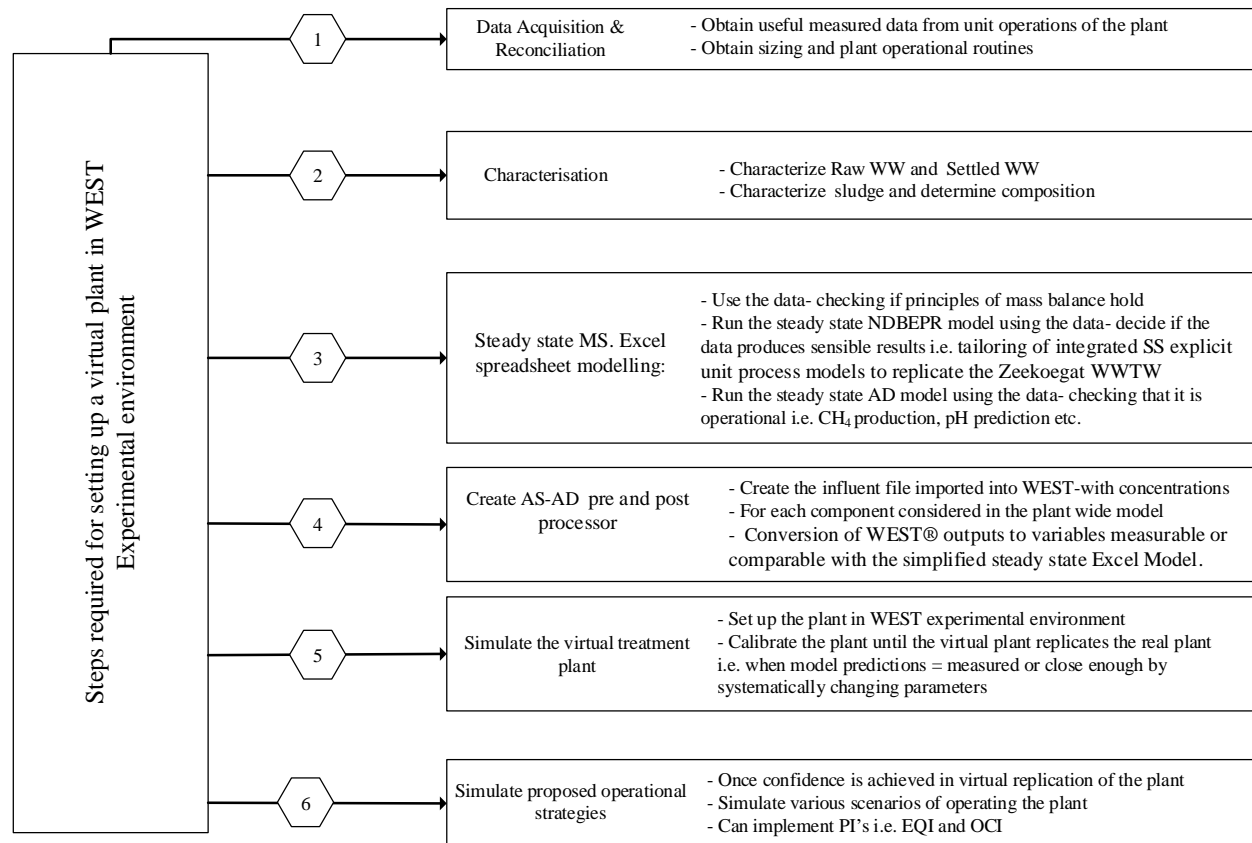
## 2.4. Closure

Water and resource recovery facility (WRRF) models have been developed for use by technically adequate professionals or researchers. Consequently, the currently developed models cannot be used by those who do not have the technical expertise and knowledge of the biological and chemical processes that happen in these models. The question of WRRF model simplification has been at the centre of discussion among modellers. For instance, in a recent debate about the issue of simplicity versus the complexity of these models at the WWTmod2016, 56 % of modellers voted for developing more complex models, while 44% voted against such models (Lizarralde *et al.*, 2018).

Developing easy-to-use WRRF models with trusted outcomes (results) is not an easy task. However, these models have been developed and are beginning to get used in various studies as decision support tools for full scale systems. Some examples of recently published examples of model application South African full-scale systems include studies by Flores- Alsina *et al.* (2021), Potts, 2021 and Jelliman, 2021. There have also been various attempts to simplify the steady state spreadsheet model towards generating a tool utilizable by stakeholders in the Water and Sanitation industry. Examples include (i) the design analysis program by Wu (2015) and the plant performance evaluation tool (PPET) of Nsengiyumva *et al.* (2020). In this study we shall explore the utilization of both the steady state and dynamic simulation tools for a selected full scale WRRF. With the accomplishments obtained in such a study there may be room to explore the next stage in model implementation, which involve working with stakeholders towards their uptake of such models and the development of digital twins that would be useful in introducing the water and sanitation sector to future sustainable smart cities.

### 3. Experimental methods, programme and site layout

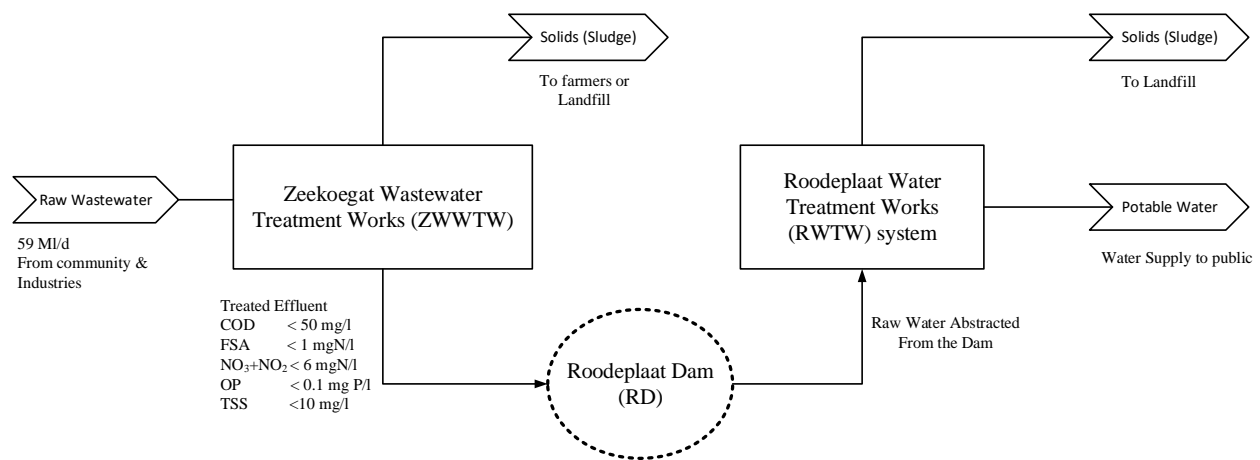
This section describes the implementation of the UCT plantwide steady state and dynamic models (Ikumi *et al.*, 2015; Ekama, 2020; Ikumi, 2020) towards simulation of the Zeekoegat WWTW. The steady state model was set up in MS. Excel and the dynamic simulation model was set up using the wastewater treatment plant engine for simulation and training (WEST®; Vanhooren *et al.*, 2003) software experimental environment. Zeekoegat WWTW. An overview of the entire process used for setting up the virtual plant and for simulation of different WWTP control strategies is summarized in Figure 6 below:



**Figure 6:** Process steps to simulating a virtual plant using a plant wide model in a simulation software

### 3.1. Zeekoegat WWTW overview and brief process description

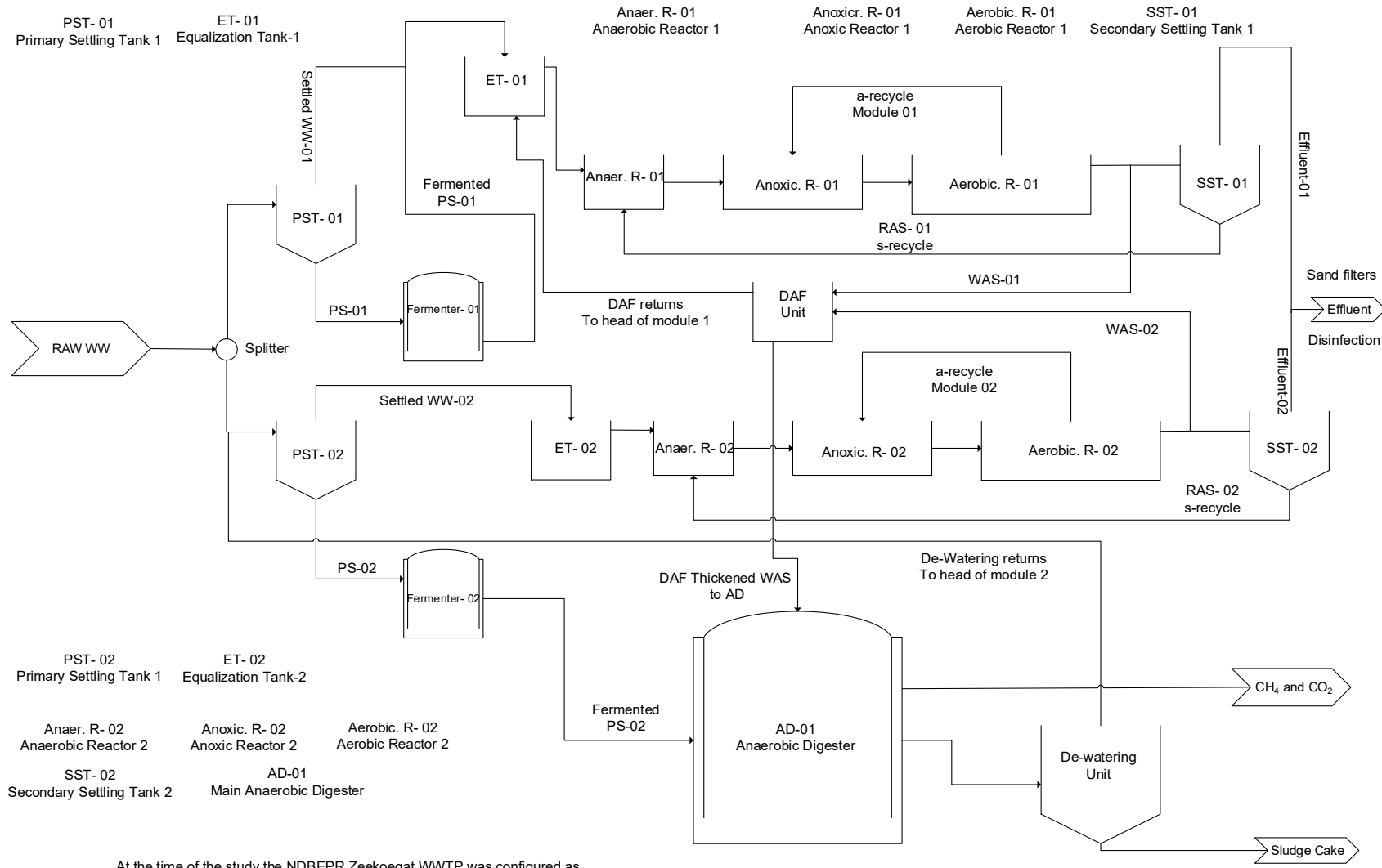
Zeekoegat WWTW was commissioned in June 1991 and is located upstream of Roodeplaat dam on the Pienaars River within the city of Tshwane metropolitan area as shown below. The effluent from Zeekoegat WWTW is discharged into the Roodeplaat Dam (RD), which sends water to the Roodeplaat Water Treatment Works (RWTW). Hence, in-direct wastewater recycling is being practiced on the Zeekoegat WWTW – RD –RWTW system as part of proactive measures to improve availability of drinking water in Gauteng, South Africa. Figure 7 below provides a depiction of the ZWWTW - RD – RWTW system.



**Figure 7:** Zeekoegat WWTW- Roodeplaat Dam - Roodeplaat WTW System

It is critical that the effluent from Zeekoegat WWTW contains minimum nutrients (see Table 6), in accordance with the compliance requirements for the Water Use License Application (WULA), from the Department of Water Affairs (DWA) and to prevent the occurrence of environmental problems such as eutrophication in RD and potential problems in the RWTW. There is a possibility of excess nutrients being discharged to Zeekoegat WWTW to RD, if the design and operational conditions are not adequate to meet the effluent quality criteria. For instance, if the AD dewatering liquor containing high nutrients remains untreated or is recycled to the AS system to levels beyond the treatment capacity that the AS system could handle.

Figure 8 on the next page shows a frozen process flow diagram for the Zeekoegat WWTW. The treatment process is also briefly explained below.



At the time of the study the NDBEPR Zeekoegat WWTW was configured as 3 stage Bardenpho system

**Figure 8:** Process flow diagram for Zeekoegat WWTW- 3 Stage BARDENPHO system

The raw wastewater (mainly domestic, with a bit of industrial WW) into Zeekoegat WWTW is first screened and degrittied, then fed by gravity to the splitter box, where it is split between two WWTW treatment modules. Each module consists of primary settling tanks (PSTs), equalization tanks, NDBEPR reactor, secondary settling tanks (SSTs) and final effluent disinfection (by direct chlorination). The treatment process can be broken down into (i) the primary treatment phase, (ii) secondary treatment and (iii) treatment of the sludge generated through AD and disinfection of the effluent.

i. Primary treatment and equalization (flow balancing) tanks

Pre-treated raw wastewater is split to four PSTs (each 22 m in diameter) and three PSTs (34 m diameter) in module 1 and module 2 respectively. The primary sludge (PS) from the PSTs is pumped to two fermenters (each module has a fermenter), where the PS is fermented to produce volatile fatty acids (VFAs).

For module 1, the fermented sludge together with the supernatant are fed to an equalization tank (11 150 m<sup>3</sup>)- the supernatant from the dissolved air floatation (DAF) unit is also fed to the balancing tank. In module 2, the PST supernatant flows to the equalization tank (10 000 m<sup>3</sup>), whilst the PS is fermented and fed to the AD system where it is anaerobically digested together with waste activated sludge (WAS). The PS fed to AD is gravity thickened but the WAS, being from a biological nutrient removal (BNR) AS system is thickened by dissolved air floatation (DAF), to avoid phosphorus release during thickening (i.e. via possible anaerobic polyphosphate breakdown).

ii. Secondary treatment (NDBEPR activated sludge system)

The settled WW is charged (from equalization tanks) to the biological reactors one (39 150 m<sup>3</sup>) and two (32 548 m<sup>3</sup>) for module one and two respectively. Each module is equipped with two SSTs and the flow is split equally between the two SSTs for settling, and the thickened return activated sludge (RAS) is pumped to the anaerobic zone of the bioreactor (during the study the system was operated as 3-stage Bardenpho- also known as A2O in the USA).

