UNIVERSITY OF CAPE TOWN
IYUNIVESITHI YASEKAPA • UNIVERSITEIT VAN KAAPSTAD

DEPARTMENT OF CIVIL ENGINEERING

PRIMARY SEDIMENTATION TANK MODEL WITH CHARACTERIZED SETTLING VELOCITY GROUPS

By

Christian Leprince Polorigni

The present Dissertation is submitted as partial fulfilment of the requirements for the degree of Master of Science in Water Quality Engineering

Supervisor: Dr David S. Ikumi

February 2020

University of Cape Town

The copyright of this thesis vests in the author. No quotation from it or information derived from it is to be published without full acknowledgement of the source. The thesis is to be used for private study or non-commercial research purposes only.

Published by the University of Cape Town (UCT) in terms of the non-exclusive license granted to UCT by the author.

University of Cape Town

Abstract

Primary sedimentation involves the separation of solids and liquid in primary settling tanks (PSTs) of wastewater treatment systems. These physical processes are described by various settling conditions such as discrete and flocculent settling, along with other phenomena such as flocculation, coagulation, ammonification or hydrolysis. The modelling of primary sedimentation has often been overlooked because (i) it involves various intricacies that are difficult to replicate and (ii) primary sedimentation has been assumed to be an input to most of the main unit process models, including the activated sludge (AS) system and the anaerobic digestion (AD) models. Though there has been a wide range of proposed mathematical models to describe how PSTs function, the need to correctly disaggregate the total suspended solids (TSS) into realistic fractions of unbiodegradable particulate organics (UPO), biodegradable particulate organics (BPO) and inorganic settleable solids (ISS), remains. This is because PST models that are unable to correctly split the TSS into its characteristic components make incorrect assumptions. These assumptions lead to inconsistencies in predicting the compositions of the primary sludge (PS) that is fed to the AD unit and the settled wastewater (settled WW) that is treated in the AS system. Hence, it becomes difficult to correctly simulate the entire system (plant-wide) towards a holistic evaluation of system strategies.

In this study, a realistic PST model was developed, with characterized settling velocity groups, within a plant-wide setting, for municipal wastewater. This involved the improvement of a current TSS-based model into a more accurate and realistic model that could account for the settling of raw wastewater particles. The model was therefore expected to predict the composition of the PS that is treated in the AD system and the composition of the settled WW that is going to the AS unit processes. This could be achieved by splitting the TSS into UPO, BPO and ISS fractions. In developing preparation of such a realistic PST model, the following objectives were established:

1. Disaggregate the TSS into realistic UPO, BPO and ISS fractions, by means of discrete particle settling modelling (Kowlesser, 2014) and the particle settling velocity distribution (PSVD) approach of Bachis *et al.* (2015).
2. Verify that the model is internally consistent with wastewater treatment plant (WWTP) data, by means of mathematical material mass balances and other specific scenarios.
3. Demonstrate the application and impact of such a model by performing steady state plant-wide simulations.

Using the discrete particle settling approach of Kowlesser (2014), a discrete particle settling model was developed in Microsoft Excel and implemented into a dynamic PST framework in WEST® (Vanhooren *et al.,* 2003). The discrete particle settling model was described using steady state and dynamic calculations and the insights obtained from these calculations were implemented in the current TSS-based PST model of Bachis *et al.* (2015). This was performed towards developing the University of Cape Town Primary Sedimentation Unit (UCTPSU). The influent raw wastewater TSS was fractionated into UPO, BPO and ISS fractions and settling proportions of these fractions were assigned to five settling velocity groups. In addition, a distinct settling velocity was assigned to each settling velocity group.

Previous studies data from WRC (1984) and Ekama (2017), were used in the discrete particle settling model, which was able to reproduce PS and settled WW outputs, through steady state and dynamic calculations and under strict material mass balances. As a result, UPO, BPO and ISS settling proportions as well as settling velocities, were extracted from these calculations and used as input parameters into the UCTPSU model. This dynamic model was rigorously verified to be internally consistent with regards to strict material mass balances. The verification scenarios also included variations of high and low settling velocities as well as a combination of both high and low velocities and checking that the model was behaving as expected.

The application and impact of the UCTPSU model were demonstrated using plant-wide scenarios in proposing a preliminary integration, under steady state conditions. It showed how incorrect disaggregation of the TSS into UPO, BPO and ISS fractions can lead to incorrect predictions in terms of the settled WW composition, the AS system capacity, the effluent quality, as well as the energy consumption and generation in the AS system and AD unit respectively. The investigation also revealed the need to measure key wastewater parameters such as particle settling velocities and the unbiodegradable particulate COD fraction, when it comes to realistically modelling of primary sedimentation of municipal wastewater, with the view of optimizing plant operations and tactical decision making.

The study thereafter recommended the need to conduct an extensive experimental campaign to measure in-situ diurnal data, mainly in terms of settling velocities and settling proportions of UPO, BPO and ISS. It was also suggested to use the settleometer as a tool to extract these settling velocities and settling proportions, after performing biodegradability tests. As such, the data collected from the experimental campaign and the biodegradability tests could be used in calibrating the UCTPSU model and validation could be undertaken by means of full plant scale data.

Plagiarism Declaration

I know the meaning of plagiarism and declare that all the work in the document, save for that which is properly acknowledged, is my own. This thesis/dissertation has been submitted to the Turnitin module (or equivalent similarity and originality checking software) and I confirm that my supervisor has seen my report and any concerns revealed by such have been resolved with my supervisor.

Signature Signed by candidate

Date: 9th February 2020

Acknowledgements

I want to first praise and thank **Jehovah** for carrying me through this journey. May His Hand rest forever upon my life, in **Jesus**’ name.

I would then like to express my sincere gratitude to the following people for their support and assistance throughout this investigation:

Doctor David S. Ikumi, for your constant help in thoroughly understanding the research project, concepts, working with WEST® as well as your valuable feedback in the different drafts,

Professor George A. Ekama, for your invaluable input into this investigation as well as the feedback in the write up of this document,

My parents **Ignace** and **Amele**, my brothers **Jean Legrand Woulo**, **Angelo de Dieu** and **Wilfried**, for your enduring love and support during my entire degree and particularly in preparing this report,

My **friends and family of faith, home cell, small groups, and ushering team of Every Nation Baxter Cape Town, my Togolese brothers in Cape Town, and all the friends, colleagues, acquaintances** for encouraging me through various means throughout these years and towards the completion of this report.

The **Mandela Rhodes Foundation** (MRF), the **Water Research Commission** (WRC), the **Water Research Group** (WRG), the **department of Civil Engineering** of the University of Cape Town (UCT), for providing financial support as well as personal growth.

Glossary

A	Area in m^2
ABMP	Augmented Bio Methane Potential
ABSP	Augmented Bio Sulphide Potential
AD	Anaerobic Digestion
ADM	Anaerobic Digestion Model
ADM1	Anaerobic Digestion Model Number 1
$Al_2(SO_4)_3$	Aluminum Sulphate
AS	Activated Sludge
ASM	Activated Sludge Model
ASM1	Activated Sludge Model Number 1
ASM2	Activated Sludge Model Number 2
ASM3	Activated Sludge Model Number 3
BMP	Bio Methane Potential
BPO	Biodegradable Particulate Organics in mgVSS/l
C	Carbon in mgC/l
C_s	Solids concentration in the UCTPSU in g/m^3
CBIM	Continuity-Based Interface Model
CEPT	Chemically Enhanced Primary Treatment
CFD	Computational Fluid Dynamics
CH4	Methane gas
CHON	Carbon, Hydrogen, Oxygen, Nitrogen
C_l	Solids concentration of the n^{th} layer in g/m^3
COD	Chemical Oxygen Demand in mgCOD/l
CSTR	Continuously Stirred Tank Reactors
FBSO	Fermentable Biodegradable Soluble Organics in mgCOD/l
$Fe_2(SO_4)_3$	Ferric Sulphate
$FeCl_3$	Ferric/Iron Chloride
FSA	Free and Saline Ammonia in mgN/l
$f_{S'up}$	Unbiodegradable Particulate Organic fraction
$f_{S'us}$	Unbiodegradable Soluble Organic fraction
GT	Gravity Thickener
H	Height in m
H_L	Height of the layer in m
ISS	Inorganic Suspended Solids in mgISS/l
J_{DN}	Downwards bulk liquid flux
JG	Gravity settling flux
J_{UP}	Upwards bulk liquid flux
N	Nitrogen in mgN/l

OP	Ortho Phosphate in mgP/l
OU	Oxygen Utilization
OUR	Oxygen Utilization Rate
P	Phosphorus in mgP/l
PS	Primary Sludge
PST	Primary Settling Tank
PSVD	Particle Settling Velocity Distribution
PVC	Polymerizing Vinyl Chloride
PWM_SA	Plant Wide Model of South Africa
PWSSM	Plant Wide Stoichiometric and Kinetic Steady State Model
PWWF	Peak Wet Weather Flow
$\mathbf{Q_I}$	Incoming flow
$\mathbf{Q_{OUT}}$	Exiting flow
SCFA	Short Chains Fatty Acids
SS	Suspended/Settleable Solids in mgVSS/l
SST	Secondary Settling Tank
TKN	Total Kjeldhal Nitrogen in mgN/l
TOC	Total Organic Carbon
TP	Total Phosphorus in mgP/l
TSS	Total Suspended Solids in mgTSS/l
UCTPSU	University of Cape Town Primary Sedimentation Unit
UCT-PW	University of Cape Town Plant-Wide
UPO	Unbiodegradable Particulate Organics in mgVSS/l
USO	Unbiodegradable Soluble Organics in mgCOD/l
$\mathbf{V_{DN}}$	Downwards liquid bulk velocity
VFA	Volatile Fatty Acids in mg COD/l
ViCAs	Vitesse de Chute en Assainissement
$\mathbf{V_L}$	Volume of the layer in m^3
$\mathbf{V_S}$	Settling velocity in m/hr or m/d
VSS	Volatile Suspended Solids in mgVSS/l
$\mathbf{V_{UP}}$	Upwards liquid bulk velocity
WAS	Waste Activated Sludge
WRC	Water Research Commission
WRG	Water Research Group
WRRF	Water and Resource Recovery Facility
WW	Wastewater
WWTP	Wastewater Treatment Plant
$\mathbf{X_{LIM}}$	Maximum threshold concentration in mg/l
$\mathbf{X_{MIN}}$	Minimum sludge blanket concentration in mg/l

Table of Contents

List of Figures

List of Tables

1. Introduction

1.1. Terms of Reference

This study proposes the modelling of a realistic primary settling tank (PST), with characterized settling velocity groups. The project will seek to improve on a current total suspended solids (TSS)-based PST model into a more accurate and realistic model that can predict the settling of municipal raw wastewater in the PST as well as the generated primary sludge (PS) and settled wastewater (settled WW) characteristics, in terms of unbiodegradable particulate organics (UPO), biodegradable particulate organics (BPO) and inorganic settleable solids (ISS). This shall be done in a plant-wide context because the settling of biodegradable organics in the PST determines the extent of energy recovery from the connected unit process of anaerobic digestion (AD) and energy consumption in the activated sludge (AS) system. The investigation was conducted in the Water Research Group (WRG) of the department of Civil Engineering, at the University of Cape Town (UCT), under the supervision of Dr David S. Ikumi.

1.2. Background to Problem

Throughout the development of wastewater engineering, wastewater treatment plants (WWTP) have been designed mainly to ensure effluent quality, through the removal of organics and nutrients such as nitrogen (N) and phosphorus (P). This is performed before discharging the effluent into the environment. Due to the problems associated with water scarcity, and the increasing need to look for other sources of energy and nutrients (N and P), it has become obvious that WWTPs must be able to treat the wastewater for reuse, nutrients recovery and energy self-sufficiency purposes. Hence, the current paradigm shift from WWTPs to water and resource recovery facilities (WRRFs), towards more economically, environmentally and socially sustainable waste treatment systems. In this context, the modelling of primary sedimentation processes is becoming more relevant, to optimize the PS production and the associated energy generation via the AD of PS, as well as the AS system energy efficiency.

Primary sedimentation refers to physical processes of solid-liquid separation in primary clarifiers or settlers, which are usually referred to as primary settling tanks (PSTs). These physical processes include settling of particles, which occur under the force of gravity (gravitational settling), alongside with flocculation and coagulation (when chemically enhanced treatment is implemented). However, it is possible that some biological processes, such as ammonification and hydrolysis, take place (Lessard & Beck, 1988; Gernaey *et al.,* 2001) . The role of primary sedimentation has been overlooked over many years, due to the difficulties arising in describing the above-mentioned processes, from both optimization and modelling perspectives.

Furthermore, the PST has been weakly replicated in the virtual plant-wide model setup, because it is mostly considered as an input to the main unit process models (i.e., AS and AD systems) and, hence, not directly influential in the modelling processes (Bachis *et al.,* 2015).

A wide range of mathematical models have been proposed to describe how PSTs function. Some models were quite simplistic by making use of retention time with a single variable (Otterpohl & Freund, 1992) or addressing scouring with the PST hydraulic behavior (Lessard & Beck, 1988), in an empirical fashion. Other models comprised of combined physical and biological processes that were extremely complex to develop and calibrate (Lessard & Beck, 1988; Gernaey *et al.,* 2001). Hence, there is a need to redefine the development of PST models with the objective of a better WRRF processes description and a holistic plant-wide optimization. This led to a new generation of promising models using the particle settling velocity theory (Vallet, 2011; Maruéjouls *et al.,* 2012; Bachis *et al.,* 2015).

However, the TSS in these models is incorrectly disaggregated due to inappropriate assumptions made about its composition. In fact, the TSS is made of UPO, BPO and ISS fractions that settle in different proportions in the PST, from observed experiments (Wentzel *et al.,* 2006; Ikumi *et al.,* 2014). In addition, the TSS characterization in terms of these parameters which can be easily determined or measured experimentally, would be much more accurate and realistic, unlike other TSS fractionation methods (carbohydrates, lipids and proteins, etc.). Subsequently, predictions that do not reflect reality are made in terms of TSS composition and energy generation, as well as energy recovery, in a plant-wide context. Since, it is crucial to realize that the accuracy of models depends on the accuracy of input parameters, it is therefore imperative to improve primary sedimentation modelling in such a way that realistic and accurate predictions are made to optimize energy estimations and plant operations.

1.3. Research Aspects

1.3.1. Problem Statement

Primary settling tanks are used for primary sedimentation of wastewater, to generate primary sludge, which is then fed into the anaerobic digester for energy recovery purposes. Mathematical models have been developed to simulate the removals of particles in the PST, by means of different particle settling principles. However, these models are all TSS-based and, as such, it has been increasingly difficult to accurately predict the PS composition, which is an input into downstream unit processes, such as the anaerobic digestion. The knowledge of the particles' characteristic component compositions would be useful when applying plant-wide mathematical models in the prediction of PS fed AD performance and the performance of the AS system that is fed the settled wastewater (the supernatant generated after primary sedimentation).

PSTs have not been modelled extensively because of the complexity in representing the sedimentation phenomena. Moreover, prior to the development of plant-wide models, the mathematical models focused on the prediction of effluent quality from distinct unit processes, such as the AS system. Since the various WRRFs unit processes are linked, their operations impact the performance of other downstream (and upstream, where recycling is involved) unit processes (Sötemann *et al*., 2006). Furthermore, the tracking of energy (chemical oxygen demand - COD), nutrients (N and P) and water became essential with the utilization of plant-wide models to provide more holistic solutions for the recovery of resources and generation of good effluent quality. Within these plant-wide models, the current PST unit process models have not been able to track the organic and inorganic materials removals appropriately; hence, the compositions of the PS (to the AD unit process), as well as the settled wastewater (to the AS system), are not properly estimated. Therefore, this project works towards the development of a model that realistically depicts the removals of municipal wastewater particles (grouped in UPO, BPO and ISS) and caters for the determination of the PS and settled WW compositions, such that resource recovery strategies can be optimized at a plant-wide level.

1.3.2. Key Questions

The following key questions were prompted, in response to the above-mentioned problem statement.