To achieve one of the general objectives of a WWTP i.e., maximizing nutrient removal (N & P), the plant was designed so that it can be operated in any of the following configurations:

- ❖ 3-Stage Bardenpho (configuration at the time of the study)
- ❖ UCT system
- ❖ Modified UCT system (MUCT)
- ❖ Johannesburg system



iii. Chemical treatment, sludge treatment and effluent quality

Orthophosphate (Ortho P) precipitation using ferric chloride is effected whenever required to comply with stringent Ortho P effluent quality legal requirement for discharge. The effluent from each module's SSTs is sand filtered before disinfection using chlorine in two contact tanks before discharged to the maturation dam, thereafter overflowing to Roodeplaat dam.

**Table 6:** Zeekoegat WWTW effluent quality requirements as per DWA Licence 27/2/2/A223/101/8

Parameter	Unit	Limit
COD	mg/l	50
Free and Saline Ammonia	mgN/l	1
Nitrate/Nitrite	mgN/l	6
Ortho-P (2009 -2011)	mgP/l	0.9
Ortho-P (2012 - 2015)	mgP/l	0.5
Ortho-P (2012 - 2018)	mgP/l	0.1
Total Suspended Solids	mg/l	10
pH		6.5 < pH < 8.5
Electrical Conductivity	mS/m	80
Faecal Coliform	CFU/100 ml	0

At the time of the study, primary sludge from module 2 was fermented and thickened before being mixed with DAF thickened WAS and charged to the anaerobic digester for biogas generation. Digested sludge is de-watered through belt-press and the liquor sent to liquor treatment tank-attempting to precipitate excess phosphorus.

### 3.2. Model Implementation

Various mathematical models have been developed for activated sludge (AS) and anaerobic digestion (AD) in wastewater treatment systems. These models (both steady state and dynamic simulation models) are based on basic principles of mass balanced stoichiometry.

When it comes to mathematical simulation models, Ekama and Wentzel (2008) cautioned that, these models need to be checked by conducting steady state calculations on the system to check the simulation model outcome predictions. If the simulation results, in this case on WEST® under steady state conditions give similar predictions as the steady state model calculation (e.g., using an excel spreadsheet), then the model can be applied in its wider range of capabilities like dynamic simulation (Ekama and Wentzel, 2008).

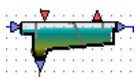

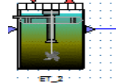

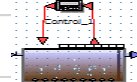

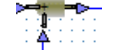
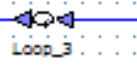
*In the case of Zeekoegat WWTW, the steady state AS model (Marais and Ekama, 1976; Ekama and Wentzel, 2008)) together with AD model (Sötemann *et al.*, 2006; Ikumi and Ekama, 2019; Quavauvilliers, 2021) were used in Microsoft excel environment, using explicit equations and could be checked for mass balanced stoichiometry for widespread use with confidence. This*

*plantwide steady state model* has been described in Section 2.2.3 of the *Literature review*. The plant-wide (PWM\_SA model) of Ikumi *et al.* (2015) was used for the dynamic simulation of the plant in WEST®. This PWM\_SA model has been described in Section 2.2.8 of the literature review. When the virtual plant was set up in WEST® experimental environment, certain icons were used representing unit operations containing model equations for the processes taking place in those unit operations to allow for calibration and simulation of the WWTP. Those key unit operations and the icons used are shown in the page overleaf.

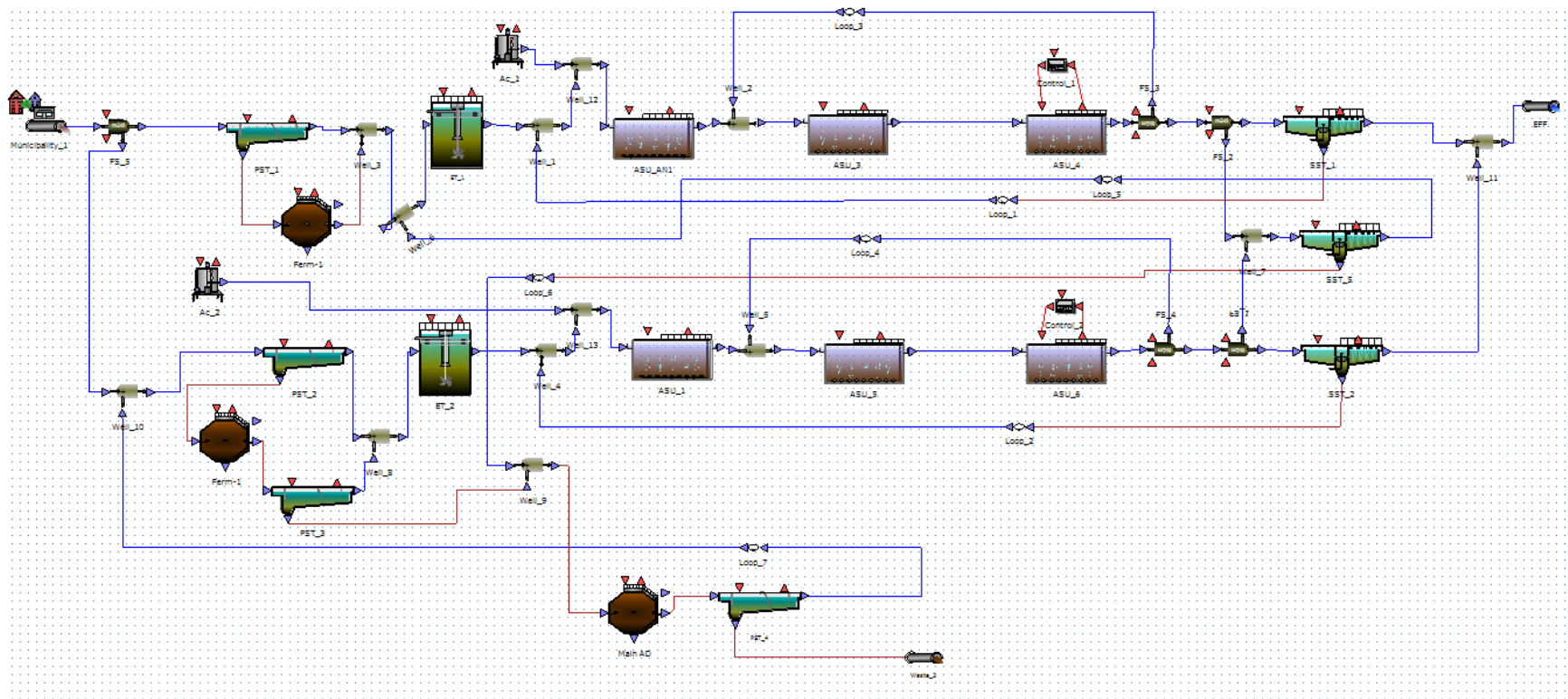
The UCT steady state model described in Section 2.2.3 of the Literature review was tailored to replicate the Zeekoegat WWTW configuration. Hence, the configuration used during steady state calculations was also set up the same way as the one added in WEST® simulation environment (See Figure 9).

The results (steady state vs dynamic) were compared at the beginning to have a good verification of the model, to have more confidence in the data generated by the dynamic models.

**Table 7:** Icons used for the individual unit operations & models used for the simulation of Zeekoegat WWTW

Unit Operation	Class-Name	Parameter/Dimension Specified	Unit Process Model & description	Comment (or model rationale)	Symbol/Icon
SSTs, PSTs, Thickeners & flotation	Primary/Secondary point settlers	Underflow rate (m <sup>3</sup> /d)	All these units are described as ideal splitters ( Jeppsson et al., 2007 ). All assumed to be non-reactive ( Flores-Alsina et al. 2021)	The settling tank has no volume (i.e. no retention time) and acts as an ideal phase separator. Flotation unit may have some P release with minimal impact on effluent quality ( Flores-Alsina et al. 2021)	
Fermenters (short sludge age ADs)	UCTAD_BSM3P operated at very short sludge age	Liquid space-volume m <sup>3</sup> of the AD	UCTSDM3P (extended model of Sotemann et al. (2006) to include multiple organic types (e.g. WAS with PAOs), P release stoichiometry & MMP (Brouckaert et al. (2010); Ikumi et al., 2014)	Volume m <sup>3</sup> based on incoming flow rate and chosen short Rs- modelled as 'failed AD' to inhibit the growth of methanogens.	
Equalization/ Balancing Tanks (ET)	Fixed- Volume- Equalisation-Tank	Volume of the ET in m <sup>3</sup> based on operational routine data	Assumed to be non-reactive, but simply balances the flow.	The model describes an ideally mixed equalization tank, with a constant volume: $Q_{in} = Q_{out}$	
Activated Sludge Unit	Fixed Volume ASU	For Anoxic & Anaerobic zone-only Volume m <sup>3</sup>	The UCT plant-wide "three-phase" (aqueous-gas- solid) model that includes P, PWM_SA (Ikumi et al., 2014) was used to simulate the virtual Zeekoegat WWTW	The model describes an ideally mixed, activated sludge tank with constant volume (Dimension)- Obtained from steady state model of the NDBEPR system	
		For Aerobic Zone- volume and DO			
Anaerobic Digester	UCTAD_BSM3P	Volume of the ET in m <sup>3</sup> based on operational routine data	UCTSDM3P (extended model of Sotemann et al. (2006) to include multiple organic types (e.g. WAS with PAOs), P release stoichiometry & MMP (Brouckaert et al. (2010); Ikumi et al., 2014)	Modelled as proposed by PWM_SA - combination of AS and AD. Extension of ADM1 to 3-phase model by Ikumi et al. (2011)	
Combiners/ Splitters	2,3,4 or 5 stream Combiner	Specify the outflow	-	For Example: two-Combiner -specify 1 outgoing stream, other is calculated	
Loop breaker	Differential Loop Breaker	Time constant 'Tau' The model introduces a small exponential delay	-	It is to be used to 'break' algebraic loops, e.g. on return flows, for wwtp type terminals.	

The figure below shows how the virtual treatment plant appears on the WEST® experimental environment.



**Figure 9:**Virtual Zeekoegat WWTW plant, on the WEST® experimental environment

### 3.3. Model evaluation and sensitivity analysis

The steady state model was evaluated by simply performing mass balance and the explicit nature of the stoichiometric equations for the processes allow for intuitive knowledge of important parameters, according to the identifiable links between significant model variables and parameters.

The plant-wide (PWM\_SA model) of Ikumi *et al.* (2015) used for WEST® simulations was evaluated through the protocol developed by Vanrolleghem *et al.* (2003). This process includes a model verification step, whereby the stoichiometric equations for the processes were checked for internal consistency by performing COD, CHONP, Mg, K, Ca and charge balances (Hauduc *et al.*, 2010). This mass balance verification spreadsheet is also included as part of the thesis supplementary material, together with the models. It's also important to determine significant parameters and to identify those with negligible impact during simulations (sensitivity analysis). It was emphasized by Ikumi (2020) that “The importance of sensitivity analysis in model calibration is prompted by the notable limitation in the applicability of various WWTP dynamic models, based on the complexities brought about by wide ranges of parameters and the intricate dependence of output variables on these parameters and other state variables” and the extensive analysis for the PWM\_SA simulation model, used in this study can be found in Ikumi (2020). Further, the model simulation results were compared to experimental data generated by various laboratory-based systems for activated sludge connected to anaerobic digestion and anoxic aerobic digestion (Harding, 2009; Ikumi *et al.*, 2015, Ikumi and Ekama, 2019, Ikumi and Harding, 2020).

#### Model Application

With the UCT steady state model and PWM\_SA dynamic simulation model having a reasonable calibration base, they were selected to be used towards simulation of the Zeekoegat WWTW (Section 4.2) shows the tailoring of these models to replicate the full scale WWTW). The reason for simulating the two systems with both the simpler steady state and WEST® simulation models, is to generate tools that could be used for the required applicable functions of design and optimized operation.

The simplified steady state excel model and the WEST® PWM\_SA model were run in parallel for the same system parameters for Zeekoegat WWTW and the variables dictating system performance were compared. without any strategies implemented.

#### Economic and Environmental Evaluation of System Performance

Simulation and evaluation of proposed operational strategies was done using performance indices (PI's: operational cost index (OCI) and effluent quality index (EQI)) derived from a previous investigation by the International Water Association (IWA) benchmark simulation modelling task

group (Copp, 2002, Nopens *et al.*, 2010). This framework for WWTP model output evaluations was modified by De Ketele *et al.* (2018) for compatibility with South African WWTPs.

### Effluent Quality Index and extensions

The two control strategies/scenarios considered in the study were evaluated for environmental impact using the EQI equation as modified by De Ketele *et al.* (2018), to include phosphorus, site specific effluent discharge restrictions (obtained from the effluent permit) and extended (from original 7 days) time horizon to account for all seasonal changes through the year (Paleker *et al.*, 2018):

$$EQI = \frac{1}{T \times 1000} \int_{t_0}^{t_{end}} [\beta_{COD} \times (Limit_{COD} - COD(t)) + \beta_{FSA} \times (Limit_{FSA} - FSA(t)) + \beta_{OP} \times (Limit_{OP} - OP(t)) + \beta_{NO} \times (Limit_{NO} - NO(t)) + \beta_{TSS} \times (Limit_{TSS} - TSS(t))] \times Q_e(t) dt \dots\dots\dots (Eq 80)$$

Where,

EQI, is Effluent quality index: kg pollution per day

T, is time horizon (length of the evaluation period): days

Q<sub>e</sub>, is effluent flowrate: m<sup>3</sup>/day

PU<sub>x</sub> = β<sub>x</sub> × (X<sub>Limit</sub> - X(t)), this term contains the concentration of the pollutant (X)

**Table 8: Beta factors :Weighting factors to determine the weight of each pollutant relative to COD**

Variable in the EQI	Unit	Limit	Beta (β)
COD	mg/l	50	1,00
Free and Saline Ammonia	mgN/l	1	50,00
Nitrate+Nitrite	mgN/l	6	8,33
Ortho-P (2009 -2011)	mgP/l	0,9	55,56
Ortho-P (2012 - 2015)	mgP/l	0,5	100,00
Ortho-P (2012 - 2018)	mgP/l	0,1	500,00
Total Suspended Solids	mg/l	10	5,00
pH		6.5 < pH < 8.5	
Electrical Conductivity	mS/m	80	
Faecal Coliform	CFU/100 ml	0	

When EQI is evaluated, the PU<sub>x</sub> term will be negative whenever the effluent concentration of pollutant X(t) exceeds the regulated limit (X<sub>Limit</sub>) and positive whenever the pollutant concentration is lower than the limit, and zero when the concentrations match the limit. The negative and positive values of EQI were segregated to form EQI negative (effluent limits violated) and EQI positive (effluent discharged is within limits) respectively for the entire period of simulation.

An acceptable/better effluent quality is obtained when  $EQI_{neg}$  is zero i.e. none of the pollutants contravene the relevant regulatory limit. Therefore to maintain better effluent quality the value of  $EQI_{neg}$  must be brought closer to zero and the value of  $EQI_{pos}$  maximized (De Ketele *et. al.*, 2018).

When both  $EQI_{pos}$  and  $EQI_{neg}$  are not zero, then one or more of the pollutants have contravened the effluent quality regulatory limits and can be identified by analyzing the data (De Ketele *et. al.*, 2018).

Current EQI equations predicted the impact of treated effluent on the receiving water bodies, these have been extended by Coothen (2021) to include evaluating the impact of WWTP processes on land and atmosphere.

The following equation was formulated to evaluate the impact of greenhouse gases such as carbon dioxide ( $CO_2$ ), methane ( $CH_4$ ) and nitrous oxide ( $N_2O$ ) from the plant on the atmosphere.

$$EQI_{gas} = \frac{1}{T \cdot 1000} \int_{t_0}^{t_{end}} \left( \beta_{CO_2} \cdot FCO_2(t) + \beta_{CH_4} \cdot FCH_4(t) + \beta_{N_2O} \cdot FN_2O(t) \right) \cdot dt \dots\dots (Eq 81)$$

Where:

- T : Total length of evaluation period (days)
- $\beta$  : Pollutant weighting factor
- F : Flux of gas evolved (kg/d)

The expression below was formulated to account for the impact of sludge disposal on land.

$$EQI_{sludge} = \frac{1}{T \cdot 1000} \int_{t_0}^{t_{end}} \frac{38}{x(t)} \cdot \left( \beta_{AS} \cdot AS(t) + \beta_{Cd} \cdot Cd(t) + \beta_{Cr} \cdot Cr(t) + \beta_{Cu} \cdot Cu(t) + \beta_{Pb} \cdot Pb(t) + \beta_{Hg} \cdot Hg + \beta_{Ni} \cdot Ni + \beta_{Zn} \cdot Zn + \beta_{CFU} \cdot CFU + \beta_{ova} \cdot ova \right) \cdot F Sludge(t) \cdot dt \dots\dots (Eq 82)$$

Where:

Where:

- SP : Sludge produced for disposal (kg/d)
- T : Total length of evaluation period (days)
- $M_{TSS}(t_{end})$  : Total mass of solids at the end of evaluation period (kg)
- $M_{TSS}(t_{start})$  : Total mass of solids at the start of evaluation period (kg)
- $TSS_x$  : Total settleable solids concentration in sludge flow ( $g/m^3$ )
- $Q_x$  : Waste sludge flow rate ( $m^3/d$ )
- AS : Activated sludge reactors
- SC : Secondary clarifier
- PC : Primary clarifier
- AD : Anaerobic digester
- SS : Sludge storage tank

## Operational Cost Index (OCI) and extensions

De Ketele *et al.* (2018) modified the OCI equation to include weighting economic factors which are country dependent (such as energy tariffs), to perform a realistic economic assessment associated with each control strategy (Paleker *et al.*,2018). The following OCI equation (as detailed in Section 2.3) was used to obtain the economic performance of the system for each simulated control strategy:

$$OCI = ((AE + PE - MP + ME + HE) + SP \times Energy\ cost) + SP \times Disposal\ cost + EC * Carbon\ cost \dots\dots (Eq\ 83)$$

Where,

Energy cost in ZAR/kWh

Disposal cost in ZAR/kgTSS

Carbon cost in ZAR/kgCOD

The EQI & OCI as amended by De Ketele *et al.* (2018) formed part of the calibrated plant-wide (PWM\_SA model) of Ikumi *et al.* (2014) for implementation in WEST® simulation platform.

**Table 9:** Components of the Operation Cost Index (OCI)

Unit Operation	OCI Component						
	Aeration (AE)	Pumping (PE)	Methane Production (ME)	Mixing (ME)	Heating (HE)	External C Addition (EC)	Sludge Disposal
PST Module 1 (PST-1)		✓					
Carbon dosing -module 1		Negligible				✓	
Anaerobic Reactor-1 (ASU_ANA1)				✓			
Anoxic Reactor-1 (ASU_3)				✓			
Aerobic Reactor -1 (ASU_4)	✓			✓			
AS internal a-Recycle module 1		✓					
RAS 1 Transfer (s-recycle)		✓					
PST Module 2 (PST-2)		✓					
Carbon dosing -module 2		Negligible				✓	
Anaerobic Reactor-2 (ASU_1)				✓			
Anoxic Reactor-2 (ASU_5)				✓			
Aerobic Reactor -6 (ASU_6)	✓			✓			
AS internal a-Recycle module 2		✓					
RAS 2 Transfer (s-recycle)		✓					
WAS (1&2) from DAF (SST-3)		✓					
Main AD			✓		✓		
AD Dewatering unit		✓					✓



Given the paradigm shift, involving the transition of wastewater treatment plants (WWTPs) into water resource recovery facilities (WRRFs) there's a need to quantify the benefits through modelling. As a result, the current OCI equations as used by De Ketele *et al.* (2018) were extended by Coothen (2022) to include operating cost factors and potential savings associated with implementation of WRRF design or control operating strategies.

$$OCI = (AE + PE - MP + ME + HE) \cdot \text{Energy cost} + SP \cdot \text{Sludge disposal cost} + EC \cdot \text{Carbon cost} + \text{Metals dosed} \cdot \text{Metal cost} + \text{Lime dosed} \cdot \text{Lime cost} - NR \cdot \text{Market price} + \text{Fines} \dots\dots \text{(Eq 84)}$$

Where:

AE : Aeration energy (kWh/d)

PE : Pumping energy (kWh/d)

SP : Sludge produced (kgTSS/d)

EC : External carbon addition (kgCOD/d)

ME : Mixing energy (kWh/d)

MP : Energy from methane produced (kWh/d)

HE : Total heat energy required by anaerobic digester for sludge treatment (kWh/d)

NR : Nutrient recovered; e.g Struvite (kg/d)

### **3.4. Data reconciliation, characterization and input to the simulation plant wide model (on WEST®)**

The process of data reconciliation and characterization requires that samples be collected from unit operations of the plant and gathering information regarding sizing and operational routines. Then characterized wastewater and operational parameters are then used as input to the mathematical model. The data obtained from Musvoto and Ikumi (2015) was used for this project. It contained the wastewater characteristics from the period of 2012 to 2014 for Zeekoegat WWTW. Once the available data is reconciled and raw sewage characterized, an influent file for model components is created and imported to the WEST® modelling software.

The list of components is provided in Table 10 below containing concentrations in mg/l for each model component. It is a requirement to have an entry (value) for each component before the simulation is started. For this reason, components not/with negligible concentration in the raw WW were allocated very small values close to zero (e.g., 0.001) for mathematical equations to work, such as biomass concentration components including OHOs (X\_OHO), PAOs (X\_PAO), acidogens (X\_AD), endogenous residue (X\_U\_Org) etc.

**Table 10:** Pre-processed influent raw WW concentrations supplied to the WEST® software before virtual replication of the plant on the experimental environment

Component	Notation	Concentration (mg/l)	Mass Flux (mg/d)
Water (solvent)	H2O	59000.000 (m <sup>3</sup> /d)	59000.00
Hydrogen	S_H	4.628	273069.91
Sodium	S_Na	2666.350	157314626.34
Potassium	S_K	10.000	590000.00
Calcium	S_Ca	5.000	295000.00
Magnesium	S_Mg	10.000	590000.00
Ammonium	S_NH	30.857	1820571.43
Chloride	S_Cl	4111.792	242595713.31
Acetate	S_VFA	26.674	1573750.19
Propionate	S_Pr	0.001	59.00
Carbonate	S_CO3	263.047	15519770.42
Sulphate	S_SO4	0.001	59.00
Phosphate	S_PO4	5.254	309997.05
Dissolved hydrogen	S_H2	0.001	59.00
Unbiodegradable Soluble Organics	S_U	11.150	657861.27
Fermentable Biodegradable Soluble Organics	S_F	72.813	4295978.96
Glucose	S_Glu	0.001	59.00
Unbiodegradable particulate organics	X_U_Inf	21.918	1293185.01
Biodegradable particulate organics	X_B_Org	81.790	4825601.93
Polyphosphate	X_PAO_PP	0.001	59.00
Poly-hydroxy-alkanoate	X_PAO_Stor	0.001	59.00
Struvite	X_Str_NH4	0.001	59.00
Calcium Phosphate	X_ACP	0.001	59.00
K-struvite	X_Str_K	0.001	59.00
Ordinary heterotrophic organisms	X_OHO	0.001	59.00
Phosphate accumulating organisms	X_PAO	0.001	59.00
Acidogens	X_AD	0.001	59.00
Acetogens	X_AC	0.001	59.00
Acetoclastic Methanogens	X_AM	0.001	59.00
Hydrogenotrophic methanogens	X_HM	0.001	59.00
Endogenous residue	X_U_Org	0.001	59.00
Carbon dioxide	G_CO2	0.001	59.00
Methane	G_CH4	0.001	59.00
PS biodegradable particulate organics	X_B_Inf	0.001	59.00
Influent inorganic settleable solids	X_ISS	32.147	1896652.36
Dissolved oxygen	S_O	0.001	59.00
Nitrogen	G_N2	0.000	0.00
Nitrate	S_Nox	0.001	59.00
Autotrophic nitrifying organisms	X_ANO	0.001	59.00
Calcite	X_Cal	0.000	0.00
Magnesite	X_Mag	0.000	0.00
Newberyite	X_Newb	0.000	0.00

## **4. Results and discussions**

In this chapter the comparison of the steady state MS Excel and the WEST® dynamic simulation model predictions are presented and discussed. Simulation and evaluation of proposed operational strategies was done using performance indices (PI's: operational cost index (OCI) and effluent quality index (EQI)) derived from a previous investigation by the International Water Association (IWA) benchmark simulation modelling task group (Copp, 2002, Nopens et al., 2010) and these results are presented in Section 4.2.

### **4.1. Comparison of steady state Microsoft excel model and dynamic plant-wide predictions in WEST®**

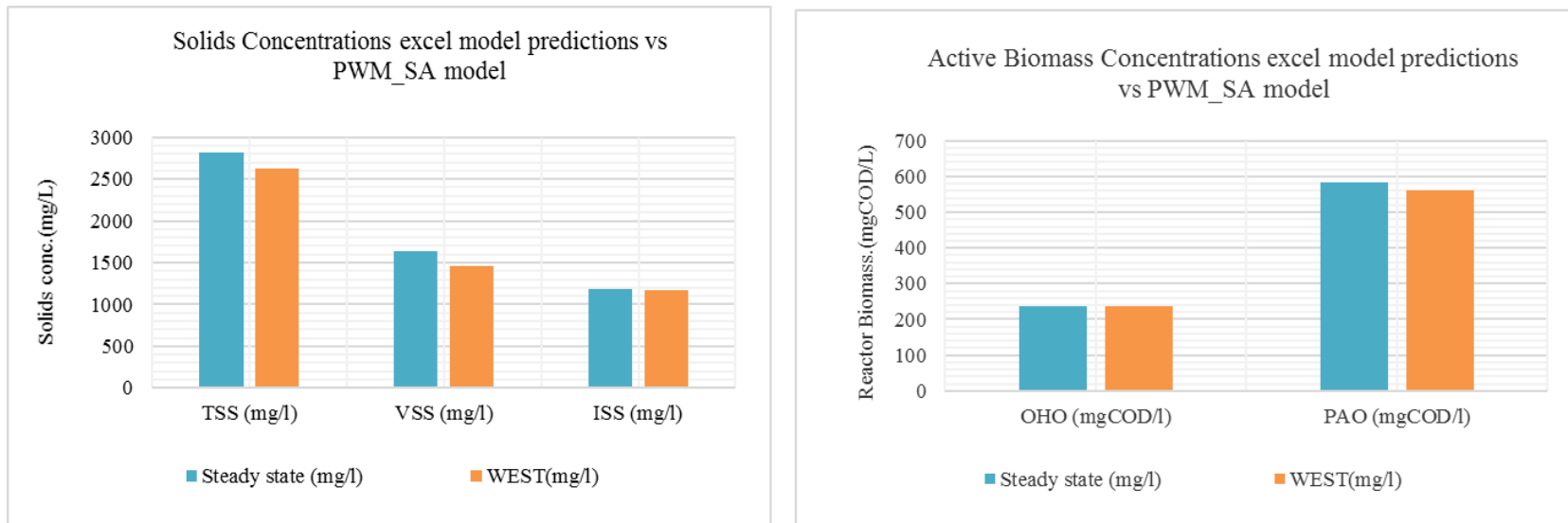
The results obtained from explicit steady state model equations using MS Excel were compared with the dynamic model (PWM\_SA) predictions. Once the confidence was achieved, then the plant wide model together with performance indices (PIs) were used to evaluate the two scenarios considered during the comparative study.

The steady state MS Excel model predictions matched very well with the dynamic plant-wide model in WEST®, with reasons provided whenever minor differences were noticed. The major reason for slight discrepancies observed is due to various assumptions made in the steady state model which the dynamic model seeks to include/simulate. One of the assumptions is that with the SS model the RBCOD is used in the anaerobic reactor and this process is catered for by applying fermentation kinetics in the dynamic model. Aeration is also assumed to work very well in the SS model and in the dynamic model aeration is modelled as process. The water generated in the activated sludge process under SS conditions is assumed to evaporate completely to keep the reactor volume constant, whereas the dynamic model caters for the accumulation of water which to some extent might dilute the concentration of solids in reactor, as observed in real life. The prediction of important system variables is presented in the next page.