1. How can the current TSS-based models be improved to extract UPO, BPO and ISS fractions with the aim of generating an improved (realistic) PST model, within the integrated plant-wide context and whereby the predicted PST outputs are the required, realistic and useful inputs to the other connected unit processes of the WRRF?
2. Can the improved model in (1) accurately predict primary sludge and settled wastewater characteristics, adequately, under both steady state and dynamic conditions?

1.4. Scope and Limitations

The project is primarily focused on developing and verifying an improved mathematical model of a PST. It includes two main components, which are listed below.

1. The utilization of particle settling velocity distribution (PSVD) theory (Maruejouls *et al.,* 2012; Bachis *et al.,* 2015) towards representing a realistic picture of the PST sedimentation processes,

as described in Wentzel *et al.* (2006) and Ikumi *et al.* (2014), and with regards to UPO, BPO and ISS fractions. This is to be performed by extending a discrete particle settling model (Kowlesser, 2014), to perform calculations under steady state and dynamic conditions.

2. The development of a dynamic PST model by implementing the previous modelling approach and results obtained, in the current TSS-based model of Bachis *et al.* (2015), to reflect realistic PST predictions, in terms of UPO, BPO and ISS fractions.

Furthermore, it is worth noting that the proposed dynamic model development will only include implementation and verification stages. The calibration and validation procedures, as well as other evaluation processes, fall outside the scope of the present work.

1.5. Aim and Objectives

The purpose of this research is to develop a dynamic mathematical model of a PST that accounts for a realistic settling of municipal raw wastewater and disaggregation of its TSS, in fractions of UPO, BPO and ISS. Therefore, the model is expected to predict under steady state and dynamic simulations, the primary sludge composition in terms of UPO, BPO and ISS, as well as the composition of the settled wastewater that is treated in subsequent unit processes. The detailed objectives of the project are as follows:

1) Make use of a discrete particle settling approach (Kowlesser, 2014) and the current TSS–based model of Bachis *et al.* (2015) to develop a dynamic PST model that can disaggregate the TSS into realistic fractions of UPO, BPO and ISS.
2) Verify the model with WWTP data from the literature, by making sure that it is internally consistent with strict material mass balances.
3) Propose a preliminary integration of the developed PST model in a plant-wide context to demonstrate its application and impact.

1.6. Thesis Structure

This dissertation is made of 6 Chapters, as well as References and Appendices.

Chapter 1 gives a background to the problem, presents the aim and scope of the project, as well as the research aspects.

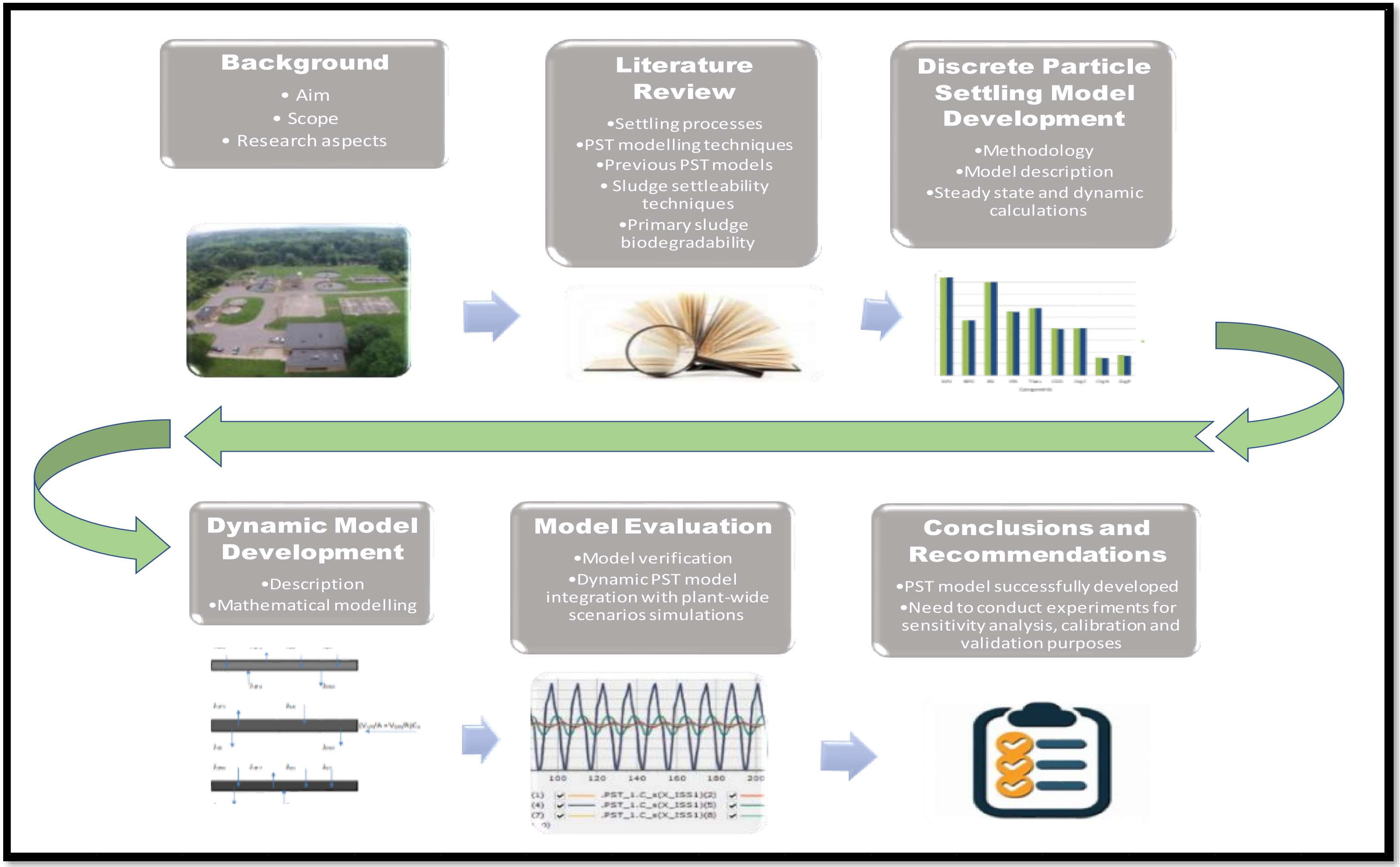
Chapter 2 reviews the literature which details the previous works completed on primary sedimentation modelling, to find the gaps that still require further investigation. It, therefore, elaborates on the different particles settling processes and critically reviews the modelling techniques, as well as the different PST models that have been developed over the years. It also expands on the primary sludge characterization which includes different sludge settleability techniques and primary sludge biodegradability.

Chapter 3 presents the development of a discrete particle settling model, which can mimic steady state and dynamic calculations. It extends the work done by Kowlesser (2014) and makes use of the PSVD approach of Bachis *et al.* (2015). The methodology underlying the discrete particle settling model, as well as the mathematical modelling development, are thoroughly described. Results of steady state and dynamic calculations, using data from previous studies (WRC, 1984; Ekama, 2017) are also presented.

Dynamic developments of the PST model are discussed in Chapter 4. The discrete particle settling approach is implemented into a PST unit, to build up a mathematical model (the University of Cape Town Primary Sedimentation Unit -UCTPSU) that can predict the TSS removals in terms of UPO, BPO and ISS fractions. In this regard, the current TSS-based model of Bachis *et al.* (2015) is firstly described and thereafter modified accordingly into the UCTPSU model.

Chapter 5 presents the evaluation of the UCTPSU model and its preliminary integration in a plant-wide setting. First, the model is rigorously verified by using multiple loading conditions and sanity checks. Thereafter, specific plant scenarios are presented to demonstrate the application of such a model and show the impact of its integration in a plant-wide model context.

Chapter 6 provides the concluding remarks and proposes recommendations to further improve primary sedimentation modelling of municipal wastewater, in the view of a better plant-wide model integration for resource recovery. The structure of this thesis is summarized in Figure 1.



Background

- Aim
- Scope
- Research aspects

Literature Review

- Settling processes
- PST modelling techniques
- Previous PST models
- Sludge settleability techniques
- Primary sludge biodegradability

Discrete Particle Settling Model Development

- Methodology
- Model description
- Steady state and dynamic calculations

Dynamic Model Development

- Description
- Mathematical modelling

Model Evaluation

- Model verification
- Dynamic PST model integration with plant-wide scenarios simulations

Conclusions and Recommendations

- PST model successfully developed
- Need to conduct experiments for sensitivity analysis, calibration and validation purposes

Figure 1: Thesis Structure Diagram

2. Literature Review

2.1 Introduction

The main function of a primary settling tank (PST) in a wastewater treatment plant (WWTP) is to perform preliminary treatment by allowing settlement of readily settleable particles, thus reducing the organic load on the activated sludge system reactors. Unlike most of the unit operations (activated sludge systems, anaerobic digesters, secondary settling tanks) which have been modelled for better plant optimization and resource recovery, few investigations have been conducted (and therefore built models) to understand PST operations. This was due to the complexity of settling processes description (Bachis *et al.,* 2015).

Empirical models have been developed (Otterpohl & Freund, 1992; Christoulas *et al.,* 1998) using empirical relations and regression techniques. These models do not use scientifically sound principles to link the measured influent characteristics and the model outputs. Hence, there is a need for transition towards a more glass box approach to modelling, such that the principles of material mass balance could be applied towards connecting the PST model inputs to its predicted outputs. Such an improved (scientifically verifiable) model shall add value towards tracking important components (those influencing resource recovery, sludge stability and effluent quality) along the unit processes of the WRRF (including the PST).

Furthermore, these empirical models as well as recently improved ones, mostly generate outputs in total suspended solids (TSS) form, which is not enough in making tactical decisions with regards to energy costings (recovery and consumption), for instance. Therefore, incorrect assumptions have been made with regards to the desegregation of the TSS removed, into biodegradable particulate organics (BPO), unbiodegradable particulate organics (UPO) and inorganic settleable solids (ISS) fractions. In addition to that, the output of the PST becomes input to other unit processes, such as the primary sludge (of the anaerobic digester), as well as the settled wastewater (of the activated sludge system) and these unit processes operate with components such as UPO, BPO and ISS.

As such, if the fraction of settleable particulates (biodegradable and unbiodegradable organics, as well as inorganic) is accurately represented in the PST model, like experimental studies on municipal primary sludge have revealed (Wentzel *et al.,* 2006; Ikumi *et al.,* 2014), then the other unit process outputs (mainly energy requirements and sludge mass generation) can be adequately predicted. In that respect, linking a PST model to the abovementioned unit processes, within a plant wide modelling context, is crucial, as displayed in Figure 2.

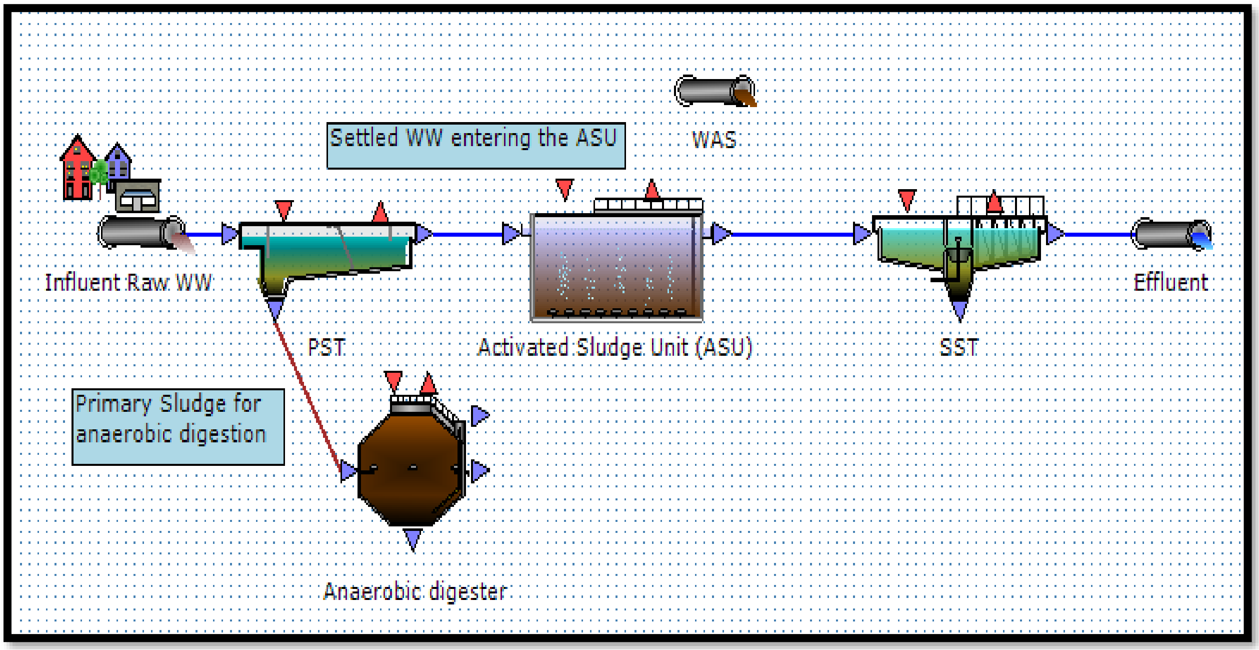


Figure 2: Typical WWTP with Different Units and their Links to the PST

Various investigations have been undertaken to propose dynamic models that can adequately simulate the sedimentation processes in a PST and, eventually, bridge the gaps with the subsequent unit processes (Gernaey *et al.,* 2001; Maruejouls *et al.,* 2012; Bachis *et al.,* 2015).

2.2 Primary Sedimentation Overview

2.2.1 Description

Primary settling is the last stage of a series of different processes of the primary treatment, which includes pumping, screening, grit removal, flow distribution and balancing. A portion of the total suspended solids (TSS) referred to as settleable solids (SS), flocculates and gets enmeshed to settle in the sedimentation basin. That portion is eventually disposed as primary sludge (PS). Hence, the remaining suspended solids which are non-settleable, as well as the dissolved compounds, constitute the supernatant (settled wastewater) that is conveyed to the biological reactors for secondary treatment and mediated by the organisms performing biological wastewater processes. Since settleable particles naturally gravitate in the wastewater, due to their density compared to water, it appears that settling is the common solid/liquid separation technique (Piro *et al.,* 2011). In addition, the fundamental parameter controlling in primary sedimentation is the particles' settling velocity (Davis, 2011), which is investigated in the next section.

2.2.2 Settling Processes

“Sedimentation involves the removal of suspended particles from a liquid stream by gravitational settling” (Cheremisinoff, 2002). Gravitational settling occurs in several ways, as pointed out by Metcalf & Eddy (2003), such as discrete particle settling, flocculent particle settling, ballasted flocculent settling, hindered or zone settling, compression settling, accelerated gravity settling and flotation. This review will highlight discrete, flocculent and zone settlings, since these regimes are more applicable to particle removals in primary clarifiers (Davis, 2011).

2.1.1.1. Discrete Settling

This type of settling is referred to as Type I sedimentation. Particles settle individually, at a constant settling velocity and without any significant interaction with others (Davis, 2011). Hence, particle sizes, shapes, as well as densities, are not altered and assimilated to spheres (Chebbo & Gromaire, 2009). This directly implies that the terminal velocity is instantaneously reached and remains constant. As such, the wastewater is a suspension of a low solids concentration (Metcalf & Eddy, 2003). Sand and grit are usually removed under discrete settling.

Davis (2011) expresses the settling velocity from Stokes’ law which, under laminar flow conditions, states that:

$$V_s = \frac{g\,(\rho_s - \rho)d^2}{18\,\mu}$$

Where

V_s is the particle settling velocity in m/s

d is the particle diameter in m

g is the acceleration due to gravity in m^2/s

ρ_s is the density of particle in kg/m^3

ρ is the density of fluid in kg/m^3

μ is the dynamic viscosity in Pa.s

Furthermore, Metcalf and Eddy (1991) established that to design a sedimentation basin, a particle of terminal velocity V_c is selected and the basin is designed such that particles having a settling velocity equal or greater than V_c will be removed. It follows that the overflow rate is given by the equation:

$$V_c = \frac{Q}{A}$$

Where

Q is the overflow rate in m^3/s

A is the surface area of the basin in m^2

In practice, even though particles are not settling in a discrete fashion in a PST, discrete modelling could still be used to provide a realistic representation of primary sedimentation with the aid of particle settling velocities.

2.1.1.2. Discrete Particle Modelling Technique

A discrete settling particle model has been developed by Kowlesser (2014), based on the particle settling velocity distribution (PSVD). The model allows a description of the distribution of particles, in terms of their settling velocities, towards developing a vertical flow model that can be applied to describe particle removals in PSTs.

An influent sample of known concentration (200 mg/l) was used to simulate a batch settling column. In this column, the concentrations are measured at a fixed collection depth (z) of 1.22 m and this was done at different time intervals (t). Hence, at every time interval, particles that are removed need to have settled with a specific terminal settling velocity. This velocity is determined by the following equation:

$$V_s = \frac{z}{t}$$

Where V_s is in m/s, z is in m and t is in s.

Therefore, the influent sample was divided into 15 settling velocity groups, to which different concentration proportions and different settling velocities were assigned. As such, the concentration proportions and settling velocities were varied such that the total concentration predicted at a specific time t could best match the measured concentration (X_t) for that same time. The settling processes were bound by the following conditions and assumptions:

- The sum of the percentages of concentrations, which are assigned to the 15 settling velocity groups, must add up to 100% and, therefore, to the measured total concentration.
- The values of settling velocities are assumed to vary between 0.18 m/min and 3 m/min.
- Since the concentrations were discretized, only two scenarios were possible: the concentration at the collection depth is (i) 0 mg/l if no particles settle, or (ii) the initial assigned value, if all particles settle.

To determine whether a particle in a settling velocity group settles and gets removed or not, its terminal velocity is compared to the assigned settling velocity of the settling velocity group. At a time, t, if the particle terminal velocity is less than the assigned velocity to the settling velocity group, that particle does not settle. Should the particle terminal velocity be greater than the assigned velocity to the settling velocity group, the particle settles out completely. Therefore, this model allows a description of the velocities' distribution across the different settling groups, in a vertical flow fashion.

2.1.1.3. Flocculent Settling

Flocculent settling is quite dominant in primary settling tanks, as well as in the upper layer of second clarifiers (Takacs *et al.,* 1991). In this type of sedimentation, particles coalesce and increase in mass to settle at a faster rate. The wastewater is usually a dilute suspension of particles and there is removal of a portion of the untreated water, as well as chemical flocs (Metcalf & Eddy, 2003). Described by Davis (2011) as Type II sedimentation, this settling phenomenon cannot be accurately modelled by Stokes' law, since particles vary in size and shape through flocculation, as well as the specific gravity variation due to the air entrapped into the flocs. As such, settling column tests (ViCAs, for instance) can, instead, be used to model this behavior (refer to Section 2.4.1 below).

2.1.1.4. Zone Settling

It is a settling regime that is also referred to as hindering settling. Because of the high concentration of particles, the free area between them decreases and, hence, the inter-forces hamper the processes. As a result, particles settle as a mass of unit, in a "zone" or "blanket" fashion (Takacs *et al.,* 1991; Davis, 2011). Column tests are also used to determine the settling characteristics pertaining, associated with the solid (or particle) flux theory (Metcalf & Eddy, 2003).

2.2.3 Advanced Primary Treatment

Primary sedimentation can be improved by dosage of chemicals to enhance the fraction of TSS removal. Suspended solids (SS) flocculate better and become more settleable to be deposited in the PST. This process is called chemically enhanced primary treatment (CEPT). Metal salts and/or polymers such as ferric or iron chloride ($FeCl_3$), aluminum sulphate ($Al(SO_4)_2$) or ferric sulphate ($Fe_2(SO_4)_3$) are added in the form of organic polyelectrolytes, towards coagulation and flocculation (Chagnon & Harleman, 1992). Davis (2011) stated that the CEPT promotes an increased contact between particles. As a result, there is an increase in primary sludge production which is superior to simple or conventional primary sedimentation, in terms of chemical oxygen demand (COD) and nutrient removal (nitrogen - N and phosphorus - P). On the other hand, many WWTP in South Africa for instance, do not have adequate primary sludge treatment facilities. Therefore, additional primary sludge is a concern when it comes to overall treatment capacity.

Thus, the treatment capacity of the WWTP is increased and low capital costs can be achieved. In addition, the surface overflow rate can be increased or the requirement for biological reactor size (in design) and secondary settling tanks (SSTs) surface area can be reduced (Harleman & Murcott, 2001; Aiyuk *et al.,* 2004). Furthermore, Rashed *et al.* (2013) showed that the settling time can be significantly reduced from 2 hours to 30 min. However, Davis (2011) has found that the CEPT can present various disadvantages. It can incur high operational costs due to chemical consumption costs and require chemical handling facilities. Moreover, it is possible to remove too much phosphorus by precipitation and create a deficiency in the settled wastewater nutrient capacity. This can be negative to downstream biological processes that require phosphorus. In addition, this enhanced sedimentation process may decrease the sludge settleability in the biological reactors.

As far as primary sedimentation modelling is concerned, considering CEPT processes would be an interesting aspect to explore. This is because the settling velocities will significantly change with the dosing of flocculants and coagulants which, in turn, will affect the settleability of the particles. In this regard, Bachis *et al.* (2015) investigated the CEPT impact on the particle settling velocity distributions and found a significant improvement in the settling rate of slower particles which, eventually, yielded to a better TSS removal.

2.2.4 Importance of Primary Sedimentation

When only primary sedimentation is implemented, it promotes the removal of a substantial fraction of the organic load which would have polluted receiving waters when discharged in it. In addition, sedimentation tanks can provide sufficient retention time required to allow overflows to be disinfected (Metcalf & Eddy, 2003).

Since primary settling aims at reducing the influent organic load (COD) on secondary treatment processes, it follows that the design costs (associated with reactor sizing) and operational costs (associated with oxygen demand from breakdown of biodegradable organics in the settled wastewater – PST supernatant) can be substantially optimized, with accurate PST model predictions (Ekama & Wentzel, 2008). According to Lessard and Beck (1988), other advantages of PSTs include increasing the rate of soluble substrate degradation during aeration, and a reduction in waste activated sludge (WAS) volume. There is also potential to produce energy (biogas) from anaerobic digestion of the primary sludge (Ekama, 2017).

However, primary sedimentation has many disadvantages. An additional footprint from a plant perspective is required and also space is needed, to store the primary sludge collected. In addition, odors can be generated if the hydraulic retention time is not properly monitored (Davis, 2011). Furthermore, the COD removed can be detrimental to the influent COD composition, towards better nutrient removal and reduced energy demand. Moreover, primary sedimentation necessitates further treatment of the primary sludge before disposal, mainly through anaerobic digestion (Gori *et al.*, 2013; Nowak, 2015). This treatment process is well known to be a very sensitive and complex (Wentzel *et al.,* 2006).

Towards mitigating these shortcomings and optimise primary sedimentation, it is recommended that the hydraulic retention is kept under 1.5 hours to minimize odors (Davis, 2011). But odor control measures still need to be implemented in a plant operating with primary sedimentation. The COD removal through primary sedimentation has to be monitored since it affects the N:COD ratio of the plant , which subsequently impacts on the energy demand (Nowak, 2015). Lastly, primary sedimentation needs to be carefully evaluated in conjunction with the associated treatment and costs implications of anaerobic digestion and as well as sludge disposal, before its implementation. This will assist in determing if the implementation is realistic from a plant capital costs and lifecycle costs perspective.

In order to maximize the accrued benefits from utilization of PSTs, models have been developed to describe these primary sedimentation processes for plant design, optimization and maintenance.

2.3 Primary Sedimentation Modelling

To represent the physical processes that occur in a PST, different modelling techniques have been utilized to generate the models reviewed below.

2.3.1 Modelling Techniques

According to Amerlinck (2015), there are many techniques used to model PSTs, ranging from linear regression techniques, which yield to empirical models, to more advanced methods using artificial neural networks. Three techniques will be particularly explored in this review, namely (i) the removal efficiency correlations with one variable, (ii) computational fluid dynamics (CFD) methods, and (iii) phenomenological techniques.

Regression methods or empirical based models are used by empirically linking the removal efficiency with one variable. Most of the variables used are the suspended solids (SS) influent concentration or the hydraulic retention time. Sets of data (concentrations) are used to produce model fits for removal efficiency curves (Otterpohl & Freund, 1992; Amerlinck, 2015). These methods are simple to use, well documented and can predict the effluent quality with good confidence. However, they do not take into account flow patterns, solid distribution and tanks geometry (Matko *et al.,* 1996).

Computational fluid dynamics (CFD) techniques can better describe the flow patterns which significantly affect sedimentation performance. They can be further used to optimize sedimentation tank shapes. However, the complexity associated with hydraulic characterization can lead to modelling deficiencies of the settling processes. In addition, these models require large amounts of data for validation, enough computational power, and it is difficult to link them to the other unit processes for plant integration and urban wastewater management (Maruejouls *et al.,* 2012; Amerlinck, 2015).

Finally, phenomenological methods are used for primary sedimentation modelling, as well as secondary clarifier models. They can describe the dynamics of water and particles in one dimension, as well as optimizing the design and operation of sedimentation tanks from an integrated management perspective (Maruejouls *et al.,* 2012). Amerlinck (2015) distinguished between models: (i) applying the particle pathline concept linked with particle settling velocity, (ii) relating scouring with the settling tank hydraulic behavior, (iii) applying a one-dimensional discretization in the vertical direction, and (iv) using the PSVD theory, which is of interest in this proposed investigation. The velocity distribution theory was noted to predict the TSS with reasonable accuracy, by fractionating it into a limited number of particle groups. These groups were each defined by a distinct mean settling velocity that is extracted from lab scale experiments (Tik *et al.,* 2014). The problems associated with the PSVD theory include the difficulties in incorporating biological processes and a non-rigorous discretization procedure to increase the model confidence when applying different conditions (Amerlinck, 2015).

2.3.2 Review of Some Existing Models

As discussed in Section 2.1, the requirement for primary sedimentation modelling is to adequately replicate the removal of particles, through primary settling and, hence, predict the concentrations in the settled wastewater (settled WW), from the given raw sewage influent concentrations, and other provided design parameters. A wide range of models have been developed through various studies (Lessard & Beck, 1988; Otterpohl & Freund, 1992; Gernaey *et al.,* 2001; Maruejouls *et al.,* 2012; Bachis *et al.,* 2015) and by means of the techniques elaborated in Section 2.3.1. Each model developed has its advantages and disadvantages, as laid out in Table 1.

Table 1: Comparison of the Models Reviewed

Model	Description	Strengths	Gaps
Dynamic Lumped-Parameter Model (Lessard & Beck, 1988) **Aim**: Settling characteristics of influent components and capacity of soluble removal	• Use of continuously stirred tank reactors (CSTR) • A distinction is made between the removable and non-removable compounds • The soluble removal is included	• The removable fraction is modelled into settleable and non-settleable fractions • The model attempted to assign settling velocities to different types of sewage • The soluble COD and ammonium removals are described	• The sludge settling velocity is not adequately described • The primary sludge is not characterized • The solid profile distribution is not considered
Simple Model of a Primary Clarifier (Otterpohl & Freund, 1992) **Aim**: Predict the PST buffering behavior and consider the change of inflow characteristics	• Dilution of wastewater fractions per reactor volumes • The removal of particulate fractions is based on hydraulic retention time	• The regression analysis makes the model easy to be built • A good COD particulate removal could be predicted	• The biodegradability is not considered • Only COD is modelled • The solids distribution and flow patterns cannot be described
Dynamic Model of Clarification-Thickening (Takacs *et al.,* 1991) **Aim:** Propose an alternative settling velocity model to dynamically replicate the clarification and thickening functions of a clarifier	• The solid flux theory and a mass balance around each layer of a one-dimensional settler are used • A special settling velocity equation for simulation of dilute and concentrated suspensions is developed	• The model can simulate the solids profile in a column test under steady state and dynamic conditions, by means of the underflow and effluent suspended solids concentrations • It can be applied to primary and secondary clarifiers	• The settling velocity equation only holds for zone settling and fails to properly describe discrete and flocculent settlings • The velocity profile distribution is not properly described as it makes use of a single concentration to determine the velocity
Reactive Clarifier Model (Gernaey *et al.,* 2001) **Aim**: Model development of a primary clarifier to be used in WEST	• Based on Takacs *et al.* (1991) model • Use of a settling velocity model for clarification and thickening	• The influent COD is split into characteristics compatible with ASM1 • Good prediction of effluent COD • An extensive description of biological reactions (COD and ammonium removal through hydrolysis, ammonification) • An attempt to link the model to the ASM1 is highlighted	• Soluble COD is not well described by incorporating a particulate fraction • Particles are assumed to have the same velocity • Settling parameters not completely determined • Primary sludge characterization is not addressed

Model	Description	Strengths	Gaps
Phenomenological Retention Tank Model with PSVD Theory (Maruejouls *et al.,* 2012) **Aim**: Improve sedimentation model by incorporating particle settling velocity distribution (PSVD)	• It is based on Lessard & Beck (1991) model • Particle settling description under dynamic flows • The ViCAs protocol is used for velocity characterization	• Successful full-scale data testing • The solid distribution is addressed by a PSVD model using three particle classes with assigned time varying fractions of the influent TSS • A good effluent TSS prediction	• A validation with many other events is limited • Organics and nutrient fractionation are not considered • The incorporation of WWTP state variables linking unit processes with the PST model has not been done
New Dynamic Water Quality Model for Stormwater Basins (Vallet *et al.,* 2014) **Aim:** Replicate the behavior of particulate pollutants in a basin	• A distribution explains the particle settling velocities • ViCAs experiments are used for velocity characterization • Hydraulic and soluble models are also included, alongside to the particles' component	• Three settling velocities are used to describe the distribution of particles associated with the pollutants • The ViCAs results proved to be a good input into the model and virtual settling simulations were successful	• In the context of a PST, this model needs to characterize the different particles with regards to their biodegradability • The theoretical simulations are not enough to validate the model performance
PST Modelling Approach with PSDV Theory (Bachis *et al.,* 2015) **Aim**: Sedimentation modelling with PSVD and primary sludge characterization	• PSVD model used for solids distribution • ViCAs protocol is used for velocity characterization	• PSVD model improved by using five particle classes with assigned time varying fractions of the influent TSS • Good effluent TSS prediction • Implementation on the CEPT strategy • ASM1 fractionation from primary treatment	• Biodegradability is partially addressed • PST model is still to be properly linked to the ASM • Lack of links to other unit processes (such as the anaerobic digester and the activated sludge system)

After evaluating these models, it appears that their predicted PST solid removals are TSS sensitive but do not characterize the removed TSS according to the relevant TSS components of UPO, BPO and ISS. This is because the data used to calibrate these models was measured in terms of TSS only, of which the composition was not included in these data collections. It is also worth noting that these parameters can be reasonably measured experimentally, unlike other characterization parameters, as elaborated in Section 1.2.Therefore, the research gaps to be addressed in this project will include the development of a model which allows for the incorporation of these components (UPO, BPO and ISS) towards achievement of such detailed predictions. Furthermore, the composition of the TSS removed is usually incorrect with respect to the fractions of its components - the TSS in these models is assumed to be removed in equal fractions of its constituents (and, subsequently, at the same settling velocity). This was first noted by Sötemann *et al.* (2005b) and recently highlighted in the plant-wide configuration of the Benchmark Simulation Model No 2 for Phosphorus (Solon *et al.,* 2017*)*. However, Wentzel *et al.* (2006) and Ikumi *et al.* (2014) have observed that UPO, BPO and ISS settle out in the PST in different percentages of 60-70%, 30-40%, and 70-90%, respectively. PST models that do not model the removals of the UPO, BPO and ISS materials well, do not model the split of these materials, between the primary sludge of the anaerobic digester (where energy is generated) and settled wastewater of the activated sludge system (where energy is consumed) well, with the result that the energy self-sufficiency of the wastewater treatment plant is not adequately predicted. Hence, a better PST model for the fractionation of the primary sludge and the settled wastewater subsequently, is required.