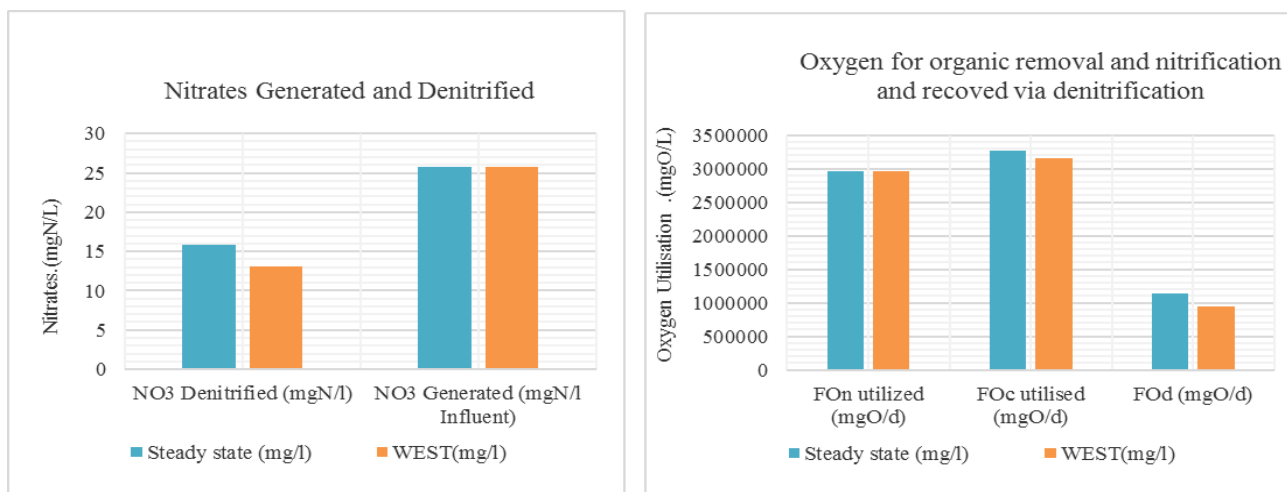
### **Module one comparisons (Postprocessor)**

The simplified steady state MS Excel model and the WEST® PWM\_SA model were run in parallel for the same system parameters for Zeekoegat WWTW. This was done mainly because (i) the steady state model contains explicit equations (the link between the parameters and output variables can be directly identified and for better understanding of predicted data) that allows for easy evaluation of the output results, while the dynamic model contains algebraic equations that are run in parallel at various kinetic rates (more complex with higher levels of intricacy between parameters and variables). (ii) Because the simplified steady state model in MS Excel and the complex dynamic simulation model have the same conceptual background (both are mechanistic models, that are largely dependent on the behavior on microorganisms mediating the wastewater treatment process and principles of material mass balance), then it is expected that at steady state, they would provide similar outcomes. These comparisons assist to identify the current limitations that the steady state model may have due to the assumptions made to ensure its simplicity relative to the dynamic simulation model in their possible application as a decision-support tool for full scale WWTWs.

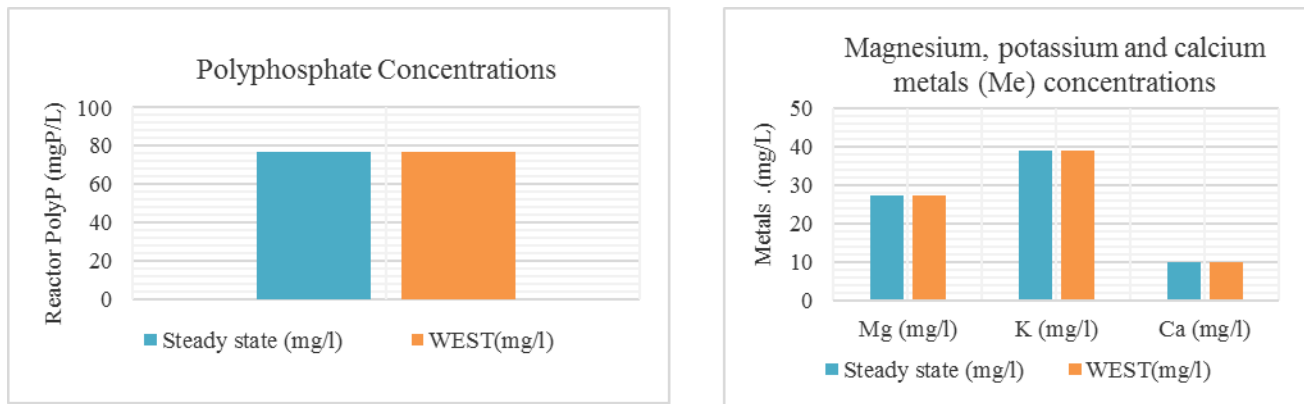
The most important variables to showcase AS system performance in terms of reactor solids concentration (see Figure 10), oxygen utilized, nitrates generated and nitrates denitrified (Figure 11) and concentrations of polyphosphate chains and key metals like magnesium (Mg), potassium (K) and calcium (Ca) (Figure 12). which are important in the potential for multiple mineral precipitates (such as struvite) in the AD system that treats the WAS generated.



**Figure 10:** Comparison of solids concentration in the reactor and active biomass concentrations for module one



**Figure 11:** Comparison of nitrate generation and denitrification (left) and oxygen utilization rate and recovery via denitrification in module 1



**Figure 12:** Prediction of polyphosphate concentrations and metals in module 1

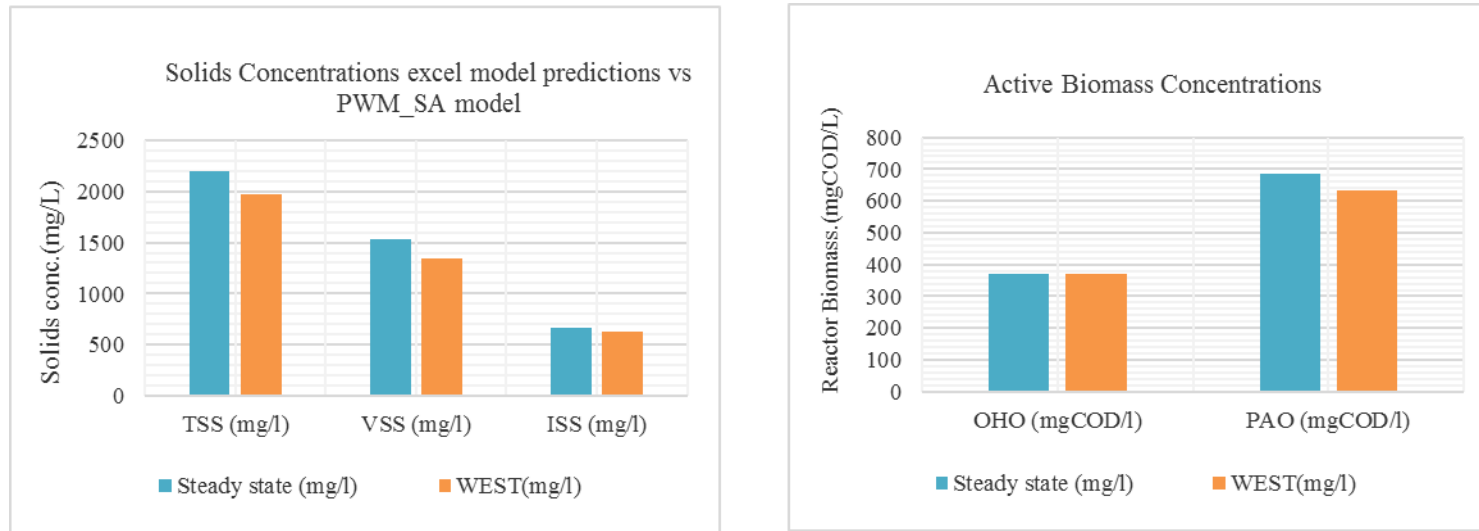
Reasonable matches can be observed between the explicit mass balanced steady state MS Excel model and the PWM\_SA WEST® model. There are few minor discrepancies in the active PAO biomass, volatile suspended solids (VSS) and total suspended solids (see Figure 10). In the simplified MS Excel SS model, the substrate for the growth of PAOs (VFAs) is largely determined by the quantity of readily biodegradable organics present in the influent that can be anaerobically sequestered by the PAOs to form internally stored poly hydroxy-butyrate (PHB), which they later use aerobically for growth. This is done via an iterative process that includes a calculation of the quantity of biodegradable COD that would be used in the ‘anaerobic’ zone by OHOs to break down organics, using any recycled nitrates and/or oxygen. Hence, the anaerobic zone is deemed truly anaerobic after all the nitrates and oxygen are depleted and only then could the PAOs have access to the RBCOD. Further, despite anaerobic hydrolysis of biodegradable particulate organics (BPO) not being included in the steady state AS model, the fermentation rate is deemed to be sufficiently high such that all the fermentable biodegradable soluble organics (FBSO) is assumed to have been converted to VFAs. This is different from the dynamic simulation model (PWM\_SA) which includes the kinetics of hydrolysis and fermentation. Hence the PAOs only have access to the VFAs in the influent and the quantity that is available after the hydrolysis and FBSO fermentation processes are complete. Further the OHOs are also modelled to take up VFAS and FBSO in the ‘anaerobic’ zone at prescribed rates, with the utilization of any oxygen or nitrates recycled to this zone. The nitrates are hence denitrified both in the anoxic zone and the anaerobic zone (as long as nitrates are available in an unaerated zone). Further, the ‘anoxic’ zone could also allow for PAO substrate uptake, as long as the nitrates have been depleted (Ikumi, 2020). A

higher growth in PAOs results in increased VSS (hence also TSS) and oxygen consumption because the PAOs are known to have a much lower death rate (0.04/d) than OHOs (i.e., 0.62/d) (Wentzel and Ekama, 2008).



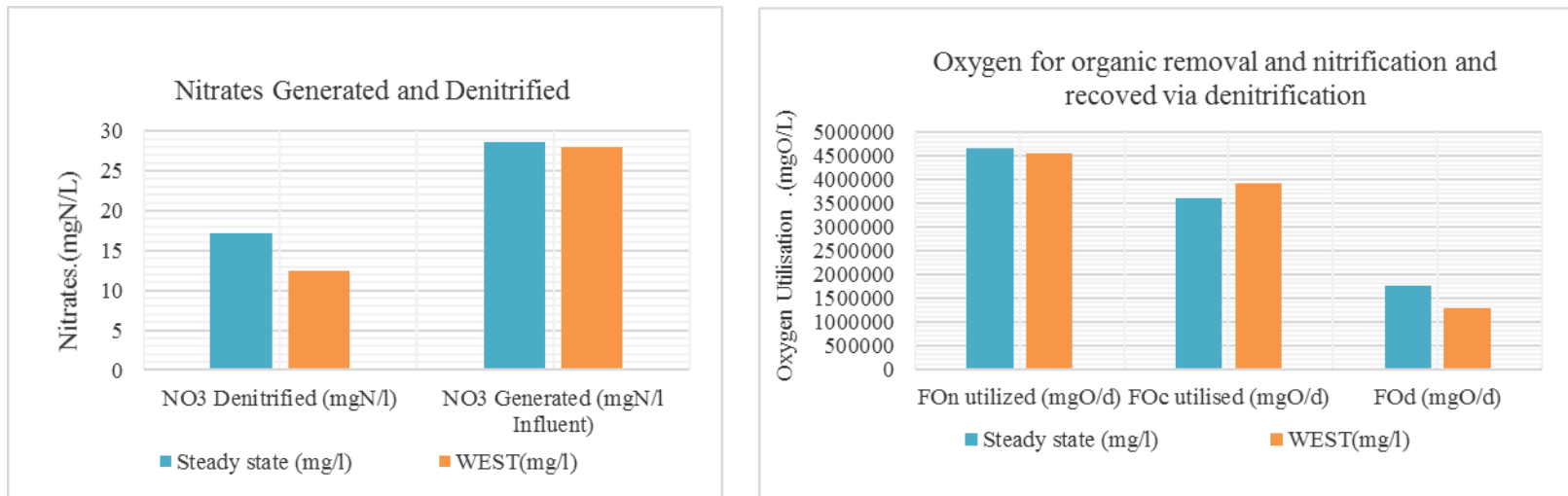
### Module two comparisons (Postprocessor)

Similar comparisons were made also for the second module and system variables matched well i.e., the mass balanced (CHONP & charge) stoichiometric equations of both the steady state model and PWM\_SA predicted similar results as seen in Figures 13,14 & 15).

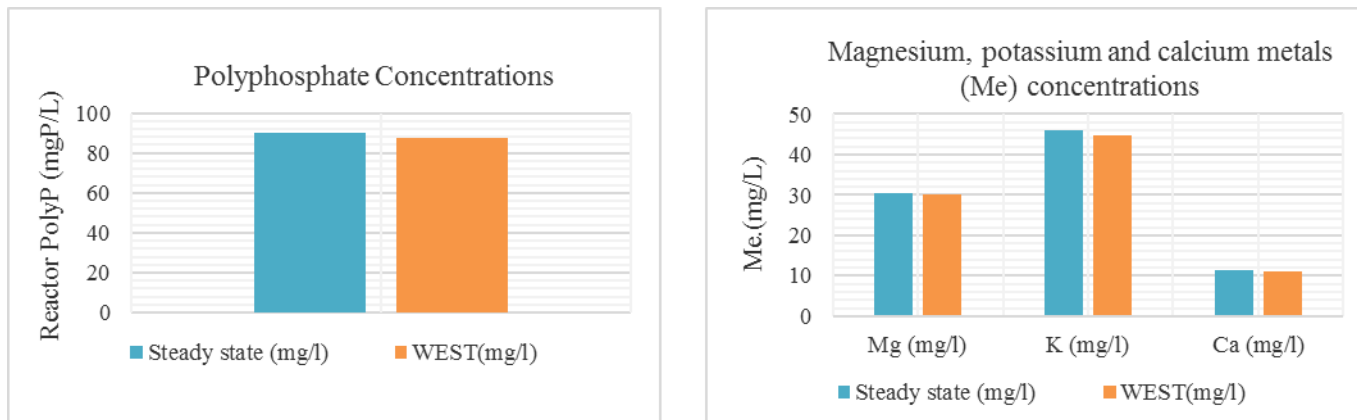


**Figure 13:** Comparison of solids concentration in the reactor and active biomass concentrations for module two

The rest of the system variables were predicted quite well as seen below.