It then follows that the particle settling velocity distribution (PSVD) theory can serve as a good tool to model the removals of these components, under different settling velocities. In fact, this theory can account for solids distribution, based on the settling velocity of particles (Matko *et al.,* 1996). Furthermore, if the primary sludge is characterized, it will be possible to provide a more detailed prediction in terms of the settled WW composition.

2.4 Primary Sludge Characterization

To model PST removals in realistic percentages, as well as accurately predicting the inputs into subsequent unit processes, the primary sludge needs to be comprehensively characterized. This characterization can be split into two experimental phases. The first phase consists of characterizing the primary sludge based on their settling velocities and settling mass proportions, and the second section determines the biodegradability of these different proportions.

2.4.1 Sludge Settleability Methods

Settleability characteristics of primary sludge (PS) generates particle velocity distributions that can adequately feed into a PSVD model. Owing to the density of particles, the PS can be characterized in different mass proportions. Methods, such as the particle settling effluent (ViCAs) protocol (Chebbo & Gromaire, 2009) and the settleometer method (Poinapen *et al.,* 2009) can be used. These protocols are described further in the subsequent sections.

2.1.1.5. Particle Effluent Velocity Protocol

Chebbo and Gromaire (2009) have elaborated on the well-known particle effluent velocity (ViCAs) operating protocol, highlighted in some of the above-mentioned PST models (Maruejouls *et al.,* 2012; Vallet *et al.,* 2014; Bachis *et al.,* 2015). It has been developed to measure settling velocities of suspended particles (carried by stormwater or combined sewage) and, hence, generate the distribution of these velocities. The protocol is based on the principle of homogeneous suspension to avoid pre-treatment and sample modification. This requires the tests to be performed immediately after sampling.

The apparatus (displayed in Figure 3) consists of a sedimentation column made of PVC, with an internal diameter of 70 mm and a height of 64 cm. The column is filled with a homogeneous wastewater sample to about 60 cm and allowed to settle at defined time intervals. At every time interval the sludge mass, which is later analyzed to determine its TSS content, is collected by a receptacle and replaced by another one for the next time interval. From these cumulated masses at different time intervals, it is possible to generate the distribution curves of settling velocities. Since particles do not settle over the same height, statistical tools are used to generate settling velocities distribution curves. Mass balances verifications are performed to determine losses or gains throughout the experiment and evaluate the accuracy of the measurements.

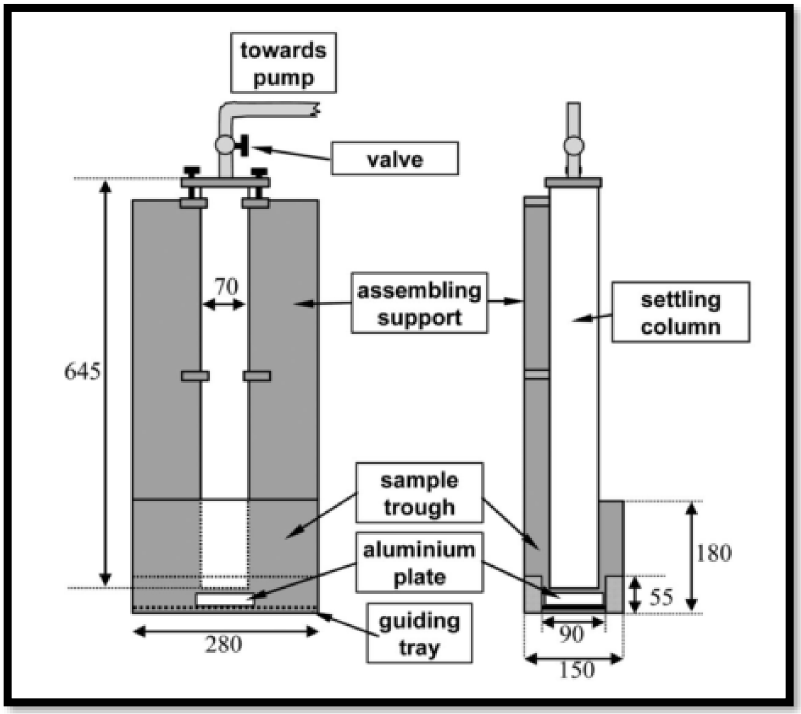


Figure 3: ViCAs Protocol Experimental Set Up (dimensions in mm) (Chebbo & Gromaire, 2009)

2.1.1.6. Settleometer Experiment

Similar to the ViCAs protocol, to a certain extent, the settleometer method was described by Poinapen *et al.* (2009). The device (shown in Figure 4) is made of five vertical transparent PVC columns of equal height and increasing internal diameters. The columns are interconnected with a plastic tube and the raw wastewater is pumped from the smallest column to the largest, at a constant flow rate.

The fastest settling particles settle and remain in the first column, which has the smallest diameter, and where the upflow velocity is highest. The slowest settling particles settle and remain in the last column with the largest diameter where the upflow velocity is slowest. The particles that do not settle at all are non-settleable and flow out of the largest column. Hence, by collecting the sludge mass that settles in each tube (since their settling velocity is higher than the upflow velocity), the sludge can be fractionated according to the size and density of particles. Hence, it could be used to reasonably model discrete settling and flocculent settling further. As such, once the percentage of sludge mass per column is estimated, as well as the sludge mass concentration, those two parameters can be plotted against their respective upflow velocities to describe the PS settling profile at various upflow and settling velocities. The settleometer can be a useful tool that can generate settling velocities and settling mass proportions to aid in calibrating the proposed PST model.

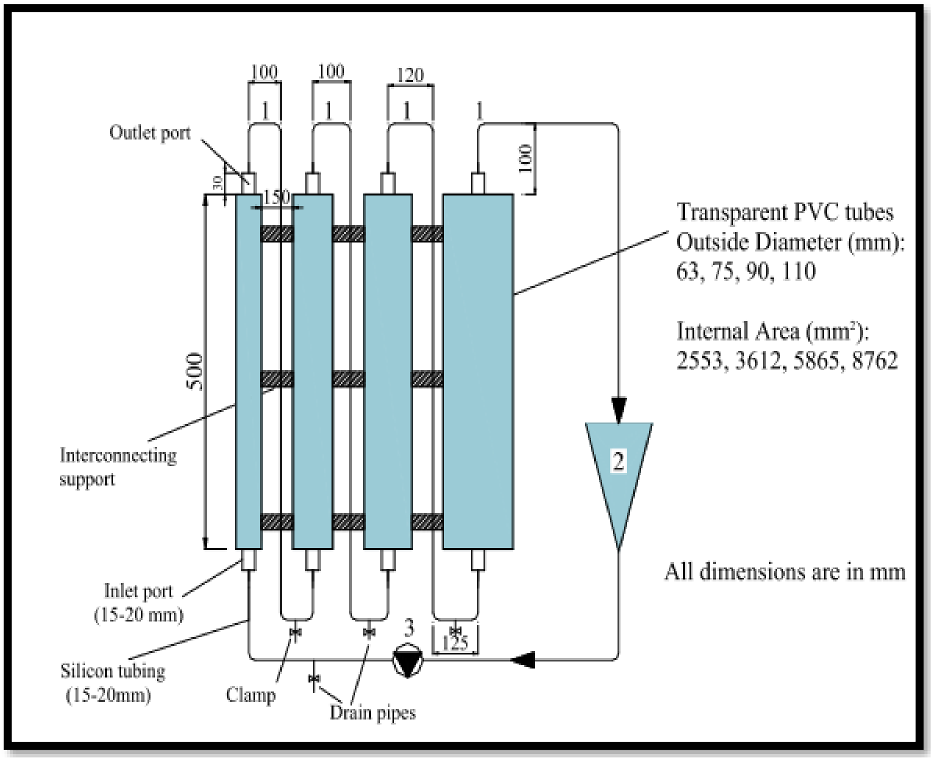


Figure 4: Settleometer Experimental Set Up from Poinapen *et al.* (2009)

2.4.2 Biodegradability and Elemental Analysis

If the BPO (of the primary sludge) elemental composition, in terms of x, y, z, a and b of $C_xH_yO_zN_aP_b$, can be determined, this will assist in making better predictions of the composition of the inputs in the anaerobic digestion and activated sludge models, and further allow an integration of a PST model in a plant-wide context.

Biodegradability tests consist of determining the biodegradable fraction of a substrate by measuring its anaerobic digestion output. The bio methane potential (BMP) test measures the amount of organic carbon (from digesting the organic waste) which is used to estimate the potential methane produced. It is commonly used because it is not expensive and can be reproducible between various substrates for comparisons (Moody *et al.,* 2009).

However, it was improved to the augmented bio methane potential test (ABMP) which measures additional tests of the aqueous phase (free and saline ammonia – FSA, orthophosphate - OP, and H_2CO_3 alkalinity) to the usual tests of carbon dioxide, methane, COD and volatile suspended solids (VSS). Furthermore, the augmented bio sulphide potential (ABSP) can be performed as well, since it measures the sulphide in the aqueous phase with the H_2CO_3 alkalinity, FSA, OP, VSS and COD (Botha & Ekama, 2015).

These measurements are added as inputs to a mathematical model parameter estimation procedure that determines the properties of the primary sludge, including its biodegradability (BPO content) and the empirical formula of the BPO ($C_xH_yO_zN_aP_b$). As such, the data obtained from an ABMP test performed on primary sludge, can be used together with the settling velocities (extracted from a settleometer in this case) to model a PST that can give detailed predictions of the primary sludge composition in terms of organics (UPO and BPO) and inorganics (ISS), as summarized in Figure 5.

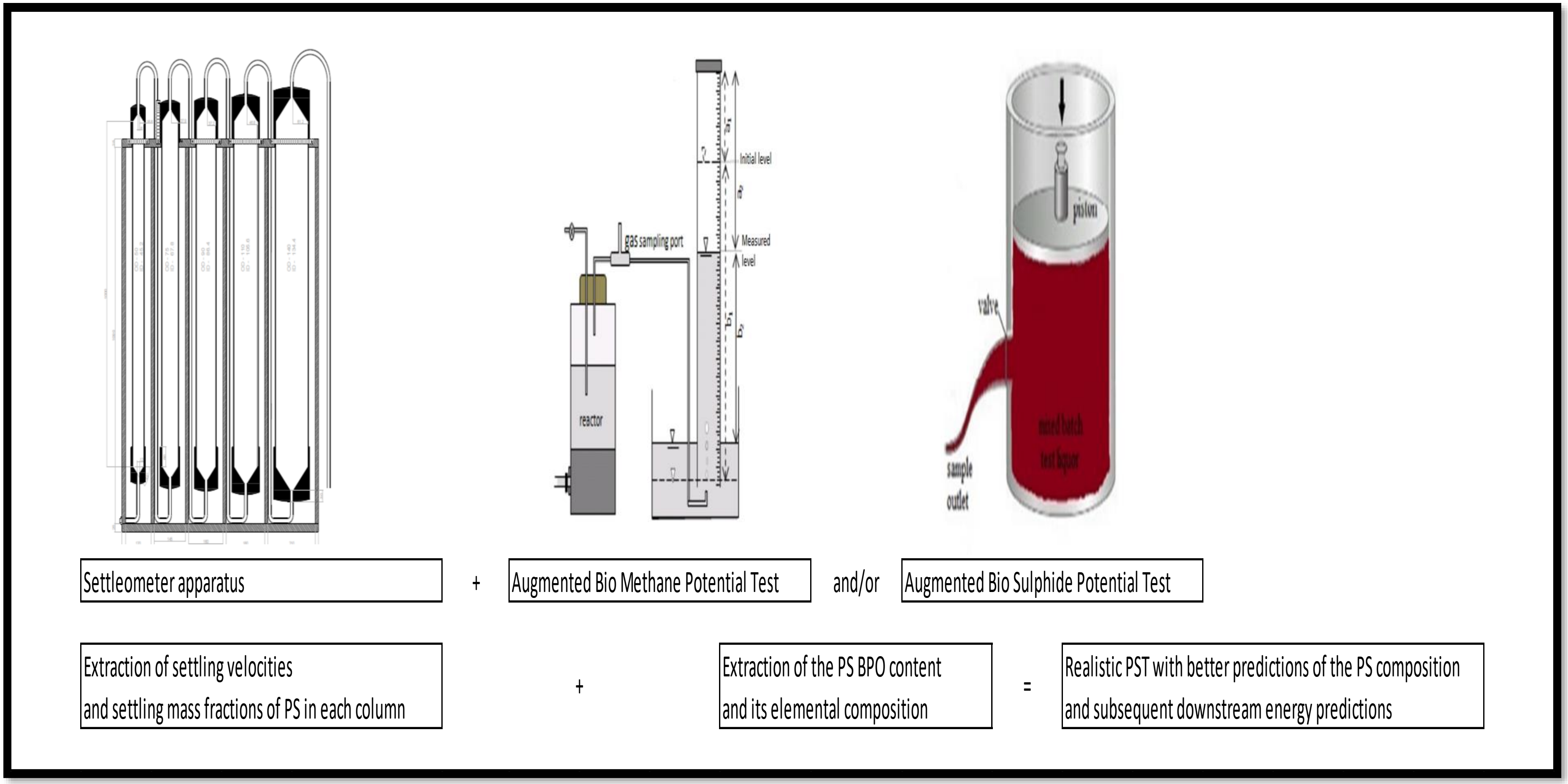


Figure 5: Relationships between the Settleometer and the ABMP/ABSP Tests towards Building a Realistic PST Model

2.5 Unit Processes Integration

With the recent drive towards plant-wide modelling and integrated systems, it is evident that modelling a PST, which cannot be used in a WWTP plant-wide context, will be incomplete. As such, the model must be able to connect to the other unit processes, which are the activated sludge model (ASM) and the anaerobic digestion model (ADM). In that way, the different compounds can be tracked throughout the plant. Unit processes models such as ASM1, ASM2(d), ASM3, as well as ADM1, have been mostly developed in isolation with state variables, composition and units that are difficult to match (Volcke *et al.,* 2006; Zaher *et al.,* 2007). It was, therefore, important to come up with integrative systems that can link these models. Among the different methods, two approaches were analyzed for this investigation, namely the continuity-based interfaced model (Volcke *et al.,* 2006) and the supermodel approach (Jones & Takacs, 2004).

2.5.1 Continuity-Based Interfaced Model Approach

The continuity-based interface model (CBIM) constructs model interfaces between different wastewater sub-systems (modelled in isolation) while ensuring the continuity of elements (C, H, O, N, P), charges and COD (Volcke *et al.,* 2006). It first formulates the elemental mass fractions and charge density, then defines a composition matrix and develops a set of algebraic equations, based on a Gujer matrix description of the two models to be linked. Conversion processes are thereafter defined to ensure the continuity of elemental fractions and charge before making use of transformation equations (Zaher *et al.,* 2007).

Although this method has been used by many studies (Volcke *et al.,* 2006; Zaher & Chen, 2006; Zaher *et al.,* 2007), it is quite cumbersome to make use of conversion processes and transformation equations, which may still not be compatible.

2.5.2 Supermodel Approach

The supermodel approach maintains the same model component structure, across the different unit treatments (Jones & Takács, 2004). A general set of components, that serve as inputs and outputs to the different models, is used. As such, it needs a set of pre-processed elements that are entered from the influent characteristics and recognized by the subsequent models, through the various physical, biological and chemical processes. This approach is more consistent and capable of generating less errors or incompatibility. The Plant-Wide Model of South Africa (PWM_SA) of Ikumi *et al.* (2013) is an example.

2.5.3 Discussion

Due to the increasing complexity in water resource recovery modelling, Vanrolleghem *et al.* (2014) have debated on whether accepting a mass continuity interface approach is the best approach to connect unit processes in a plant-wide set up, or whether adopting of a supermodel approach (where all components and transformations from the sub-model of each unit process are combined to form the plant-wide model) such as that of Grau *et al.* (2009), would improve the modelling process. It appears that moving towards the supermodel approach would require the description of all components according to their elemental composition, which would allow for the virtual tracking of all material elements in the models, using the principle of mass balances for the stoichiometric processes. In addition, the electroactivity of various species, prompted Lizarralde *et al.* (2016) to favour the supermodel approach, which links slower reacting components that are simulated using differential equations to much faster physicochemical reactions, which are calculated algebraically at each iteration. Therefore, that method (the supermodel approach) can be used to integrate the different unit processes in a plant-wide context. As such, the PST model can be built as an extension in PWM_SA and, eventually, linked to predict anaerobic digestion, as well as activated sludge system outputs.

2.5.4 Anaerobic Digestion and Activated Sludge System Models

The primary sludge generated can either be digested in an aerobic or an anaerobic digester. To recover the energy associated with the organics through methane production, as well as nutrients (phosphorus) via struvite precipitation, the digestion in an anaerobic digester (AD) is preferred. Depending on the system conditions (hydrogen partial pressure, mainly), four groups of organisms, namely the acidogens, acetoclastic methanogens, hydrogenotrophic methanogens and acetogens, mediate the bioprocesses. It includes conversion of complex organics to acetic acid and hydrogen, and then to methane or conversion of high volatile fatty acids (VFAs) to acetic acid, hydrogen and, finally, methane (Ikumi, 2011). These bioprocesses are very sensitive to pH changes and weak acid base conditions which, ultimately, dictate the failure or system recovery of the AD (Wentzel *et al.,* 2006). It then follows that being able to accurately predict these parameters, by knowing the composition of the input in terms of UPO, BPO and ISS and, subsequently, the BPO empirical elemental formula $C_xH_yO_zN_aP_b$, will assist in better optimizing the abovementioned bioprocesses in the AD model.

In addition, since acidogenic bacteria transform and convert fatty acids to short chain fatty acids (SCFA) through fermentation (Ikumi, 2011) and, considering that degradation of soluble components (including volatile fatty acid – VFA) can occur in a real PST, depending on the retention time (Lessard & Beck, 1988; Gernaey *et al.,* 2001), it would be useful to incorporate some biological process such as hydrolysis and fermentation in the modelling process, should the PST be linked to other unit processes (anaerobic digester and activated sludge system). In fact, Lessard & Beck (1988) noted that a long retention time could have led to COD removal through flocculation of colloidal particles with non-filterable particles or metabolic uptake. Furthermore, Gernaey *et al.* (2001) suggested the inclusion of an hydrolysis reaction to account for the variation in COD concentrations, from the influent to the effluent in the PST. They further included an ammonification factor to also account for the ammonia discrepancy in the predictions.

However, the purpose of this investigation is not to model a primary reactive clarifier by including bioprocesses such as hydrolysis and ammonification but to, rather, propose a configuration that can permit the PST outputs to be linked to subsequent unit treatments (anaerobic digestion and activated sludge system) in a plant-wide modelling context. Furthermore, the proposed PST model can give an indication of the settled wastewater composition of the activated sludge (AS) model, since the primary sludge characteristics can be predicted. The energy line can, therefore, be tracked more accurately since the AS is known to consume energy through oxygen demand, whereas the AD generates energy via methane production.

2.6 Closure

This literature has presented an overview of primary sedimentation and expanded on the different settling processes. Discrete and flocculent settlings, which are the most relevant for primary settlers, were reviewed, towards their application in primary sedimentation modelling.

To depict the physical processes that are occurring in primary settlers, various modelling techniques have been utilized and presented. Regression methods and computational fluid dynamics (CFD) are some of the techniques used, with the recent one being the phenomenological methods, which include the particle settling velocity distribution technique, a technique of interest for the proposed modelling investigation of this project. Using these techniques, different models that mimic solids removals and effluent concentrations, as best as possible, have been developed and critically reviewed. It was established that most of these models are TSS sensitive and fail to characterize that TSS into UPO, BPO and ISS fractions. Hence, incorrect fractionations are being assumed and propagated towards incorrectly predicting the composition of the primary sludge composition, as well as the settled wastewater. As such, there was a need for primary sludge characterization, which could be addressed through settling velocities tests and biodegradability tests.

Sludge settleability methods, to characterize the primary sludge according to the different settling velocities of particles, were described. It included the particle effluent (ViCAs) protocol and the settleometer experiment. Biodegradability tests, namely the ABMP (Augmented Bio Methane Potential) and ABSP (Augmented Bio Sulphide Potential) tests, were also presented to determine the BPO content and the elemental composition of the primary sludge. It was concluded that the combined settleometer experiment and the ABMP/ABSP tests could be used to build a realistic PST model with accurate primary sludge composition and subsequent downstream energy predictions.

It was further established that there is the necessity of proposing a PST model that can be integrated in a plant-wide context. In this regard, two main unit process integration techniques were reviewed, namely the continuity-based interface model approach and the supermodel approach. Since the proposed PST model is to be developed as an extension of PWM_SA, the supermodel approach was deemed to be the best method. Finally, the importance of linking the PST to downstream unit processes, such as the anaerobic digester and the activated sludge system, was also highlighted.

3. Discrete Particle Settling Model Development

3.1 Introduction

To propose a realistic model of the primary settling tank (PST), a discrete particle settling approach was developed into Microsoft Excel. This approach was applied to the particles making up the total suspended solids (TSS), which is categorized into unbiodegradable particulate organics (UPO), biodegradable particulate organics (BPO) and inorganic settleable solids (ISS). Discrete particle settling, which is referred to as Class 1 or Type I sedimentation, assumes a constant velocity and no significant interaction between particles (Davis, 2011). Therefore, a discrete particle settling model was primarily developed for constant (steady state) flow and load and then extended to dynamic (changing) flows and load conditions, such that it could be, subsequently, implemented into a PST model which can mimic the same conditions. In fact, model predictions under steady state conditions can be checked against expected results. This is to ensure that the model is working correctly before applying dynamic flow and load conditions, for which expected results cannot be simply generated. This section, therefore, presents the development of a discrete particle settling model in terms of its theoretical approach and mathematical description, as well as calculated results obtained under steady state and dynamic conditions.

3.2 Rationale

The discrete particle settling approach was chosen because it allows particles to be categorized into different settling velocity groups with a different settling velocity assigned to each group, to describe the particle settling distribution (Bachis *et al.,* 2015). It is possible that flocculent particle settling would provide a better description of settling particles in a PST (Takacs *et al.,* 1991). However, the challenges associated with modelling particles that are increasing in mass by coalescing and, subsequently, settling faster (due to a change in settling velocity), make the discrete particle settling approach a more easily achievable method. Flocculent (Class 2) settling may be required for modelling PSTs to which coagulants, like Iron or Aluminum, are dosed for chemically enhanced primary treatment (CEPT). However, that aspect falls outside the scope of this research.

A discrete particle settling model has been developed by Kowlesser (2014) and a similar discretization framework has been utilized in the PST model of Bachis *et al.* (2015), to predict removals of particles in terms of single parameter TSS only. However, this modelling approach fails to account accurately the removal of different fractions of UPO, BPO and ISS (Wentzel *et al.,* 2006; Ikumi *et al.,* 2014), which together make up the TSS and can be reasonably measured experimentally (refer to Section 1.2), to be removed in the PST. In fact, it has been observed that ISS and UPO are removed in greater fractions in the PST than BPO. To overcome the current deficiency in PST models, that remove equal fractions of UPO and BPO under changing upflow rates caused by dynamic flow conditions, a discrete particle settling model has been developed in this thesis in such a way that the TSS disaggregates into these three different components, i.e. TSS = UPO + BPO + ISS. The aim of this settling model is to mimic and realistically describe sedimentation patterns in a PST of a wastewater treatment plant with diurnal data, such that removals of UPO, BPO and ISS settleable particles is achieved in observed fractions, which yield the observed primary sludge unbiodegradable and VSS/TSS characteristics, so that the settled wastewater characteristics can be predicted from the raw wastewater characteristics and the PST performance. Therefore, an understanding of principles behind these removals under discrete particle settling conditions will provide a detailed insight into the parameters and variables to consider when developing more complex conditions for dynamic modelling.

3.3 Influent Wastewater Characteristics

The influent wastewater (WW) characteristics used in the calculations with the discrete particle settling model were the same as those used in previous publications, i.e. WRC (1984), Ekama (2009, 2011) and Ekama (2017). This wastewater data is made of steady state inputs (constant flow and load) and dynamic inputs (changing flows and loads) and comprise all the required measurements for developing the PST model. The rationale behind selecting this data set in describing the PST settling model stems from its rigorous data reconciliation process to produce typical sewage characteristics for South African wastewater systems, in terms of raw wastewater (raw WW), settled wastewater (settled WW), as well as primary sludge (PS) characteristics, while maintaining mass balances over the PST.

The raw influent chemical oxygen demand (COD) concentration, used as input to the settling model, is fractionated into 5 organics components, i.e.:

- Volatile fatty acids (VFA)
- Fermentable biodegradable soluble organics (FBSO)
- Unbiodegradable soluble organics (USO)
- Biodegradable particulate organics (BPO)
- Unbiodegradable particulate organics (UPO).

To these organics components, are added 3 inorganics components, which are:

- Free and saline ammonia (FSA)

- Orthophosphate (OP)
- Inorganic suspended solids (ISS).

The UPO, BPO and ISS are divided into settleable and non-settleable fractions, as observed in Wentzel *et al.* (2006) and Ikumi *et al.* (2014) and, together, make up the total TSS. The five organics groups each have a COD, C, N and P to VSS mass ratio (denoted as f_{cv}, f_c, f_n and f_p respectively). Hence, once the raw WW component COD (i.e. organics) concentrations are determined (computed from parameterized raw wastewater COD fractions), they are utilized, together with the mass ratios, to calculate the organically bound N and P concentrations (OrgN and OrgP). The total Kjeldhal nitrogen (TKN) and total phosphorus (TP) are calculated as the respective sums of the organic N and FSA, as well as the organic P and OP (TKN = OrgN + FSA; TP = OrgP + OP).

The soluble components are, theoretically, the same for the raw WW, settled WW and PS (i.e. the PST is considered as a non-reactive tank). With the unbiodegradable particulate fraction ($f_{S'up}$) of the settled WW (0.029) being independent from the raw WW (0.130) and only dependent on the PST performance, the soluble and non-settleable concentrations make up the settled WW, and the PS is made of the soluble and settleable concentrations. Furthermore, the PST is modelled as a point settler in this set of data, and removes 100% of settleable solids, while ensuring a 100% water, COD, N, P and ISS material mass balance. In other words, the % UPO, BPO and ISS settled out in the PST are set, depending on the PST performance. The % UPO, BPO and ISS removed in the PST of the WRC (1984) wastewater data, to yield the settled wastewater characteristics, are 84.0% UPO, 47.2% BPO and 80.3% ISS and show that the UPO (and ISS) is removed in greater proportion than the BPO. An influent flow rate (average dry weather flow - ADWF) of 15.0 Ml/d is selected and the underflow recycle of the PS is fixed at a percentage of that influent flow rate (0.5% of ADWF in this case). The flows and loads of the raw WW, settled WW and PS characteristics, as well as the mass ratios, have been summarized in Table 2, Table 3, Table 4, Table 5 and Table 6. Details of the influent characteristics, in terms of the block diagrams and complete dynamic loads, can be found in Appendices 8.1.

Table 2: Flows and Loads of Raw WW

Time dt (h)	Flow (m^3/h)	VFA (mgCOD/l)	FBSO (mgCOD/l)	USO (mgCOD/l)	Settleable BPO (mgCOD/l)	Non-Settleable BPO (mgCOD/l)	Settleable UPO (mgCOD/l)	Non-Settleable UPO (mgCOD/l)	FSA (mgN/l)	TKN (mgN/l)	OP (mgP/l)	TP (mgP/l)	Settleable and Non-Settleable ISS (mgISS/l)
06H00	225.0	0.00	56.67	20.05	79.37	89.86	36.23	6.95	17.97	24.38	2.89	5.14	15.16
08H00	315.6	0.00	57.34	20.28	80.31	90.93	36.66	7.03	27.15	33.64	2.55	4.84	24.91
10H00	937.5	0.00	107.94	38.18	151.18	171.17	69.01	13.23	42.19	54.40	5.92	10.22	34.66
12H00	1075.0	0.00	148.41	52.50	207.87	235.35	94.88	18.19	49.23	66.01	8.51	14.42	51.99
14H00	906.3	0.00	167.30	59.18	234.33	265.31	106.96	20.51	54.70	73.62	9.40	16.06	56.32
16H00	731.3	0.00	171.35	60.61	240.00	271.73	109.55	21.01	58.60	77.98	9.84	16.66	60.65
18H00	637.5	0.00	188.89	66.82	264.57	299.54	120.76	23.16	48.84	70.20	10.88	18.40	64.98
20H00	725.0	0.00	175.40	62.05	245.67	278.14	112.14	21.50	44.93	64.77	9.62	16.60	56.32
22H00	662.5	0.00	161.91	57.27	226.77	256.75	103.51	19.85	40.24	58.55	8.80	15.25	47.65
00H00	606.3	0.00	155.16	54.89	217.32	246.05	99.20	19.02	31.25	48.80	8.06	14.24	43.32
02H00	425.0	0.00	141.67	50.11	198.42	224.65	90.57	17.37	29.30	45.32	7.77	13.41	38.99
04H00	275.0	0.00	94.45	33.41	132.28	149.77	60.38	11.58	23.83	34.51	5.18	8.94	23.83
Mean	625.0	0.00	134.92	47.73	188.98	213.96	86.26	16.54	39.07	54.33	7.40	12.77	43.32
FWA	625.0	0.00	147.00	52.00	205.89	233.11	93.98	18.02	43.40	60.03	8.15	14.00	48.00

FWA = Flow Weighted Average

Table 3: Raw WW Characteristics

Components	VFA	FBSO	USO	Settleable BPO	Non-Settleable BPO	Settleable UPO	Non-Settleable UPO	Settleable ISS	Non-Settleable ISS	Total
COD (mgCOD/l)	36.00	110.00	53.00	206.00	233.00	94.00	18.00	0.00	0.00	**750.00**
C (mgC/l)	13.50	36.41	18.18	65.27	75.58	32.88	6.26	0.00	0.00	**248.08**
OrgN (mgN/l)	0.00	1.70	1.83	2.52	12.52	6.35	1.22	0.00	45.00	**71.13**
OrgP (mgP/l)	0.00	1.32	0.00	1.20	1.56	1.59	0.30	0.00	11.46	**17.43**
SS/DS (mgSS/l)	33.74	77.46	37.32	119.77	156.48	63.47	12.16	38.50	9.50	**399.88**

SS = Suspended Solids; DS = Dissolved Solids

Table 4: Settled WW Characteristics

Components	VFA	FBSO	USO	Settleable BPO	Non-Settleable BPO	Settleable UPO	Non-Settleable UPO	Settleable ISS	Non-Settleable ISS	Total
COD (mgCOD/l)	36.00	110.00	53.00	0.00	233.00	0.00	18.00	0.00	0.00	**450.00**
C (mgC/l)	13.50	36.41	18.18	0.00	75.58	0.00	6.26	0.00	0.00	**149.92**
OrgN (mgN/l)	0.00	1.70	1.83	0.00	12.52	0.00	1.22	0.00	45.00	**62.27**
OrgP (mgP/l)	0.00	1.32	0.00	0.00	1.56	0.00	0.30	0.00	11.46	**14.65**
SS/DS (mgSS/l)	33.74	77.46	37.32	0.00	156.48	0.00	12.16	0.00	9.50	**178.14**

Table 5: Primary Sludge Characteristics

Components	VFA	FBSO	USO	Settleable BPO	Non-Settleable BPO	Settleable UPO	Non-Settleable UPO	Settleable ISS	Non-Settleable ISS	Total
COD (mgCOD/l)	36.00	110.00	53.00	41200.00	233.00	18800.00	18.00	0.00	0.00	**60450.00**
C (mgC/l)	13.50	36.41	18.18	13054.65	75.58	6575.56	6.26	0.00	0.00	**19780.13**
OrgN (mgN/l)	0.00	1.70	1.83	503.02	12.52	1269.41	1.22	0.00	45.00	**1834.70**
OrgP (mgP/l)	0.00	1.32	0.00	239.53	1.56	317.35	0.30	0.00	11.46	**571.53**
SS/DS (mgSS/l)	33.74	77.46	37.32	23953.49	156.48	12694.13	12.16	7700.00	9.50	**44525.76**

Table 6: Mass Ratios Used for the Characterization

Mass ratios	VFA	FBSO	USO	Settleable BPO	Non-Settleable BPO	Settleable UPO	Non-Settleable UPO
fcv (mgCOD/mgVSS)	1.067	1.420	1.420	1.500	1.500	1.481	1.481
fc (mgC/mgVSS)	0.400	0.470	0.487	0.510	0.510	0.518	0.518
fn (mgN/mgVSS)	0.000	0.022	0.049	0.019	0.019	0.100	0.100
fp (mgP/mgVSS)	0.000	0.017	0.000	0.010	0.010	0.025	0.025

3.4 Model Development

This section elaborates on the theoretical approach used in developing the discrete particle settling model, which extends on the model developed by Kowlesser (2014). It also proceeds to a step-by-step model description which is, thereafter, summarized.