**Figure 14:** Comparison of nitrate generation and denitrification (left) and oxygen utilization rate and recovery via denitrification in module two



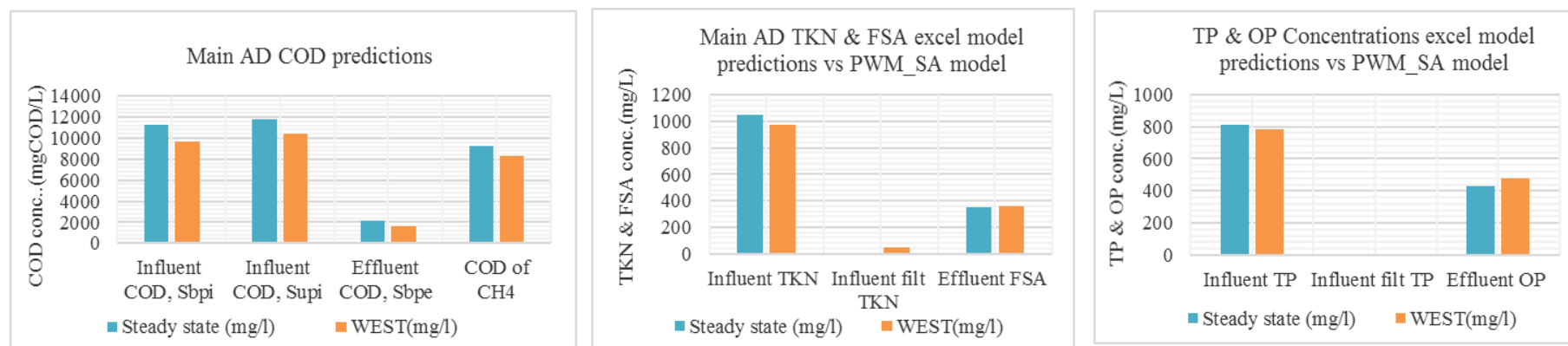
**Figure 15:** Prediction of polyphosphate concentrations and metals in module two

Similar to the module 1, the minor discrepancies can be noted between the PAO vs OHO population, due to the substrate allocation for biomass growth (i.e., the quantity that is sequestered anaerobically by the PAOs). As explained above, the predicted PAO and OHO biomass growth due to biodegradable COD utilization influences the system VSS oxygen utilization, due to the PAO death rate being lower than for OHOs. Further, depending on how much polyphosphate (PP;  $Mg_cK_dCa_ePO_3$ ) is accumulated by the PAOs aerobically,

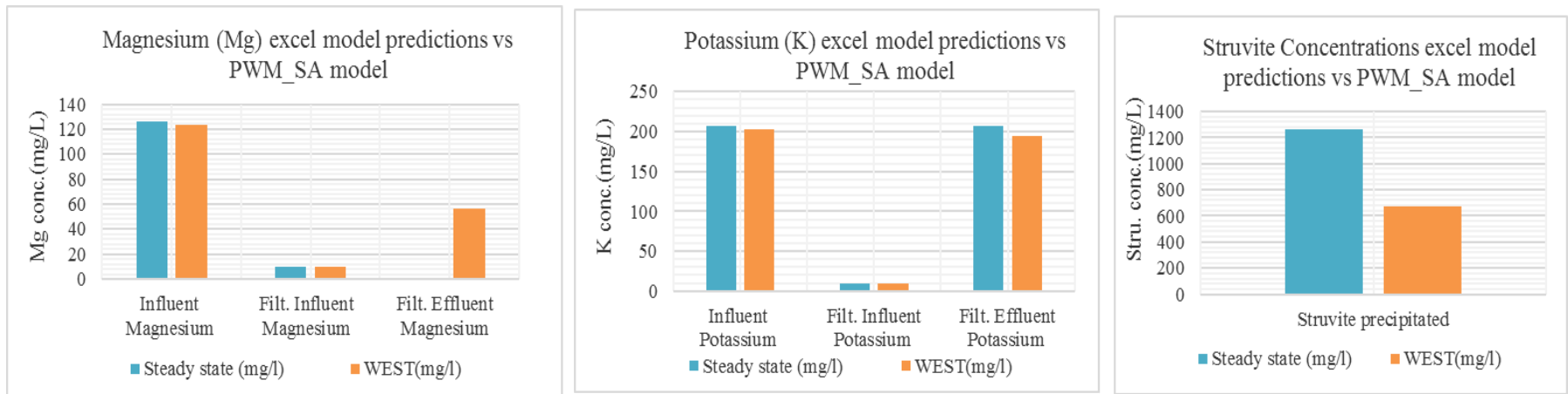
the system ISS is also influenced by quantity of PAO growth (since PP is part of ISS). According to Wentzel *et al.* (1990), the maximum amount of PP that can be taken up by PAOs is 0.35 mgP-PP/mg PAOVSS. In the simplified SS model, it is assumed that the maximum quantity of PAOs is generated, with limitations to the metal counter ions (Mg, K and Ca) and OP available for the PP formation. This means that if there is excessive amount of metals and OP, that the maximum of 0.35mgP/mgPAOVSS is formed. However, if either the metal counter ions or OP are limited, the PP formation will not allow for their concentrations to be less than zero in the effluent (hence the PP formed becomes less than the maximum of 0.35mgP/mgPAOVSS). In the complex dynamic simulation model, the PP formation includes the catabolic utilization of PHB and oxygen according to given rate kinetics. Hence the effluent OP and metals concentrations depend on the rate of aerobic PP uptake and PAO biomass available for this process. However, similar to the simplified SS model the storable PP is never above the maximum of 0.35mgP/mgVSS.

### Anaerobic Digester predictions (SS excel model predictions vs dynamic PWM\_SA in WEST)

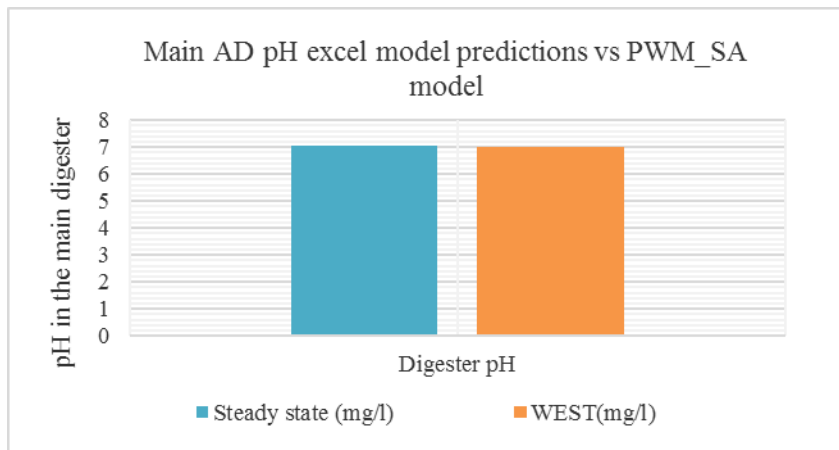
Fermented primary sludge of module two was fed to the main AD together with the DAF thickened WAS from both modules. The key system variables were predicted very well by the steady state excel model vs PWM\_SA dynamic model as seen in Figures 16 to 18.



**Figure 16:** Main AD (16a), TKN &FSA (16b) and Total phosphorus and OP (16c)



**Figure 17:** Main AD predictions for metals Mg (17a), Potassium (17b) and Struvite concentration (17c)



**Figure 18:** Main Anaerobic digester pH prediction

The breakdown of organics, including NDBEPR WAS in the AD leads to a release of OP and ammonia which ultimately leads to change in system pH and this was predicted quite well by the SS MS Excel model and PWM\_SA dynamic model (Figure 18). Because the AD system is fed both PS and WAS, the results from the parent AS system would impact the characteristics of sludge fed to the AD. As noticeable there are some marginal discrepancies between the simplified SS model and dynamic simulation model for the influent organics (which impacts the  $S_{bpi}$  and organic N contribution to TKN). The main reason for this is the lower VSS concentration from the parent AS system (see Figure 13 above). There are also very minor discrepancies for the effluent ammonia and OP concentrations due to the effluent FSA and OP being marginally higher in the values predicted by the dynamic simulation model. However, the COD removal and associated OP and FSA release from both the simplified SSS and dynamic models are very similar. The simplified SS AD model is currently only capable of predicting mineral precipitation in the form of struvite ( $MgNH_4PO_4 \cdot 6H_2O$ ). However, the dynamic AD model, is capable of simulating the kinetics of multiple minerals precipitating in parallel (struvite, magnetite, calcite, calcium phosphate, newberryte, K-struvite). Because of the number of P related minerals to precipitate in the dynamic model are different from the SS model. The OP prediction is similar for both models, while the effluent metals concentrations are different.

## 4.2. Scenario analysis: Using the fermenters vs dosing of VFAs to improve P removal

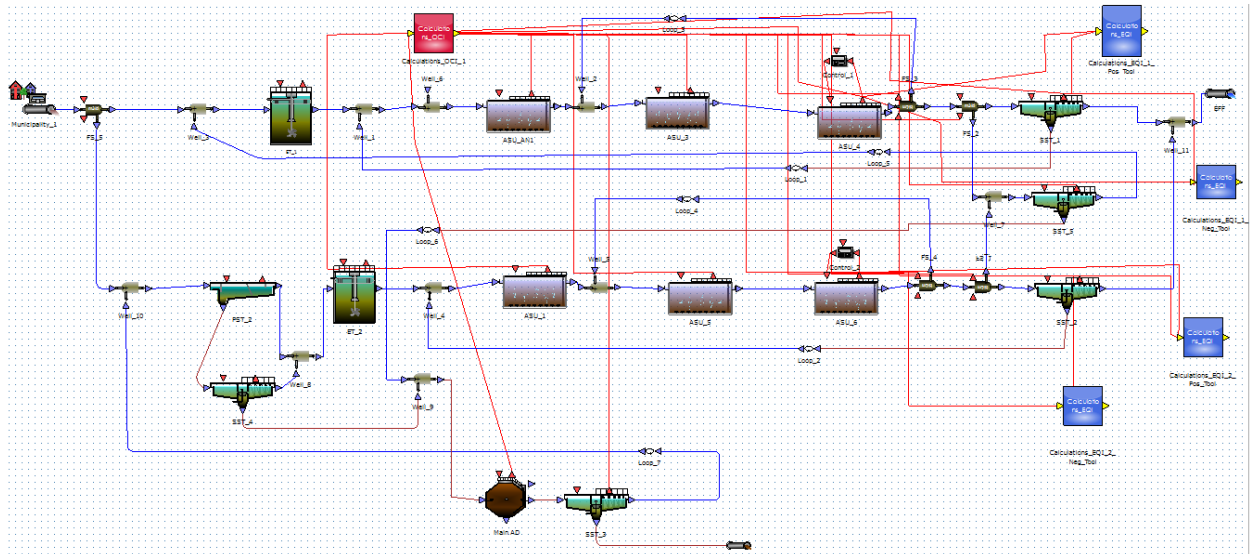
The following scenarios/control strategies were compared during the study:

**Table 11:** Scenarios/control strategies considered during the study

Control Strategy/scenario	Description	Comment
Reference	Reference layout, plant as is with no fermentation of BSO & BPO (operate the fermenters at a very short sludge age: few minutes to ensure no generation of VFAs)- All recycles & balancing tanks (BT) present.	3-stage Bardenpho system (A2O in US) on both modules
Case A_fermentation of BSO & BPO in the raw WW	The reference layout, all recycles & balancing tanks present with & fermenters present: operated at short sludge age ( $R_s = 1$ day) to allow for generation of VFAs from hydrolysis of BSO & BPO without the growth of methanogens.	
Case B_External C-dosing (VFAs)	The reference layout, all recycles & balancing tanks present with NO fermenters, but Carbon dosing.	

The plant configuration was only limited to 3-stage Bardenpho, even though it can be operated in any of the most effective configurations such as the UCT-system, modified UCT-system and the JHB system, which scenarios have been tested and shown to produce better effluent quality at relatively low operation cost by a number of researchers including De Ketele *et al.* (2018) and Paleker *et al.* (2018).

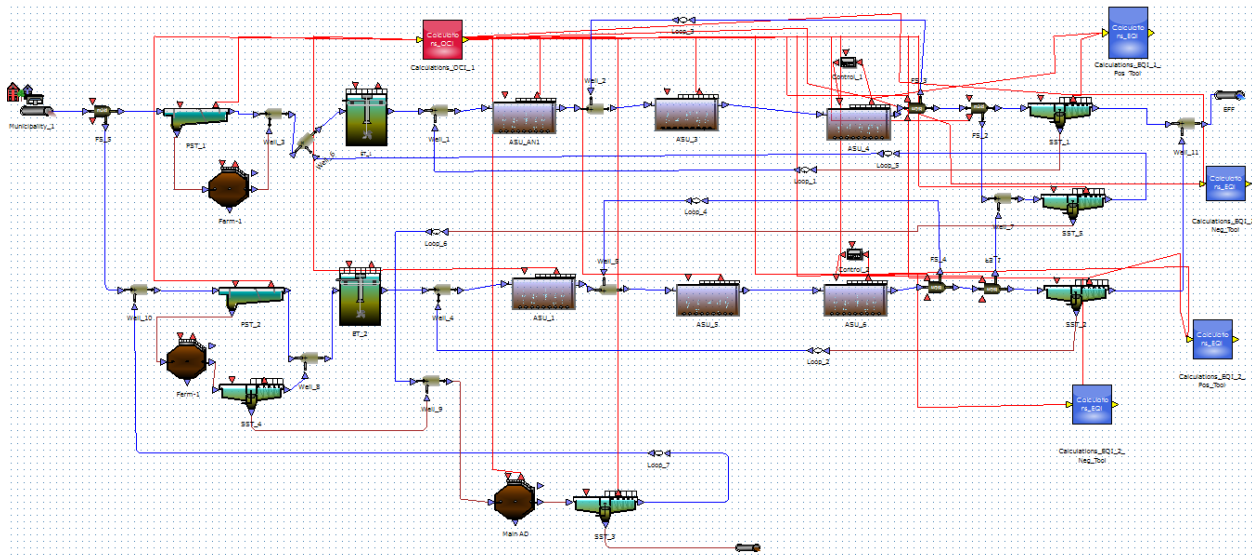
The reference layout of Zeekoegat WWTW was set up in WEST® experimental environment in the following way:



**Figure 19:** Reference layout for Zeekoegat WWTW before strategy implementation (base case)

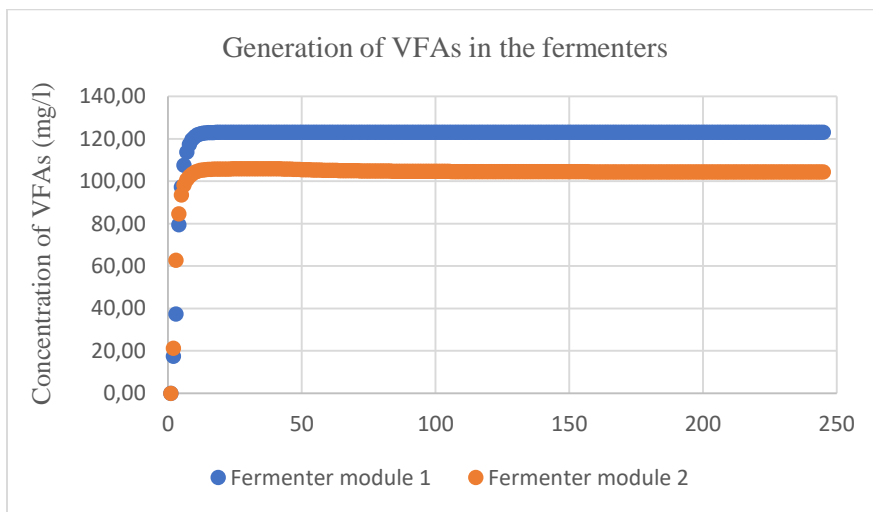
Module one of the reference layout treated raw wastewater without fermenters, so the primary settling tank was removed during simulation to retain all particulate organics to ensure meaningful comparison of scenarios.