3.4.1 Theoretical Approach

In the PST of waste resource recovery facilities (WRRFs), particles can be modelled in discrete fashion and assumed to settle in one-dimension (vertically) only. Therefore, the TSS particle settling velocity distribution (PSVD) approach, that Bachis *et al.* (2015) applied to the TSS is, in this research, applied to each of the UPO, BPO and ISS which, together, make up the TSS. It is shown that by assigning different settling velocities to the UPO, BPO and ISS, each divided in settling proportions and grouped into 5 different settling velocity groups, the observed different fractions of UPO, BPO and ISS, removed by PSTs, can be modelled. For these removals to take place, 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 wastewater exiting the PST.

As mentioned above, the influent raw WW TSS concentration is divided into UPO, BPO and ISS fractions, and each of these three components is divided into 5 settling proportions, which are contained in 5 settling velocity groups. These settling velocity groups are assigned decreasing settling velocities, which are used in combination with the influent raw WW TSS from the data set, to develop the discrete particle settling model. In fact, the settling velocities are selected (i) in a descending order, which are representative of velocity patterns that could occur in a settleometer experiment (refer to Section 2.1.1.6) and (ii) in such a way that they allow realistic removals that are in accordance with the maximum PST upflow velocities for PSTs operations at peak wet weather flow (PWWF) and average dry weather flow (ADWF), which are 2.4 m/h and 1.2 m/h, respectively (Ekama, 2018). In assigning a settling velocity to each settling velocity group, the following boundary conditions need to be met:

- The sum of the UPO, BPO and ISS settling proportions, from the respective settling velocity groups, must add up to the total UPO, BPO and ISS fractions that made up the influent raw WW TSS. This boundary condition assumes that the incoming UPO, BPO and ISS, with settling velocity faster than the PST upflow velocity, settle out completely in the PST, and those with settling velocity slower than the PST upflow velocity remain in the settled wastewater, to ensure material mass balance checks.
- Because of the previous boundary condition, the sum of the settling proportions of each of the UPO, BPO and ISS, must add up to 100% at all time steps.

It is worth noting that the number of discrete settling velocity groups is, theoretically, infinite. As such, a higher number of settling velocity groups will generate a higher accuracy in the description and prediction of particle removals by a PST. However, the more settling velocity groups, the greater the number of unknowns to calibrate, i.e. settling velocities and settling proportions. So, the number of these settling velocity groups has been limited to five for flexible model manipulation, and to manage the amount of unknown solvable variables (particle concentrations via the settling proportions), given the number of simultaneous equations, as well as parameters required for calibration (Bachis *et al.,* 2015). In a previous investigation conducted by Maruéjouls *et al.* (2013), three settling velocity groups were used and the outputs were less accurate. Furthermore, for the proposed model development, splitting the UPO, BPO and ISS fractions (from the influent TSS) into settling proportions, that are contained in each settling velocity group, generates already 15 parameters (settling proportions) that would need to be calibrated. This is all worth considering in prospective work, in order to ensure that the model can represent a reasonable level of accuracy, while containing the number of unknowns to be calibrated.

Therefore, the removal of settleable particles in the PST is carried out in the following way: the settling velocity assigned to each settling velocity group is compared to the PST upflow velocity q_i, which is defined as the ratio of the influent flow rate Q_i over the PST surface area (A_{PST}). If the settling velocity assigned to the settling velocity group is, strictly, greater than the PST upflow velocity, all the UPO, BPO and ISS settling proportions in that settling velocity group settle out and are removed. Should the settling velocity be strictly lower than the PST upflow velocity, no removal of the UPO, BPO and ISS settling proportions is achieved in that settling velocity group.

3.4.2 Model Description

From the influent raw WW characteristics, fluxes (F) of the total suspended solids (TSusps), total settleable solids (TSets) and the TSS components (UPO, BPO and ISS) of the raw WW are calculated. The same fluxes are also determined for the settled WW and the PS, as well as the removal percentages (ratios of the settleable or primary sludge over the raw WW) in the PST. Table 7 provides a summary of these results.

Table 7: Raw WW, PS and Settled WW Fluxes Calculations

Fluxes	Raw WW	Settleable (Primary Sludge)	Settled WW	Removal Percentages
TSusps (kgTSS/d)	6244.4	0.0	2641.5	-
TSets (kgTSS/d)	3602.8	3602.8	0.0	100.0%
UPO (kgVSS/d)	1134.4	953.0	181.5	84.0%
BPO (kgVSS/d)	4390.0	2071.7	2318.4	47.2%
ISS (kgISS/d)	720.0	578.2	141.8	80.3%

As mentioned in Section 3.4.1, the model comprises of five discrete settling velocity groups, and a distinct settling velocity (V_{si}) is assigned to each settling velocity group. Thereafter, the raw UPO, BPO and ISS fractions are split in settling proportions (F_{si}) across the five settling velocity groups. The assignment of settling proportions is performed in such a way that their sum, across the five settling velocity groups for each TSS component (UPO, BPO and ISS), is equal to 100%, as shown in Table 8. In this way, material mass balances are conserved in the model.

Table 8: Settling Velocity Groups and Settling Proportions Assignment

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**	**Total**
Settling Velocities (m/h)	V_{s1}	V_{s2}	V_{s3}	V_{s4}	V_{s5}	-
	5.3	3.7	2.1	0.9	0.2	-
Settling Proportions (%)	F_{s1}	F_{s2}	F_{s3}	F_{s4}	F_{s5}	-
UPO	30	25	30	13	2	**100**
BPO	11	40	10	26	13	**100**
ISS	40	20	25	5	10	**100**

The next steps in the model development are to determine the PST upflow velocity and the incremental fluxes of each TSS component ($F_{t/\text{TSS component}}$). First, for every 2h increment (dt) of a total period of 24h (T), a flow rate Q_i (constant flow rate of 625.0 m^3/h for steady state or changing flows for dynamic conditions) is assigned. In this first calculation, the influent flow and concentrations are constant over the 24h period to observe the PST performance under constant flow and load conditions. In a later calculation (see Section 3.6), the flows and concentrations at each 2h time interval will be different, to observe the PST performance under diurnal cyclic flow and load conditions. The PST surface area (A_{PST}) is determined to be the maximum area obtained from both the maximum PST upflow velocities at PWWF and ADWF, as well as knowing that the flow rate at PWWF is 2.5 times greater than the flow rate at ADWF (Ekama, 2018). That surface area is calculated to be 650.0 m^2. As such, the corresponding PST upflow velocity q_i is computed as the ratio of Q_i over A_{PST}, i.e. 625.0/650.0 = 1.0 m/h at constant flow (as shown in Table 9). With regards to the incremental flux per TSS component (TSS component flux for every two hours), it is calculated as the product of Q_i (in m^3/h) and the TSS component concentration (in mg/l) that is extracted from Table 2. For instance, the ISS incremental flux (for steady state calculations) at 06H00 is equal to:

$$F_{t/ISS} = \frac{625.0 * 48}{12} * \frac{24}{1000}$$

$$= 60.0\ kg\ ISS$$

Similarly, the same computation is done for the UPO and BPO incremental fluxes, as shown in Table 9. The mass ratios given in Table 6 are used to convert these fluxes into kgVSS units. The TSets incremental fluxes are computed as the sum of the UPO, BPO and ISS incremental fluxes.

Table 9: Determination of UPO, BPO and ISS Incremental Fluxes in Raw WW (for Steady State Calculations)

Time dt (h)	PST Upflow Velocity Number	PST Upflow Velocity (m/h)	UPO (mgCOD/l)	BPO (mgCOD/l)	ISS (mgISS/l)	UPO Incremental Flux (kgVSS)	BPO Incremental Flux (kgVSS)	ISS Incremental Flux (kgISS)	TSets Incremental Flux (kgTSS)
06H00	1	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
08H00	2	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
10H00	3	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
12H00	4	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
14H00	5	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
16H00	6	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
18H00	7	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
20H00	8	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
22H00	9	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
00H00	10	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
02H00	11	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4
04H00	12	1.0	112.00	439.00	48.00	94.4	365.8	60.0	520.4

The removals are carried out by comparing the PST upflow velocities to the settling velocity assigned to the particles in each settling velocity group, as stated in Section 3.4.1. Therefore, depending on whether the settling velocity of the particles is strictly greater or lower than the upflow velocity in the PST, 100% or 0% of the particles in that settling velocity group are removed. In the case of the first PST upflow velocity, if the percentage of particles removed in the first settling velocity group is equal to 100%, the flux of ISS removed ($F_{r/ISS}$) in that settling velocity group is determined to be the product of the ISS incremental flux, and the corresponding ISS settling proportion (refer to Table 8 for settling velocity groups and settling proportions assignment). It is, therefore, calculated as follow:

$$F_{r/ISS} = F_{t/ISS} * F_{s1/ISS}$$

$$= \ 60 * 40\%$$

$$= \ 24.0\ kgISS$$

The same calculations are performed for the UPO and BPO. Subsequently, removals in terms of chemical oxygen demand (COD), OrgN, OrgP, organic C (OrgC) and VSS can be extracted, using the mass ratios of Table 6. Table 10 provides an example of the removal calculation for the first PST upflow velocity over 2h. Since the flows and concentrations are constant, the removals in terms of incremental fluxes, at subsequent time intervals over the 24h period, are the same as those in Table 9.

Table 10: Removals Calculations for the First PST Upflow Velocity

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**	**Total**
Settling Velocities (m/h)	5.3	3.7	2.1	0.9	0.2	-
Upflow Velocity in PST (m/h)	1.0	1.0	1.0	1.0	1.0	-
Percentage of Particles Removed (%)	100	100	100	0	0	-
UPO Removed (kgVSS)	28.4	23.6	28.4	0.0	0.0	**80.4**
BPO Removed (kgVSS)	40.2	146.3	36.56	0.0	0.0	**223.2**
ISS Removed (kgISS)	24.0	12.0	15.0	0.0	0.0	**51.0**
TSets Removed (kgTSS)	92.6	182.0	80.0	0.0	0.0	**354.5**
COD UPO Removed (kgCOD)	42.0	35.0	42.0	0.0	0.0	**119.0**
COD BPO Removed (kgCOD)	60.4	219.5	54.9	0.0	0.0	**334.7**
COD Removed (kgCOD)	102.4	254.5	96.9	0.0	0.0	**453.7**
OrgC (kgC)	35.2	86.9	33.4	0.0	0.0	**155.4**
OrgN (kgN)	3.6	5.1	3.5	0.0	0.0	**12.3**
OrgP (kgP)	1.1	2.1	1.1	0.0	0.0	**4.2**
VSS (kgVSS)	68.6	170.0	64.9	0.0	0.0	**303.5**

It is worth mentioning that the dissolved constituents are not modelled in these calculations. They pass through and are removed in the PST and, at the same time, exit via the settled WW.

As such, this same procedure is applied for the other 11 PST upflow velocities. Therefore, these removals per PST upflow velocity are added to make up the total fluxes of removals over the day and compute the corresponding removal percentages.

3.4.3 Summarized Modelling Procedure

The model description above can be summarized in the following procedure:

1. Characterize the influent wastewater into its different constituents
2. Select a number of settling velocity groups and assign distinct settling velocities, as well as settling proportions of the UPO, BPO and ISS fractions, such that material mass balances are maintained
3. Calculate the incremental fluxes for these TSS components (UPO, BPO and ISS)
4. For every PST upflow velocity, compare the settling velocity assigned to each settling velocity group against that PST upflow velocity, and determine the percentage of particles removed in that settling velocity group to either be (i) 0% if the settling velocity is less than the PST upflow velocity, or (ii) 100% if the settling velocity is greater than the PST upflow velocity
5. Calculate the flux of TSS component removed to either be (i) 0 if the percentage of particles removed is 0%, or (ii) the product of the settling proportion and the TSS component incremental flux, if the percentage of particles removed is 100%
6. Add the removals of each PST upflow velocity to compute the percentage removals over the 24h period.

3.5 Steady State Flow Modelling

3.5.1 Removals Performance

To allow the removal patterns in terms of UPO, BPO and ISS, to begin to resemble reality, as experimentally observed by Wentzel *et al.* (2006) and Ikumi *et al.* (2014), constant flow and load (steady state) calculations were performed using the discrete particle settling model (described in Section 3.4) in an Excel spreadsheet. After choosing settling velocities, the settling proportions of each of these TSS components were selected by trial and error, such that the expected primary sludge removals, as fractionated from the influent characterization described in Section 3.3, were obtained.

To match the given primary sludge data set with the outputs obtained from the model, an initial set of settling proportions was applied to the UPO, BPO and ISS into the five settling velocity groups and varied. With each selection of a settling proportion, different removals of UPO, BPO or ISS are obtained. By sequentially varying the five settling proportions assigned to a selected TSS component (UPO, BPO or ISS), across the five settling velocity groups, the removal percentages obtained can be checked. The validity of the boundary conditions described in Section 3.4.1 was maintained by ensuring that each of the settling proportions, selected for the UPO fraction, added to 100% and, similarly, for the BPO and ISS. The settling velocities selected as input to the model and the matrix of settling proportions that could fit the data, a sample calculation of the removals for the first PST upflow velocity, as well as the summary of the calculated removals over 24h, are presented in Table 11 and Table 12. Table 13 and Figure 6 compare the overall UPO, BPO and ISS removals obtained from the model with the removals embedded in the raw and settled wastewater data set.

Table 11: Matching Settling Velocities and Settling Proportions

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Settling Velocities (m/h)	5.3	3.7	2.1	0.9	0.2
Settling Proportions (%)	F_{s1}	F_{s2}	F_{s3}	F_{s4}	F_{s5}
UPO	47	20	17	12	4
BPO	12	15	20	25	28
ISS	37	25	18	15	5

Table 12: Removals Calculations for the First PST Upflow Velocity of the Matching Settling Proportions Set

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**	**Total**
Settling Velocities (m/h)	5.3	3.7	2.1	0.9	0.2	-
Upflow Velocity in PST (m/h)	1.0	1.0	1.0	1.0	1.0	-
Percentage of Particles Removed (%)	100	100	100	0	0	-
UPO Removed (kgVSS)	44.4	18.9	16.1	0.0	0.0	**79.4**
BPO Removed (kgVSS)	43.9	54.9	73.2	0.0	0.0	**171.9**
ISS Removed (kgISS)	22.4	15.0	10.8	0.0	0.0	**48.2**
TSets Removed (kgTSS)	110.7	88.8	100.0	0.0	0.0	**299.5**
COD UPO Removed (kgCOD)	65.8	28.0	23.8	0.0	0.0	**117.6**
COD BPO Removed (kgCOD)	65.9	82.3	109.8	0.0	0.0	**257.9**
COD Removed (kgCOD)	131.7	110.3	133.6	0.0	0.0	**375.5**
OrgC (kgC)	45.4	37.8	45.6	0.0	0.0	**128.8**
OrgN (kgN)	5.3	2.9	3.0	0.0	0.0	**11.2**
OrgP (kgP)	1.6	1.0	1.1	0.0	0.0	**3.7**
VSS (kgVSS)	88.3	73.8	89.2	0.0	0.0	**251.4**

Table 13: Summary of Steady State Calculated Results vs Data Set Removals for the Primary Sludge

Components	Calculated Removals	Removals from WRC (1984) and Ekama (2017)	Percentage Difference
UPO	84.0%	84.0%	0.0%
BPO	47.0%	47.2%	0.4%
ISS	80.3%	80.3%	0.0%
VSS	54.6%	54.8%	0.4%
TSets	57.6%	57.7%	0.2%
COD	40.1%	40.3%	0.5%
OrgC	40.2%	40.4%	0.5%
OrgN	14.5%	15.0%	3.3%
OrgP	16.8%	17.2%	2.3%

It can be seen from Table 13 that the maximum percentage difference between the literature value and the calculated value is 3.3%. This means that the spreadsheet model could predict the removal percentages in the primary sludge of the PST, with good confidence. This is further displayed in Figure 6.