The first scenario implemented was the addition of fermenters and the experimental set up is shown below:



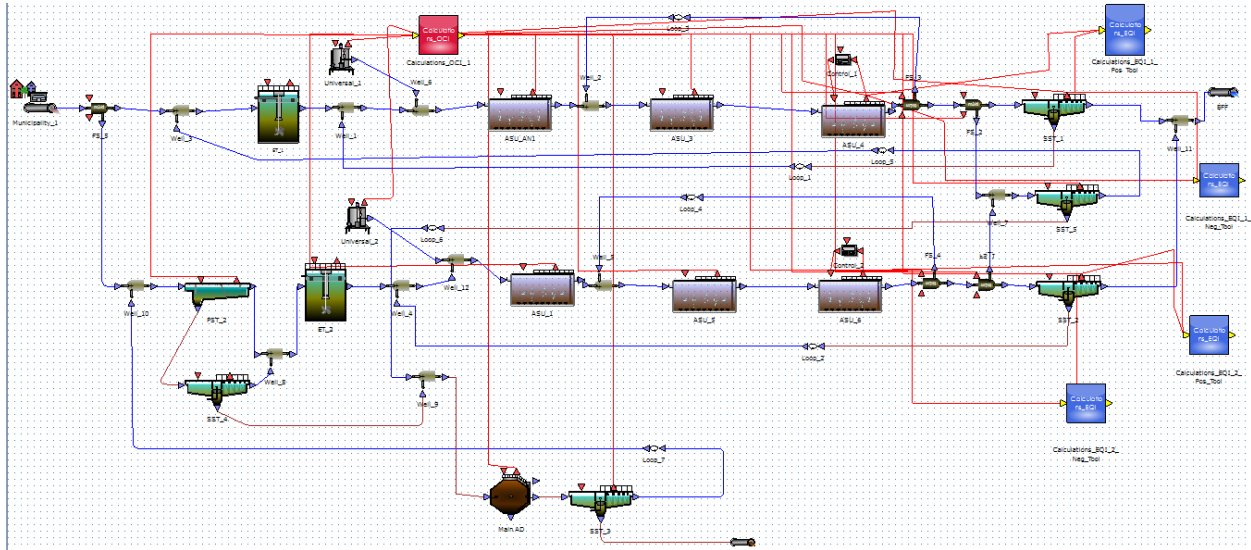
**Figure 20:** Case A\_fermentation of BSO & BPO in the raw WW

It was also important to ensure that the fermenters (Figure 21) were modelled correctly for scenario analysis i.e., the hydrolysis of biodegradable particulate organics (BPO) into fermentable biodegradable soluble organics (FBSO) and subsequently into volatile fatty acids (VFAs). The fermenter was simulated by modelling an AD that was allowed to fail (by running it at low sludge age, hence preventing methanogens from growing on the newly generated VFAs). The VFAs generated from the fermenter (i.e., AD simulated to failure) are then fed to the anaerobic zone of the AS reactor to improve P removal (see Section 2.1). Figure 21 shows the simulated quantity of VFAs generated by the fermenters using this approach.



**Figure 21:** A generated in the fermenters from BPO & BSO hydrolysed over a short sludge age

The second scenario (Case B) implemented was the addition of VFAs (via direct chemical dosing to the anaerobic zone of the AS system), and the experimental set up is shown in Figure (22). The impact of dosing VFAs was showcased under this scenario with a targeted focus on P removal through enhanced growth of PAOs.



**Figure 22:** Case B\_External C-dosing (VFAs)

### Evaluation of the two control strategies using performance indices (PIs)

Each control strategy was evaluated using the performance indices (EQI & OCI; De Ketele *et al.*, 2018) which have proven to be a useful technique to evaluate and compare different control strategies in a full scale WWTP system, using the model that has been tailored to suit the plant (i.e., in this case, Zeekoegat WWTW) operational conditions.

At the time of the study, only module two had an anaerobic digester (treating combination of module 2 PS & WAS from both modules 1 and 2). The nutrient rich stream from the AD dewatering unit is recycled back to the PST of module two and thereby overloading the activated sludge reactor with high concentrations of N&P and effectively recycling nutrients around the plant. It was noted that both operational strategies (at every time step) were able to remove COD and ammonia (by nitrification) below the regulatory limits, which achieved the first two objectives of a WWTP (Ekama and Wentzel, 2008). However, the nutrient (N&P) removal was difficult to achieve within the prescribed effluent criteria. (see Section 3.3, Table 8)



It was decided to report the performance indices (EQI) for both modules, as the effluent from module two negatively affected the effluent quality of the overall plant, this module required high dosage (10 000 kg/d) of external carbon (VFAs) to achieve near acceptable effluent quality (decreasing the magnitude of EQI<sub>neg</sub>) and as a result high operation cost. Table 12 below shows a broader view of this phenomena as observed during the experiments.

**Table 12:** Average Values for Performance indices and pollutants concentration as per effluent discharge permit

Scenario	EQI (DYN= 365 days)		COD-avg	FSA-avg	OP-avg	NO-avg	OCI (both for module 1 &2)
	EQI pos	EQI neg	[mgCOD/l]	[mgN/l]	[mgP/l]	[mgN/l]	ZAR/d
<b>Module 1</b>							
Reference layout (plant as is)	2970	-11952	22,62	0,098	1,041	12,36	13315
Case A_fermentation of BSO & BPO in the raw WW	2888	-11975	26,38	0,098	1,046	12,64	13353
Case B_External C-dosing (VFAs)	3889	-337	21,55	0,252	0,011	7,81	148570
<b>Module 2</b>							
Reference layout (plant as is)	4338	-92724	20,30	0,095	5,251	15,50	13315
Case A_fermentation of BSO & BPO in the raw WW	4288	-94783	21,81	0,095	5,393	15,55	13353
Case B_External C-dosing (VFAs)	4569	-5647	36,41	0,093	1,164	13,18	148570

The EQI negative and EQI positive values are both not zero on almost all the scenarios considered, implying that one or more of the pollutants exceeded the regulatory limits. The pollutants which exceeded the regulatory limits can be identified by analyzing the data after each simulation.

The implementation of fermenters under the current plant configuration (3- stage Bardenpho) could not improve the overall effluent quality i.e., no significant minimization of EQI<sub>neg</sub> magnitude and relatively lower EQI<sub>pos</sub> values were obtained (2.79% decrease observed). This outcome was expected because both return activated sludge (with relatively high nitrate concentration) and dewatering liquors from AD and DAF unit are fed to the anaerobic zone of the reactors, so the organics (fermented BSO and BPO) may have been first used for denitrification instead of PAO growth due to system configuration as a limiting factor.

The summary of the key drivers of the OCI for the plant is provided below:

**Table 13: Overview of major OCI drivers**

Tested Scenario	Major components of the OCI						Savings	OCI
	Aeration	Pumping	Heating	Mixing	Sludge Disposal	Chemical Addition	Methane Production	Total Costs
	kWh/d	kWh/d	kWh/d	kWh/d	kg/d	kg/d	kWh/d	ZAR/d
Reference layout (plant as is)	10622	14773	0	139	3832	0	4809	13315
Case A_fermentation of BSO & BPO in the raw WW	10662	14772	44	139	3844	0	4270	13353
Case B_External C-dosing (VFAs)	18538	14772	68	139	5334	Module 1 : 7200 kg/d Module 2: 10000 kg/d	10592	148570

It was observed that implementation of fermenters as a control strategy would not be preferred for the 3-stage Bardenpho configuration of Zeekoegat WWTW (no improvement observed) in terms of performance indices. The outcome may have been different for a configuration such as UCT-System, JHB-system or modified-UCT system since the loading of the anaerobic zone with nitrates would have been avoided to enable exclusive VFA uptake by PAOs to remove P. Furthermore, the inclusion of fermenters led to a slightly more operation cost due to more aeration and sludge disposal requirements.

As expected, the addition of external carbon (VFAs) improved P removal by 98% and 77% for module one and two respectively. The effluent quality was improved and with an impressive minimization of  $EQI_{neg}$  of 97% and 93% in module 1 and 2 respectively due to improvement of the most influential pollutants such COD, FSA, OP and  $NO_3^-$  and TSS which are direct inputs in the evaluation of the effluent quality index.

It was emphasized by De Ketele *et al.* (2018) that the addition of the carbon source in a 3-stage Bardenpho system could be more effective when dosed to the anoxic zone of the bioreactor, leading to an improvement of EQI by even 36%. This could perhaps lead to a better P removal in module two, since the main AD dewatering liquor is recycled and hence causes accumulation of nutrients which ultimately lead to limited N & P removal in the system and the  $EQI_{neg}$  not reaching zero (a sign of 100% compliance with respect to regulated pollutants). Notwithstanding that there was significant denitrification achieved in both modules (36% and 15% in modules 1 & 2 respectively) due to more/supplemental terminal electron donors (imported VFAs) available for OHOs in the anoxic zone. This benefit came, albeit with more operating cost from chemical cost (VFAs) and more aeration requirements due to increased sludge from rapid growth of PAOs and OHOs. This also meant that more sludge was sent to the main AD and hydrolyzed for methane production as seen from 50% increase in significant savings from biogas production. Therefore, the strategy of importing C-source can improve effluent quality but at unsustainably high operation cost (OC). However, it is notable that the OC can be also be avoided by simply configuring the plant differently, avoiding the recycle of untreated streams from AD & DAF dewatering liquors.

## 5. Conclusion

The main aim of the study was to utilize the PWM\_SA model to simulate Zeekoegat WWTW and hence propose operational strategies that could be useful in proposing future design or optimized operation of the system. This objective was achieved by first establishing the WWTP layout using explicit steady equations in Microsoft excel and thereafter the dynamic model (PWM\_SA) was applied to the plant' operation to minimize energy and operating cost while maximizing nutrient recovery without compromising effluent quality.

The two operational strategies were simulated and evaluated using performance indices (PI's: operational cost index (OCI) and effluent quality index (EQI)) derived from a previous investigation by the International Water Association (IWA) benchmark simulation modelling task group. These PI's were proven to be a useful approach to evaluating the environmental (EQI) and economic (OCI) impact of a WWTP based on an operational strategy implemented (i.e., optimizing WRRFs and troubleshooting problems to improve our wastewater treatment systems in South Africa).

The addition of fermenters could not improve the plant performance in terms of performance indices, this was due to recycling the nutrient rich stream from the main AD and also the current configuration (3- stage Bardenpho). This configuration overloads the anaerobic zone with nitrates and effectively converts this zone into an anoxic zone until all the nitrate is denitrified before the PAOs are able to sequester the newly formed VFAs from fermentation of FBSO and BPO. Notwithstanding that, the addition of an external carbon source (VFAs) proved to be the most optimum operating strategy, but at a relatively high operating cost.

## 6. Recommendations

Based on the above conclusion, the following recommendations are made:

- Zeekoegat WWTW should be set up (virtually) in any of the most effective configurations such as UCT-system, Modified UCT system (MUCT) and Johannesburg system to enable a holistic evaluation of the benefit of adding fermenters as an operational strategy to optimize the system. More operating strategies should also be considered, such as the exclusion of the nutrient rich stream from the AD dewatering unit.
- The SS AD should be applied to include multiple mineral precipitation beyond struvite by use of iterative processes that include various loop breakers. This will involve coding in Visual Basic to include the kinetics of various minerals precipitating and nutrients used to calculate the saturation points and solubility products of various components simultaneously.
- The PWM\_SA mathematical proved to be a useful tool to bridge the gap that exist due to complexity of WWTP processes and its resilience should be showcased by application to more wastewater treatment plants around the country to help with planning, design and operation of WWTPs.

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## Appendices

The PWM\_SA model WEST® simulation files for the experiments and the steady state excel model are provided in a separate flash drive/CD.