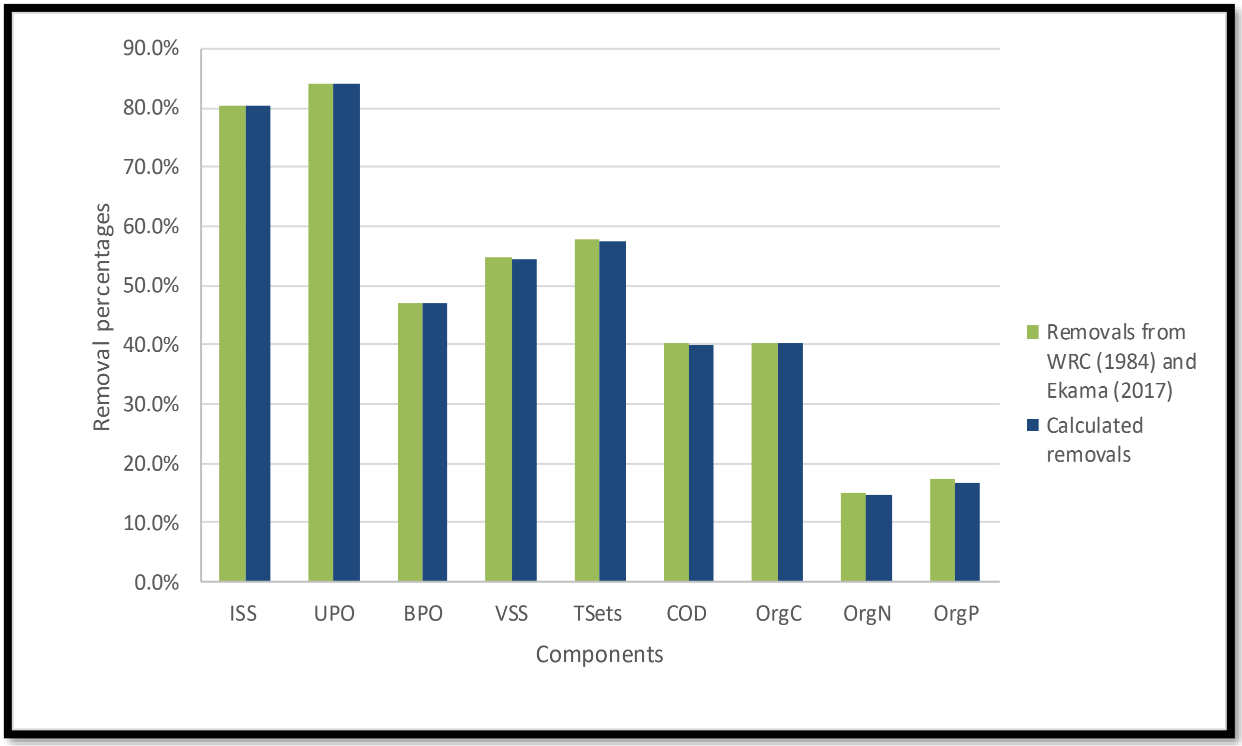


Figure 6: Removals from the Data Set vs Calculated Removals

The minor discrepancies between the WRC (1984) data and the calculated removals are due to the fact that the discrete settling model does not account for the PST underflow and the dissolved constituents in the calculations, which are factored in the WW characteristics used (WRC, 1984; Ekama, 2009, 2011; Ekama, 2017). Furthermore, since particles can either be removed (100%) or not (0%) with the number of settling velocity groups and settling velocities used (discretization), the calculated removals cannot be exact.

3.5.2 Settling Proportions

Knowing that the settling proportions had to be varied to obtain the results above, it was observed, after a few trials, that the calculated removal percentages were converging to the expected primary sludge data, when the settling proportions across the five settling velocity groups were varied in a descending order for the UPO and ISS and, interestingly, in an ascending order for the BPO. These observations were confirmed with the set of settling proportions (refer to Table 11) that matched the calculated results, as displayed in Figure 7.

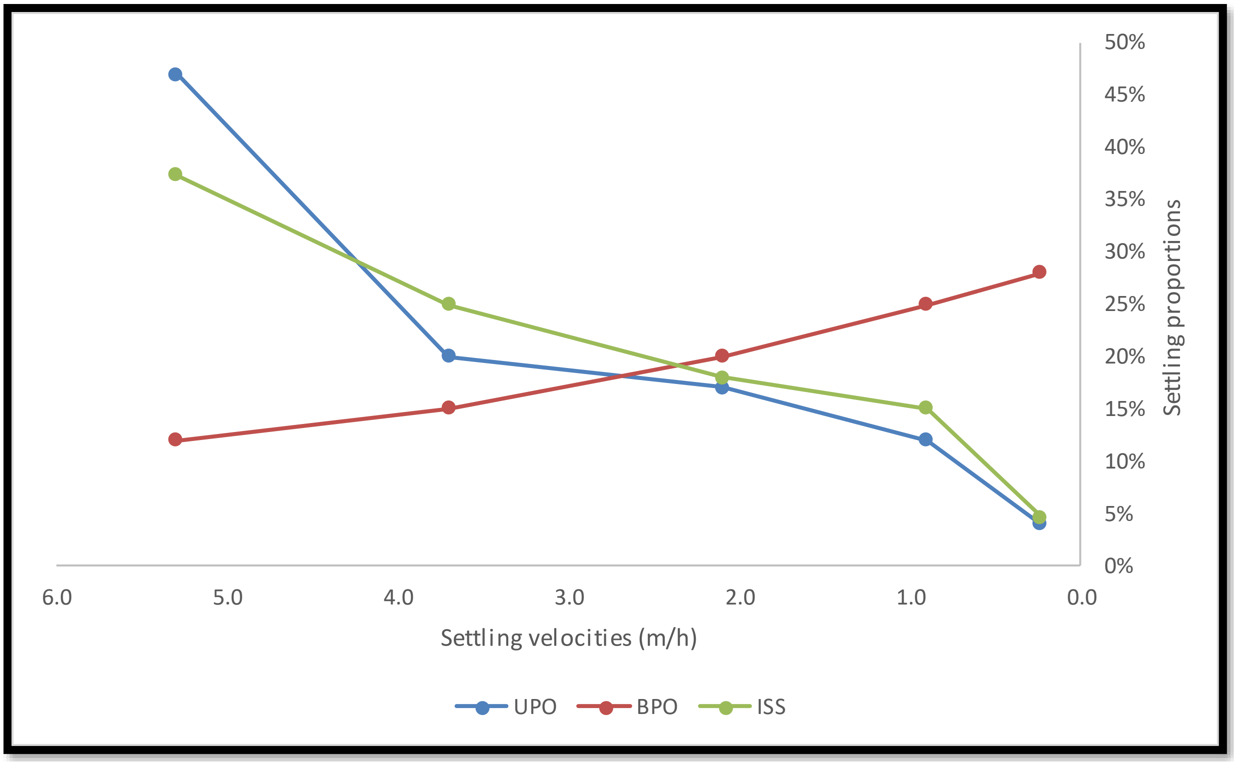


Figure 7: Settling Velocities vs Corresponding Settling Proportions Distribution

Therefore, under steady state conditions, the discrete particle settling model confirms that the UPO and ISS are removed in higher fractions than the BPO. In fact, the UPO and ISS are removed in high proportions (because of the larger settling proportions) in the fastest settling velocity groups and decrease towards the slowest settling velocity groups. On the other hand, the BPO are removed in low proportions in the fastest settling velocity groups and gradually increase towards the slowest settling velocity groups. However, it is worth noting that this graph represents a theoretical expectation of the distribution of the settling velocities and the proportions of particles settling or not settling. A calibration of these settling velocities and proportions of particles settling, using the settleometer, will be presented in subsequent investigation which is falling outside of the scope of this current model development.

3.5.3 Impact of the PST Surface Area on Removals

The impact of the PST surface area on the removals was further analyzed in these calculations. The settling velocities and settling proportions, obtained in Section 3.5.1, remained unchanged. If the flow rate is kept constant, the PST upflow velocity is indirectly proportional to the surface area. Therefore, as the surface area increases, the PST upflow velocity will decrease and vice versa. This means that if the settling velocities of the particles are compared against the varying PST upflow velocity, different removal percentages will be achieved.

Six different PST surface areas were selected (including the initial PST surface area used for the calculations above) and the PST upflow velocities were computed. The removal percentages of UPO, BPO, ISS, as well as TSS were, thereafter, calculated and the results are presented in Table 14 and Figure 8.

Table 14: Removal Percentages Calculations with PST Area Variation

Area (m^2)	100.0	150.0	250.0	650.0	1000.0	3000.0
Area Number	1	2	3	4	5	6
Flow Rate (m^3/h)	625.0	625.0	625.0	625.0	625.0	625.0
PST Upflow Velocity (m/h)	6.3	4.2	2.5	1.0	0.6	0.2
UPO Removed	0.0%	47.0%	67.0%	84.0%	96.0%	100.0%
BPO Removed	0.0%	12.0%	27.0%	47.0%	72.0%	100.0%
ISS Removed	0.0%	37.3%	62.3%	80.3%	95.3%	100.0%
TSS Removed	0.0%	21.3%	38.3%	57.6%	79.0%	100.0%

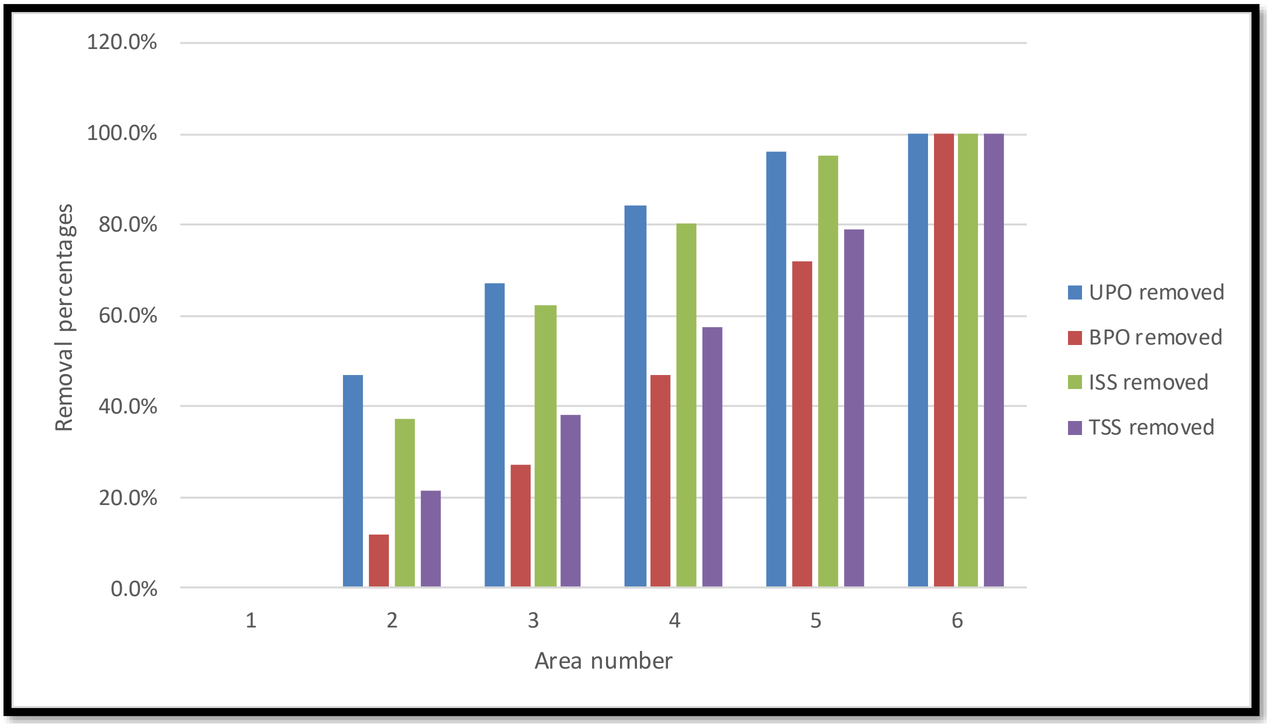


Figure 8: Variations of the Removal Percentages against the PST Surface Area

It can be seen that there is, initially, no removals when the area is reduced to 100.0 m^2. This is because the PST upflow velocity is so high (6.3 m/h) that no particles can settle. Therefore, as the PST surface area increases, the PST upflow velocity decreases. This means that more particles settle out in the different settling velocity groups, if their settling velocities are higher than the PST upflow velocity. At 3000.0 m^2, the PST upflow velocity is so low that all the particles in the settling velocity groups settle out completely. Hence 100.0% of removal percentages are achieved. This analysis further confirms that the calculation outputs generated by the discrete particle settling model are consistent and verified.

3.6 Dynamic Flow Modelling

After successfully performing steady state calculations, the discrete settling model was extended to mimic dynamic calculations where flows and loads change. The settling processes configuration, used to develop the model in Section 3.4, remained unchanged. Furthermore, the settling velocities and matching set of settling proportions of UPO, BPO and ISS obtained in Section 3.5 (refer to Table 11) were used as inputs to these dynamic calculations.

3.6.1 Key Modelling Aspects

The only modification to the dynamic calculations is the input of diurnal flows and concentrations extracted from WRC (1984), Ekama (2009, 2011) as well as Ekama (2017) and summarized in Table 2. These diurnal data replaced the constant flow and load used for steady state calculations.

The determination of the TSS components incremental fluxes was performed exactly as described in Section 3.4.2, except now the flow and concentration changed diurnally, and so was different at each 2h. This determination is summarized in Table 15.

Table 15: Determination of UPO, BPO and ISS Incremental Fluxes in Raw WW (for Dynamic Calculations)

Time dt (h)	PST Upflow Velocity Number	PST Upflow Velocity (m/h)	UPO (mgCOD/l)	BPO (mgCOD/l)	ISS (mgISS/l)	UPO Incremental Flux (kgVSS)	BPO Incremental Flux (kgVSS)	ISS Incremental Flux (kgISS)	TSets Incremental Flux (kgTSS)
06H00	1	0.4	43.18	169.23	15.16	13.1	50.8	6.8	70.7
08H00	2	0.5	43.69	171.25	24.91	18.6	72.1	15.7	106.4
10H00	3	1.4	82.24	322.35	34.66	104.1	402.9	65.0	572.0
12H00	4	1.7	113.08	443.23	51.99	164.2	635.3	111.8	911.2
14H00	5	1.4	127.47	499.64	56.32	156.0	603.7	102.1	861.8
16H00	6	1.1	130.55	511.72	60.65	128.9	498.9	88.7	716.6
18H00	7	1.0	143.92	564.10	64.98	123.9	479.5	82.9	686.2
20H00	8	1.1	133.64	523.81	56.32	130.8	506.4	81.7	718.7
22H00	9	1.0	123.36	483.52	47.65	110.4	427.1	63.1	600.6
00H00	10	0.9	118.22	463.37	43.32	96.8	374.7	52.5	523.9
02H00	11	0.7	107.94	423.08	38.99	62.0	239.7	33.1	334.8
04H00	12	0.4	71.96	282.05	23.83	26.7	103.4	13.1	143.3

Thereafter, using the same settling proportions and velocities from the steady state calculations as initial inputs (refer to Table 11), the removals were calculated for each PST upflow velocity and added altogether to determine the removals over the 24h period. A sample calculation of the removals for the first PST upflow velocity is presented in Table 16.