### Appendix A: Selected components, ionic species and processes used in the application of PWM\_SA plant wide model

Table A1.1. The Universally Selected Model Components			
	Component Name	Empirical formula	Notation
Total Dissolved Ionic Concentrations	Water	H <sub>2</sub> O	H <sub>2</sub> O
	Hydrogen ion	H <sup>+</sup>	S_H
	Sodium	Na <sup>+</sup>	S_Na
	Potassium	K <sup>+</sup>	S_K
	Calcium	Ca <sup>2+</sup>	S_Ca
	Magnesium	Mg <sup>2+</sup>	S_Mg
	Ammonium	NH <sub>4</sub> <sup>+</sup>	S_NH <sub>x</sub>
	Chloride	Cl <sup>-</sup>	S_Cl
	Acetate	CH <sub>3</sub> COO <sup>-</sup>	S_VFA
	Propionate	CH <sub>3</sub> CH <sub>2</sub> COO <sup>-</sup>	S_Pr
	Carbonate	CO <sub>3</sub> <sup>2-</sup>	S_CO <sub>3</sub>
	Sulphate	SO <sub>4</sub> <sup>2-</sup>	S_SO <sub>4</sub>
	Phosphate	PO <sub>4</sub> <sup>3-</sup>	S_PO <sub>4</sub>
	Nitrate	NO <sub>3</sub> <sup>-</sup>	S_NO <sub>x</sub>
Soluble Organics	Dissolved hydrogen	H <sub>2</sub>	S_H2
	Dissolved oxygen	O <sub>2</sub>	S_O2
	Unbiodegradable Soluble Organics	CH <sub>Y<sub>u</sub></sub> O <sub>Z<sub>u</sub></sub> N <sub>A<sub>u</sub></sub> P <sub>B<sub>u</sub></sub>	S_U
	Fermentable Biodegradable Soluble Organics	CH <sub>Y<sub>f</sub></sub> O <sub>Z<sub>f</sub></sub> N <sub>A<sub>f</sub></sub> P <sub>B<sub>f</sub></sub>	S_F
	Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	S_Glu
Particulates	Unbiodegradable particulate organics	CH <sub>Y<sub>up</sub></sub> O <sub>Z<sub>up</sub></sub> N <sub>A<sub>up</sub></sub> P <sub>B<sub>up</sub></sub>	X_U_inf
	Biodegradable particulate organics	CH <sub>Y<sub>bp</sub></sub> O <sub>Z<sub>bp</sub></sub> N <sub>A<sub>bp</sub></sub> P <sub>B<sub>bp</sub></sub>	X_B_Org
	Primary sludge biodegradable particulate organics	CH <sub>Y<sub>bps</sub></sub> O <sub>Z<sub>bps</sub></sub> N <sub>A<sub>bps</sub></sub> P <sub>B<sub>bps</sub></sub>	X_B_Inf
	Polyphosphate	K <sub>kp</sub> Mg <sub>mp</sub> Ca <sub>cp</sub> PO <sub>3</sub>	X_PAO_PP
	Poly-hydroxy-alkanoate	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	X_PAO_Stor
	Struvite	MgNH <sub>4</sub> PO <sub>4</sub> .6H <sub>2</sub> O	X_Str_NH4
	Calcium Phosphate	Ca <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	X_ACP
	K-struvite	MgKPO <sub>4</sub> .6H <sub>2</sub> O	X_Str_K
	Calcite	CaCO <sub>3</sub>	X_Cal
	Magnesite	MgCO <sub>3</sub>	X_Mag
	Newberyite	MgHPO <sub>4</sub>	X_Newb
	Influent inorganic settleable solids		X_ISS

Microorganism Biomass	Ordinary heterotrophic organisms	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_OHO
	Phosphate accumulating organisms	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_PAO
	Autotrophic nitrifying organisms	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_ANO
	Acidogens	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_ZAD
	Acetogens	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_ZAC
	Acetoclastic Methanogens	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_ZAM
	Hydrogenotrophic methanogens	$CH_{Y_o}O_{Z_o}N_{A_o}P_{B_o}$	X_ZHM
	Endogenous residue	$CH_{Y_e}O_{Z_e}N_{A_e}P_{B_e}$	X_U_Org
Gases	Carbon dioxide	CO <sub>2</sub>	G_CO <sub>2</sub>
	Methane	CH <sub>4</sub>	G_CH <sub>4</sub>

**Table A1.2:** Ionic Species Selected for the Three Phase Modelling (Ikumi *et al.* 2014)

1	H <sup>+</sup>	Hydrogen ion	23	NH <sub>4</sub> SO <sub>4</sub> <sup>-</sup>	Ammonium sulphate
2	Na <sup>+</sup>	Sodium	24	MgPO <sub>4</sub> <sup>-</sup>	Magnesium phosphate
3	K <sup>+</sup>	Potassium	25	CaCH <sub>3</sub> COO <sup>+</sup>	Calcium acetate
4	Ca <sup>2+</sup>	Calcium	26	CaCH <sub>3</sub> CH <sub>2</sub> COO <sup>+</sup>	Calcium propionate
5	Mg <sup>2+</sup>	Magnesium	27	CaHCO <sub>3</sub> <sup>+</sup>	Calcium bi-carbonate
6	NH <sub>4</sub> <sup>+</sup>	Ammonium	28	NaSO <sub>4</sub> <sup>-</sup>	Sodium sulphate
7	Cl <sup>-</sup>	Chloride	29	MgHPO <sub>4</sub>	Magnesium hydrogen phosphate
8	CH <sub>3</sub> COO <sup>-</sup>	Acetate	30	CH <sub>3</sub> COONa	Sodium Acetate
9	CH <sub>3</sub> CH <sub>2</sub> COO <sup>-</sup>	Propionate	31	H <sub>2</sub> CO <sub>3</sub>	Di-hydrogen carbonate
10	CO <sub>3</sub> <sup>2-</sup>	Carbonate	32	MgSO <sub>4</sub>	Magnesium sulphate
11	SO <sub>4</sub> <sup>2-</sup>	Sulphate	33	HPO <sub>4</sub> <sup>2-</sup>	Hydrogen phosphate
12	PO <sub>4</sub> <sup>3-</sup>	Phosphate	34	NH <sub>3</sub>	Ammonia
13	NO <sub>3</sub> <sup>-</sup>	Nitrate	35	MgCO <sub>3</sub>	Magnesium carbonate
14	OH <sup>-</sup>	Hydroxide ion	36	ACPO <sub>4</sub> <sup>-</sup>	Calcium Phosphate
15	CH <sub>3</sub> COOH	Acetic acid	37	MgHCO <sub>3</sub> <sup>+</sup>	Magnesium hydrogen carbonate
16	CH <sub>3</sub> CH <sub>2</sub> COOH	Propionic acid	38	CaHPO <sub>4</sub> <sup>-</sup>	Calcium hydrogen phosphate
17	HCO <sub>3</sub> <sup>-</sup>	Bi-carbonate	39	NaCO <sub>3</sub> <sup>-</sup>	Sodium carbonate
18	CaSO <sub>4</sub>	Calcium sulphate	40	MgH <sub>2</sub> PO <sub>4</sub> <sup>+</sup>	Magnesium di-hydrogen phosphate
19	H <sub>2</sub> PO <sub>4</sub> <sup>-</sup>	Di-hydrogen phosphate	41	NaHCO <sub>3</sub>	Sodium hydrogen carbonate
20	MgCH <sub>3</sub> COO <sup>+</sup>	Magnesium acetate	42	NaHPO <sub>4</sub> <sup>-</sup>	Sodium hydrogen phosphate
21	MgCH <sub>3</sub> CH <sub>2</sub> COO <sup>+</sup>	Magnesium propionate	43	CaOH <sup>+</sup>	Calcium hydroxide
22	CaCO <sub>3</sub>	Calcium carbonate	44	MgOH <sup>+</sup>	Magnesium hydroxide



**Table A2: Example for Equilibrium and Mass Balance Equations for Ionic Speciation**

Weak Acid Sub-System	*Aqueous Phase Equilibrium Equations	Mass Balance Equation
Ammonia	$[NH_3] = \frac{K_{NH_4} \cdot [NH_4^+]}{(H^+)}$ $[NH_4SO_4^-] = \frac{[SO_4^{2-}] [NH_4^+]}{K_{NH_4SO_4}}$	$N_T = [NH_4^+] + [NH_3] + [NH_4SO_4^-]$
*Where $(H^+)$ is the hydrogen ion activity, $[X]$ the molar concentrations of species X and $K_X$ is the thermodynamic equilibrium		

**Table A3: Processes used in the PWM\_SA three phase UCT model (Ikumi, 2020)**

Name	Description
AerHydrol	Aerobic hydrolysis of biodegradable particulate organics (BPO)
AnHydrol	Anoxic hydrolysis of BPO
AnaerHydrol	Anaerobic hydrolysis of BPO
AerGrowthOnSf	Aerobic OHO growth on fermentable soluble organics (FBSO)
AerGrowthOnSa	Aerobic OHO growth on Acetate
AnGrowthOnSfDenitrif	Anoxic OHO growth on FBSO
AnGrowthOnSaDenitrif	Anoxic OHO growth on Acetate
Fermentation	Fermentation of FBSO
LysisOfAuto	Storage of poly-hydroxy-alkanoate (PHA) by PAOs
StorageOfXPP	Aerobic storage of PP with PHA uptake
AerGrowthOnXPHA	Aerobic growth of PAOs
LysisOfXPP	Release and hydrolysis of polyphosphate (PP)
LysisOfXPHA	Release and hydrolysis of PHA
GrowthOfAuto	Aerobic growth of ANOs with nitrification
OHO_Lysis	Lysis of OHOs in aerobic systems
LysisOfXPAO	Lysis of PAOs in aerobic systems
LysisOfAuto	Lysis of ANOs in AS system
Aeration	Oxygen supply to aerobic reactor
FSO_Hydrolysis	Hydrolysis of FBSO in AD system
BPO_Hydrolysis	Hydrolysis of BPO produced by dead biomass
BPO_PS_Hydrolysis	Hydrolysis of BPO from primary sludge (PS)
OHO_Lysis_AD	Lysis of OHOs in AD system
PAO_Lysis_AD	Lysis of PAOs in AD system
PP_Release	Release of PP with uptake of PHA in AD system
PP_Hydrolysis	Release and hydrolysis of PP in AD system
PHA_Hydrolysis	Release and hydrolysis of PHA in AD system
Acidogenesis_L	Low hydrogen partial pressure (pH <sub>2</sub> ) Acidogenesis
Acidogenesis_H	High pH <sub>2</sub> acidogenesis
AD_Decay	Lysis of acidogens
Acetogenesis	Growth of acetogens in AD system
AC_Decay	Lysis of acetogens
Acet_Methanogenesis	Growth of acetoclastic methanogens in AD system
AM_Decay	Lysis of acetoclastic methanogens
Hyd_Methanogenesis	Growth of hydrogenotrophic methanogens in AD system
HM_Decay	Lysis of hydrogenotrophic methanogens

## **Appendix B: Kinetic and stoichiometric parameters used ASM2-3P**

The parameters were checked for consistency i.e. the preprocessor parameters are the same as the ones used in WEST during simulation.

Table B1: Kinetic parameters for ASM2-3P processes (AS reactors) (Ikumi *et al.* 2014)

Parameter	Description	Value	Unit
A_20	Activation/inhibition term at 20 degrees Celcius	1	1/d
A_35	Activation/inhibition term at 35 degrees celcius	1	1/d
A_55	Activation/inhibition term at 55 degrees celcius	1	1/d
KA_CO2	CO2 liquid to gas phase equilibrium constant	1,64346E-05	-
KA_H_N	Inhibition of bacteria growth due to high pH	0,0000001	-
KI_H_N	Inhibition of bacteria growth due to low pH	0,00085	-
KL <sub>a</sub> _CO2	Rate of Active CO2 gas exchange rate with aeration	2	1/d
KS_fPP_PAO_PHAstor	Saturation coeff for poly-phosphate	0,01	-
kM_fPP_PAO_PHAstor	maximum rate for PP release with anaerobic PHA storage	0,05	-
K_F_OHO	Saturation/inhibition coeff for growth on S_F	4	-
K_I_PP_PAO	Inhibition coeff for X_PP storage	0,2	-
K_MAX_fPP_PAO	Maximum ratio of X_PP/X_PAO	1	-
K_NOx_OHO	Nitrate Half-Saturation Coefficient For Denitrifying Heterotrophic Biomass	0,5	gNO3-N/m3
K_O2	Saturation/inhibition coeff for oxygen	0,2	-
K_O2_ANO	Saturation/inhibition coeff of autotrophs for oxygen	0,2	-
K_S_ALK	Saturation coeff for alkalinity (HCO3-)	0,1	-
K_S_ALK_ANO	Saturation coeff of autotrophs for alkalinity	0,1	-
K_S_Blnf_OHO_hyd	Half Saturation Coefficient For Hydrolysis Of Slowly Biodegradable Substrate	0,1	gCOD/gCOD
K_S_F_OHO_ferm	Saturation coeff for fermentation on S_F	20	-
K_S_NHx	Ammonia Half-Saturation Coefficient For Organisms Growth	0,05	gNH3-N/m3
K_S_NHx_ANO	Saturation coeff of autotrophs for ammonium	0,3	-
K_S_PHA_PAO	Saturation coeff for PHA	0,01	-
K_S_PO4	Saturation coeff for phosphorus (nutrient)	0,01	-
K_S_PO4_PAO_PPstor	Saturation coeff for phosphorus in PP storage	0,2	-
K_S_VFA	Saturation coeff for S_A (acetate)	4	-
Q_OHO_F_VFA_ferm	Maximum rate for fermentation	20	1/d
Q_PAO_PO4_PPstor	Rate constant for storage of PP	4,5	1/d
Q_PAO_PP_PHAstor	Rate constant for storage of PHA (base: X_PP)	1,5	1/d
S_O_Sat	Oxygen saturation concentration	8,9	g/m3
Th_d_XG_20	Temperature correction factor for decay of PAOs at 20°C	1,12	1/d
Th_d_XG_35	Temperature correction factor for decay of PAOs at 35°C	1,12	1/d
Th_d_XH_20	Temperature correction factor for decay of OHOs at 20°C	1,12	1/d
Th_d_XH_35	Temperature correction factor for decay of OHOs at 35°C	1,12	1/d
Th_d_XN_20	Temperature correction factor for decay of ANOs at 20°C	1,072	1/d
Th_d_XN_35	Temperature correction factor for decay of ANOs at 35°C	1,072	1/d
Th_h_20	Temperature correction factor for hydrolysis at 20°C	1,116	1/d
Th_h_35	Temperature correction factor for hydrolysis at 35°C	0,05	1/d
Th_m_XH_20	Temperature correction factor for growth of OHOs at 20°C	1,072	1/d
Th_m_XN_20	Temperature correction factor for growth of ANOs at 20°C	1,103	1/d
b_ANO	Decay rate	0,15	1/d
b_OHO	Decay Coefficient For Heterotrophic Biomass	0,62	1/d
b_PAO	Rate constant for lysis of X_PAO	0,04	1/d
b_PHA	Rate constant for lysis of X_PHA	0,04	1/d
b_PP	Rate constant for lysis of X_PP	0,04	1/d
k_M_Blnf_OHO_hyd	Maximum Specific Hydrolysis Rate	3	gCOD/(gCOD*d)
mu_ANO	Maximum specific growth rate for ANOs	1	1/d
mu_OHO_max	Maximum Specific Growth Rate For Heterotrophic Biomass	6	1/d
mu_PAO	Maximum growth rate for PAOs	1	1/d
n_NO_Het	Reduction factor for denitrification	0,3	-
n_OHO_Blnf_ferm	Anaerobic hydrolysis reduction factor	0,1	-
n_OHO_Blnf_hyd	Anoxic hydrolysis reduction factor	0,6	-
TempCoeff	Rate temperature coefficient	0,0667	-
Temperature	System Temperature	20	degC
Tref	Reference temperature for kinetics	20	degC
kdis_cal	Dissolution/ precipitation of calcite	0,5	-
kdis_cap	Dissolution/ precipitation of calcium phosphate	150	-
kdis_mag	Dissolution/ precipitation of magnesite	50	-
kdis_mgkp	Dissolution/ precipitation of K-struvite	100	-
kdis_newb	Dissolution/ precipitation of newbervite	0,05	-
Kinetic Parameters kdis_stru	Dissolution/ precipitation of struvite	0,0001	-

Table B2: Stoichiometric parameters for ASM2-3P processes (AS reactors) (Ikumi *et al.* 2014)

	f_XU_Bio_lysis	Unbiodegradable fraction of biomass that accumulates on lysis with death reg	0,08	dUnit/dUnit
	ISS_BM	ISS to biomass for OHO and PAO	0,15	g/gCOD
	f_SU_SF	Inert Fraction in Fermentable Soluble Organics	0	-
	i_Ca_PP_mol_perP	Molar fraction of Ca/P in polyphosphate	0,053	dUnit/dUnit
	i_K_PP_mol_perP	Molar fraction of K/P in polyphosphate	0,312	dUnit/dUnit
	i_Mg_PP_mol_perP	Molar fraction of Mg/P in polyphosphate	0,297	dUnit/dUnit
	i_H_Org_mol_perC	H/C: organisms	1,535	dUnit/dUnit
	i_H_SF_mol_perC	H/C: fermentable soluble	1,984	dUnit/dUnit
	i_H_SU_mol_perC	H/C: unbiodegradable soluble	1,813	dUnit/dUnit
	i_H_XBInf_mol_perC	H/C: PS biodegradable particulate	2,408	dUnit/dUnit
	i_H_XBOrg_mol_perC	H/C: biodegradable particulate	1,535	dUnit/dUnit
	i_H_XUInf_mol_perC	H/C: unbiodegradable particulate	1,484	dUnit/dUnit
	i_H_XUOrg_mol_perC	H/C: endogenous residue	1,532	dUnit/dUnit
	i_N_Org_mol_perC	N/C: organisms	0,133	dUnit/dUnit
	i_N_SF_mol_perC	N/C: fermentable soluble	0,060	dUnit/dUnit
	i_N_SU_mol_perC	N/C: unbiodegradable soluble	0,154	dUnit/dUnit
	i_N_XBInf_mol_perC	N/C: PS biodegradable particulate	0,105	dUnit/dUnit
	i_N_XBOrg_mol_perC	N/C: biodegradable particulate	0,133	dUnit/dUnit
	i_N_XUInf_mol_perC	N/C: unbiodegradable particulate	0,091	dUnit/dUnit
	i_N_XUOrg_mol_perC	N/C: endogenous residue	0,133	dUnit/dUnit
	i_O_Org_mol_perC	O/C: organisms	0,457	dUnit/dUnit
	i_O_SF_mol_perC	O/C: fermentable soluble	0,655	dUnit/dUnit
	i_O_SU_mol_perC	O/C: unbiodegradable soluble	0,519	dUnit/dUnit
	i_O_XBInf_mol_perC	O/C: PS biodegradable particulate	0,686	dUnit/dUnit
	i_O_XBOrg_mol_perC	O/C: biodegradable particulate	0,457	dUnit/dUnit
	i_O_XUInf_mol_perC	O/C: unbiodegradable particulate	0,498	dUnit/dUnit
	i_O_XUOrg_mol_perC	O/C: endogenous residue	0,458	dUnit/dUnit
	i_P_Org_mol_perC	P/C: organisms	0,019	dUnit/dUnit
	i_P_SF_mol_perC	P/C: fermentable soluble	0,007	dUnit/dUnit
	i_P_SU_mol_perC	P/C: unbiodegradable soluble	0,012	dUnit/dUnit
	i_P_XBInf_mol_perC	P/C: PS biodegradable particulate	0,004	dUnit/dUnit
	i_P_XBOrg_mol_perC	P/C: biodegradable particulate	0,019	dUnit/dUnit
	i_P_XUInf_mol_perC	P/C: unbiodegradable particulate	0,019	dUnit/dUnit
	i_P_XUOrg_mol_perC	P/C: endogenous residue	0,019	dUnit/dUnit
	Y_ANO	Yield for autotrophic nitrifying biomass (ANO)	0,24	gCOD/gN
	Y_OHO	Yield for heterotrophic (OHO)biomass	0,67	gCOD/gCOD
	Y_PAO	Yield coeff for PAO biomass/PHA	0,67	-
	Y_PP_Stor_PAO	PP requirement (S_PO4 release) per PHA stored	0,4	-
Stoichiometric Parameters	Y_Stor_PP_PAO	PHA requirement for PP storage	0,2	-
	Y_f_PP_VFA	fraction of PP taken up with VFA uptake for PHA	0,5	-

### Appendix C: Kinetic and stoichiometric parameters used in ADM3P (UCTADM)

The parameters were checked for consistency i.e. the preprocessor parameters are the same as the ones used in WEST during simulation. The kinetic and stoichiometric parameters are provided below for the AD processes.

Table C1: Kinetic parameters for ADM3P processes (Main AD and fermenters) (Ikumi *et al.* 2014)

Parameter	Description	Value	Unit
K_I_H_AD	H+ inhibition for acidogens	0,0155	
K_I_NH3	NH <sub>3</sub> Inhibition for AD organisms	0,0018	
KS_fPP_PAO_PHAstor	Saturation coeff for poly-phosphate	0,01	-
K_O2	Saturation/inhibition coeff for oxygen	20	-
K_S_ALK	Saturation coeff for alkalinity (HCO <sub>3</sub> <sup>-</sup> )	0,0001	-
K_S_NHx	Saturation coeff for Ammonia (nutrient)	0,0001	gNH <sub>3</sub> -N/m <sup>3</sup>
K_S_PO4	Saturation coeff for phosphorus (nutrient)	0,0001	-
K_S_VFA	Saturation coeff for Acetate	10	-
KS_AC	Half Sat coeff for acetogens	0,089	g/m <sup>3</sup>
KS_AD	Half Sat coeff for acidogens	0,78	g/m <sup>3</sup>
KS_AM	Half Sat coeff for acetoclastic methanogen	0,013	g/m <sup>3</sup>
KS_OB	Half Sat coeff for acetate oxidizing bacteria	0,29	g/m <sup>3</sup>
KS_BInf_AD_hyd	Half sat coeff for BPO_PS (for sewage org)	10,12	gCOD/gCOD
KS_BOrg_AD_hyd	Half sat coeff for BPO (for organics from b	10,37	gCOD/gCOD
KS_HM	Half Sat coeff for hydrogenotrophic metha	0,156	g/m <sup>3</sup>
K_CO2	Rate constant for CO <sub>2</sub> exchange in AD	0,1	
K_CO2_eq	equilibrium constant for CO <sub>2</sub> liquid - gas p	1,21E-08	
K_I_H2	Inhibition coefficient for H <sub>2</sub> in acidogenes	9,999375	g/m <sup>3</sup>
K_I_H_AM	H+ inhibition for acetoclastic methanogen	0,00000115	Mol.kg <sup>-1</sup>
K_I_H_OB	H+ inhibition for acetate oxidizing bacteria	0,00053	Mol.kg <sup>-1</sup>
K_I_H_HM	H+ inhibition for hydrogenotrophic metha	0,00053	Mol.kg <sup>-1</sup>
TempCoeff	Rate temperature coefficient	0,0667	-
Temperature	System Temperature	35	degC
Tref	Reference temperature for kinetics	35	degC
b_AC	Decay rate constant for Xac	0,015	1/d
b_AD	Decay rate constant for Xad	0,041	1/d
b_AM	Decay rate constant for Xam	0,037	1/d
b_OB	Decay rate constant for Xob	0,041	1/d
b_HM	Decay rate constant for Xhm	0,01	1/d
b_OHO_AD	Decay rate constant for X_OHO in AD	20	1/d
b_PAO_AD	Decay rate constant for X_PAO in AD	20	1/d
kH_F_AD_hyd	Hydrolysis rate constant for FSO	10	1/d
kH_PHA_AD_hyd	Hydrolysis rate constant for PHA	5	1/d
kH_PP_AD_hyd	Hydrolysis rate constant for PP	1	1/d
kM_BInf_AD_hyd	Hydrolysis rate constant for BPO_PS	2,00	1/d
kM_BOrg_AD_hyd	Hydrolysis rate constant for BPO	1,95	1/d
kM_fPP_PAO_PHAstor	maximum rate for PP release with anaerobic	0,3	1/d
kdis_cal	Dissolution/ precipitation/ precipitation of	0,5	
kdis_cap	Dissolution/ precipitation of calcium phos	150	
kdis_mag	Dissolution/ precipitation of magnesite	50	
kdis_mgkp	Dissolution/ precipitation of K-struvite	100	
kdis_newb	Dissolution/ precipitation of newberyite	0,05	
kdis_stru	Dissolution/ precipitation of struvite	300	
mu_AC	Max specific growth rate for acetogens	1,15	1/d

Table C2: Stoichiometric parameters for ADM3P processes (Main AD and fermenters) (Ikumi *et al.* 2014)

	<b>mu_AD</b>	Max specific growth rate for acidogens	0,8	1/d
	<b>mu_AM</b>	Max specific growth rate for acetoclastic n	4,39	1/d
	<b>mu_OB</b>	Max specific growth rate for acetate oxidiz	3,25	
	<b>mu_HM</b>	Max specific growth rate for hydrogenotro	1,2	1/d
	<b>f_SU_SF</b>	Inert Fraction in Fermentable Souble Orga	0	-
	<b>f_XU_Bio_lysis</b>	Unbiodegradable fraction of biomass that	0,08	-
	<b>ISS_BM</b>	ISS to biomass for OHO and PAO	0,15	g/gCOD
	<b>i_Ca_PP_mol_perP</b>	Molar fraction of Ca/P in polyphosphate	0,0530	
	<b>i_K_PP_mol_perP</b>	Molar fraction of K/P in polyphosphate	0,3120	
	<b>i_Mg_PP_mol_perP</b>	Molar fraction of Mg/P in polyphosphate	0,2970	
	<b>i_H_Org_mol_perC</b>	H/C : organisms	1,5348	dUnit/dUnit
	<b>i_H_SF_mol_perC</b>	H/C : fermentable soluble	1,9837	dUnit/dUnit
	<b>i_H_SU_mol_perC</b>	H/C: unbiodegradable soluble	1,8133	dUnit/dUnit
	<b>i_H_XBInf_mol_perC</b>	H/C: PS biodegradable particulate	2,4076	dUnit/dUnit
	<b>i_H_XBOrg_mol_perC</b>	H/C: biodegradable particulate	1,5348	dUnit/dUnit
	<b>i_H_XUInf_mol_perC</b>	H/C: unbiodegradable particulate	1,4843	dUnit/dUnit
	<b>i_H_XUOrg_mol_perC</b>	H/C: endogenous residue	1,5315	dUnit/dUnit
	<b>i_N_Org_mol_perC</b>	N/C : organisms	0,1331	dUnit/dUnit
	<b>i_N_SF_mol_perC</b>	N/C: fermentable soluble	0,0596	dUnit/dUnit
	<b>i_N_SU_mol_perC</b>	N/C: unbiodegradable soluble	0,1538	dUnit/dUnit
	<b>i_N_XBInf_mol_perC</b>	N/C: PS biodegradable particulate	0,1055	dUnit/dUnit
	<b>i_N_XBOrg_mol_perC</b>	N/C: biodegradable particulate	0,1331	dUnit/dUnit
	<b>i_N_XUInf_mol_perC</b>	N/C: unbiodegradable particulate	0,0906	dUnit/dUnit
	<b>i_N_XUOrg_mol_perC</b>	N/C: endogenous residue	0,1331	dUnit/dUnit
	<b>i_O_Org_mol_perC</b>	O/C : organisms	0,4575	dUnit/dUnit
	<b>i_O_SF_mol_perC</b>	O/C : fermentable soluble	0,6551	dUnit/dUnit
	<b>i_O_SU_mol_perC</b>	O/C: unbiodegradable soluble	0,5190	dUnit/dUnit
	<b>i_O_XBInf_mol_perC</b>	O/C: PS biodegradable particulate	0,6864	dUnit/dUnit
	<b>i_O_XBOrg_mol_perC</b>	O/C: biodegradable particulate	0,4575	dUnit/dUnit
	<b>i_O_XUInf_mol_perC</b>	O/C: unbiodegradable particulate	0,4978	dUnit/dUnit
	<b>i_O_XUOrg_mol_perC</b>	O/C: endogenous residue	0,4577	dUnit/dUnit
	<b>i_P_Org_mol_perC</b>	P/C : organisms	0,0188	dUnit/dUnit
	<b>i_P_SF_mol_perC</b>	P/C: fermentable soluble	0,0075	dUnit/dUnit
	<b>i_P_SU_mol_perC</b>	P/C: unbiodegradable soluble	0,0120	dUnit/dUnit
	<b>i_P_XBInf_mol_perC</b>	P/C: PS biodegradable particulate	0,0043	dUnit/dUnit
	<b>i_P_XBOrg_mol_perC</b>	P/C: biodegradable particulate	0,0188	dUnit/dUnit
	<b>i_P_XUInf_mol_perC</b>	P/C: unbiodegradable particulate	0,0188	dUnit/dUnit
	<b>i_P_XUOrg_mol_perC</b>	P/C: endogenous residue	0,0188	dUnit/dUnit
Stoichiometric parameters	<b>Y_AC</b>	Acetogenesis yield (COD/COD)	0,039714286	-
	<b>Y_AD</b>	Lo H2 Acetogenesis yield (COD/COD)	0,0895	-
	<b>Y_AH</b>	Hi H2 Acetogenesis yield (COD/COD)	0,0895	-
	<b>Y_AM</b>	Acetoclastic Methanogenesis yield (COD	0,03925	-
	<b>Y_HM</b>	Hydrogenotrophic Methanogenesis yield	0,04	-
	<b>Y_OB</b>	Acetate oxidizing bacteria yield	0,104	-