Table 16: Sample Dynamic Calculation of the Removals for the First PST Upflow Velocity

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**	**Total**
Settling Velocities (m/h)	5.3	3.7	2.1	0.9	0.2	**-**
Upflow Velocity in PST (m/h)	0.4	0.4	0.4	0.4	0.4	**-**
Percentage of Particles Removed (%)	100	100	100	100	0	**-**
UPO Removed (kgVSS)	6.1	2.6	2.2	1.6	0.0	**12.6**
BPO Removed (kgVSS)	6.1	7.6	10.2	12.7	0.0	**36.6**
ISS Removed (kgISS)	2.6	1.7	1.2	1.0	0.0	**6.5**
TSets Removed (kgTSS)	14.8	11.9	13.6	15.3	0.0	**55.7**
COD UPO Removed (kgCOD)	9.1	3.9	3.3	2.3	0.0	**18.7**
COD BPO Removed (kgCOD)	9.1	11.4	15.2	19.0	0.0	**54.8**
COD Removed (kgCOD)	18.3	15.3	18.5	21.4	0.0	**73.5**
OrgC (kgC)	6.3	5.2	6.3	7.3	0.0	**25.2**
OrgN (kgN)	0.7	0.4	0.4	0.4	0.0	**2.0**
OrgP (kgP)	0.2	0.1	0.2	0.2	0.0	**0.7**
VSS (kgVSS)	12.3	10.2	12.4	14.3	0.0	**49.2**

3.6.2 Dynamic Results

The results generated by the dynamic calculations and using the steady state set of settling proportions as inputs, were close to the expected removals of the WW characteristics used. These results are presented in Table 17. The maximum percentage difference for this initial calculation, between the literature value and the calculated value is estimated to be 5.3%.

Table 17: Initial Summary of Dynamic Calculated Results vs Data Set Removals for the Primary Sludge

Components	Calculated Removals	Removals from WRC (1984) and Ekama (2017)	Percentage Difference
UPO	85.4%	84.0%	1.7%
BPO	49.7%	47.2%	5.3%
ISS	81.4%	80.3%	1.4%
VSS	57.0%	54.8%	4.0%
TSets	59.8%	57.7%	3.6%
COD	41.8%	40.3%	3.7%
OrgC	42.0%	40.4%	4.0%
OrgN	15.0%	15.0%	0.0%
OrgP	17.4%	17.2%	1.2%

Likewise, for the steady state calculations, the settling proportions of the UPO, BPO and ISS were varied to match the removals observed in the WW characteristics. The set of settling proportions that could best fit these dynamic calculations, as well as the final summary of results, are presented in Table 18 and Table 19.

Table 18: Matching Settling Proportions for Dynamic Calculations and Comparison with Steady State Calculations

Settling Velocity Groups	1	2	3	4	5
Settling Proportions (%)	F_{s1}	F_{s2}	F_{s3}	F_{s4}	F_{s5}
Dynamic Proportions					
UPO	46	19	18	9	8
BPO	11	14	20	20	35
ISS	34	25	20	18	3
Steady State Proportions					
UPO	47	20	17	12	4
BPO	12	15	20	25	28
ISS	37	25	18	15	5

Table 19: Final Summary of Dynamic Calculated Results vs Data Set Removals for the Primary Sludge

Components	Calculated Removals	Removals from WRC (1984) and Ekama (2017)	Percentage Difference
UPO	84.0%	84.0%	0.0%
BPO	47.2%	47.2%	0.0%
ISS	80.3%	80.3%	0.0%
VSS	54.7%	54.8%	0.2%
TSets	57.7%	57.7%	0.0%
COD	40.2%	40.3%	0.3%
OrgC	40.3%	40.4%	0.3%
OrgN	14.6%	15.0%	2.7%
OrgP	16.9%	17.2%	1.7%

It can be seen from Table 19 that the maximum percentage difference between the literature value and the calculated value is 2.7%. These results confirm that the discrete settling model can also generate dynamic calculations, with good confidence. Therefore, under diurnal flow and load, the ISS and UPO are also removed in higher fractions than the BPO, as observed by Wentzel *et al.* (2006) and Ikumi *et al.* (2014). It can also be seen that the trends in the settling proportions of the UPO, BPO, and ISS, which were observed in generating the steady state calculations, are almost the same for the dynamic calculations.

3.7 Closure

This chapter has presented the development of a discrete particle settling model in Microsoft Excel. The purpose of this model was to mimic observed percentages of UPO, BPO and ISS removals in the primary sludge, using raw wastewater and settled wastewater characteristics extracted from WRC (1984) and Ekama (2017).

The particle settling velocity distribution (PSVD) concept of Bachis *et al.* (2015) was adapted to this discrete settling model, which is an extension of the discrete settling model developed by Kowlesser (2014). The theoretical concept of the model was extensively described, and a full model description was presented. Five settling velocity groups were used to divide the influent raw TSS and carry out the PST settleable solids removals. Each TSS fraction contained in a distinct settling velocity group was made of UPO, BPO and ISS components, which were further split in settling proportions. From the first to the fifth settling velocity group, settling velocities were assigned in a descending order to mimic velocity patterns in a settleometer.

Influent wastewater characteristics from WRC (1984), Ekama (2009, 2011) and Ekama (2017) were used in performing calculations with the discrete particle settling model, both under steady state and dynamic conditions. It was found that to match the modelling predictions with the given data set at steady state, the UPO and ISS were removed in greater proportions from the fastest settling velocity groups and decreased towards the slowest settling velocity groups, whereas the BPO were removed in low proportions in the fastest settling velocity groups and gradually increased towards the slowest settling velocity groups. These steady state results showed that UPO and ISS are removed in high fractions in a PST, and BPO are removed in low fractions, as observed by Wentzel *et al.* (2006) and Ikumi *et al.* (2014) to obtain measured primary sludge characteristics. The analysis was, thereafter, expanded to investigate the impact of varying the PST surface area on the removal percentages. It was found, as expected, that the removal percentages of UPO, BPO, ISS, as well as TSS, increased as the surface area increased and the PST upflow velocity decreased and vice versa.

The model was further extended to mimic dynamic flow and load conditions, by inputting changing flows and loads extracted from the same data set used for steady state calculations. The same trends observed in the steady state calculations, with respect to the settling proportions, were found in the dynamic calculations. As a result, the discrete particle settling model can be implemented in a PST framework, to develop a realistic PST model and investigate if removal patterns can be mimicked in a similar fashion.

4. UCTPSU Model Implementation

4.1. Introduction

The discrete particle settling model, developed in Chapter 3, has demonstrated its capability of reproducing primary settling tank (PST) removal patterns in terms of unbiodegradable particulate organics (UPO), biodegradable particulate organics (BPO) and inorganic settleable solids (ISS) to produce primary sludge characteristics that resemble reality, as observed by Wentzel *et al*. (2006) and Ikumi *et al*. (2014). The proposed discrete settling approach, therefore, will be implemented in a PST unit which can simulate steady state and dynamic conditions, and is presented in this chapter. It is worth noting that dynamic simulations provide direct links between wastewater characteristics, that are entered as inputs, and simulated treated effluents which are outputs, by means of ordinary and partial differential equations. It aims at replicating reactions and processes in the modelled process unit operations. Therefore, dynamic simulations assist in predicting the performance of wastewater treatment plants in terms of effluent quality and product recycling effects. It further helps in evaluating the responses of the system when subjected to dynamic conditions (which include control strategies implementation, load variations, as well as optimizing design and operations), with the aim of complying to effluent standards while saving on costs (Ikumi *et al.*, 2014). As such, the PST unit, in which the discrete particle settling approach developed in Chapter 3 is implemented, is referred to as the University of Cape Town Primary Separation Unit (UCTPSU). The UCTPSU is developed in PWM_SA (Ikumi *et al.*, 2014) which is within WEST® (Vanhooren *et al.,* 2003) wastewater modelling software and simulation platform (MikeByDHI, 2016). This UCTPSU model is based on the work of Bachis *et al.* (2015), which considered total suspended solids (TSS) only. This section first reports on the modelling approach of Bachis *et al.* (2015), then elaborates on the modifications implemented to that configuration, towards developing the UCTPSU model to account for a much more realistic fractionation of the primary sludge.

4.2. The Modelling Approach of Bachis *et al.* (2015)

The particle settling velocity distribution (PSVD) model of Bachis *et al.* (2015) has been briefly described and critically evaluated in Chapter 2. In this section, the model is thoroughly elaborated, since it serves as a platform to include the discrete particle settling approach, to account for the TSS fractionation in terms of UPO, BPO and ISS. The PSVD model is based on a settling velocity distribution that is covered by five settling velocity groups representing the TSS. The settling velocities of the particles are experimentally determined through the ViCAs protocol (Chebbo & Gromaire, 2009) and assigned to the different settling velocity groups. Each settling velocity group is further assigned a fraction of the influent TSS. The fractions are determined from observing the relationship between the PSVD curves extracted from the ViCAs experiments and the TSS concentrations. As a result, a vertical gradient of the concentrations of each of these particle groups can be predicted by dividing the settler model into several layers and performing a particle mass balance around each layer.

4.2.1 Settling Processes Description

The settling processes, defined by the PSVD model approach of Bachis *et al.* (2015), are based on the settling configuration described in the settler model of Takacs *et al.* (1991) which is similar to that of secondary settling tanks (SST). The settler (of area A and height H) is divided in 10 layers of equal thickness (where V_L and H_L are respectively the volume and the height of the layer) and a particle flux analysis is applied, by considering the downwards particle (or solid) flux that continuously flows through the layers. A minimum sludge blanket concentration (X_{MIN}) is defined, as well as a maximum threshold concentration (X_{LIM}). which is established to regulate that downwards flux that can be sustained by the layer below the layer of interest.

The downwards flux is defined as the sum of the bulk liquid flux and the gravity settling flux. The bulk liquid flux (J_{UP}/J_{DN}) is due to the movement of the liquid in the settler and can either be upwards or downwards, depending on the position of the layer of interest with regards to the feed layer. It is, therefore, defined as the product of the particles concentration of the ith layer (C_I) and the liquid bulk velocity (V_{UP}/V_{DN}), from the equations:

$$J_{UP} = C_I \text{ x } V_{UP}$$

$$J_{DN} = C_I \text{ x } V_{DN}$$

The gravity settling flux (J_G), which is due to the particles settling under the gravity force, is expressed as the product of the concentration of the particles in the ith layer (C_I) and the settling velocity of the particles (V_S- these velocities extracted from the ViCAs experiments), from the equation:

$$J_G = C_I \text{ x } V_S$$

According to the particle flux analysis, the gravity settling flux can be expressed under the following constraints:

- From the 1st to the 4th layer: If $C_I < X_{LIM}$, $J_G = C_I \text{ x } V_S$. But if $C_I > X_{LIM}$, $J_G = \min(J_{Gi}, J_{Gi-1})$
- From the 5th layer (feed layer) to the 9th layer, $J_G = \min(J_{Gi}, J_{Gi-1})$

These conditions show that J_G depends on the particle concentration of the layer below the layer of interest. As such, to perform a particle mass balance around each layer, it is important to understand (i) the relationships established among layers, and (ii) how particles enter and exit these layers. First, the layers are categorized into five groups, namely the top layer, the layers above the feed layer, the feed layer, the layers below the feed layer and the bottom layer. Figure 9 depicts the layered settler configuration.

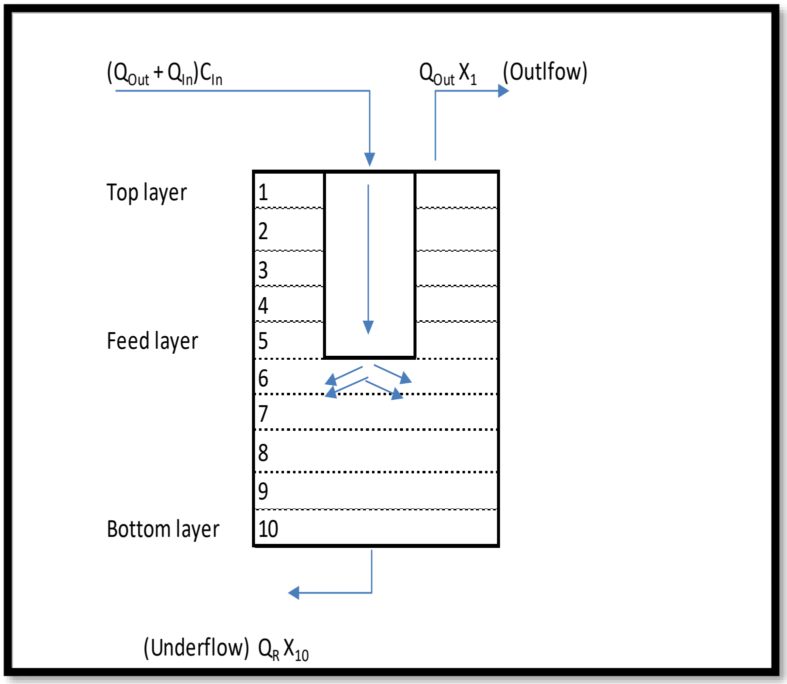


Figure 9: Layered Settler Model, Adapted from Takacs et al. (1991)

From this configuration, the settler receives the influent flow at the 5th layer, from which it is then passed through all the other layers. Takacs *et al.* (1991) state two main assumptions, which are as follow:

- The incoming particle flux distribution is instantaneous and uniform across the whole cross-sectional area of the layers
- The vertical flow is the only flow considered.

Particles, therefore, move through layers in a dynamic fashion and these movements are summarized in Table 20.

Table 20: Particles Movement Summary across the Layered Model and Adapted from Takacs et al. (1991)

	Before Settling (Input)			**After Settling (Output)**	
Layer	**Feed**	**Settling**	**Bulk Liquid Flux**	**Settling**	**Bulk Liquid Flux**
Top layer	Not considered	Not considered	Upwards	Considered	Upwards
Layers above feed layer	Not considered	Considered	Upwards	Considered	Upwards
Feed layer	Considered	Considered	-	Considered	Upwards – downwards
Layers below feed layer	Not considered	Considered	Downwards	Considered	Downwards
Bottom layer	Not considered	Considered	Downwards	Not considered	Downwards

4.2.2 Mass Balances

Based on these definitions above, as well as fluxes considered, particle mass balances are performed around each layer within the settler. It is important to note that mass balances are achieved when the particles concentration per layer is constant. This will be further illustrated through simulations, in the model evaluation chapter (refer to Section 5). Figure 10, Figure 11, Figure 12 and Figure 13 depict examples of mathematical modelling of particle mass balances that are presented for the 5th layer (feed layer) and 6th layer.

- For the 5th layer

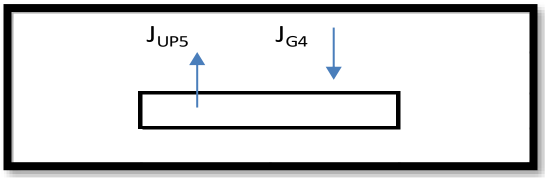


Figure 10: Input in Layer 5

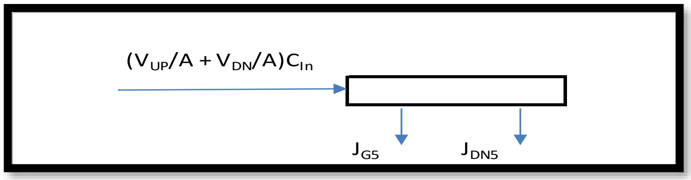


Figure 11: Output from Layer 5

Input: $J_{UP5} - J_{G4}$

Output: $- J_{G5} - J_{DN5} + (V_{UP}/A + V_{DN}/A) \times C_{In}$

Since the input must be equal to the output, it yields to:

$-J_{G5} – J_{DN5} + (V_{UP}/A + V_{DN}/A) \times C_{In} = J_{UP5} – J_{G4}$

But $(V_{UP}/A + V_{DN}/A) \times C_{In} = (Q_{Out} + Q_R) \times C_{In} = Q_{In} \times C_{In} = F_{In}$, where F_{In} is the influent flux of particles.

So $(-J_{G5} – J_{DN5} + F_{In} - J_{UP5} – J_{G4}) = 0$

Which leads to $dC_I/dt = 0$

And, subsequently, $(1/H_L) \times (-J_{G5} – J_{DN5}) + ((1/V_L) \times F_{In}) = 0$

- For the 6th layer

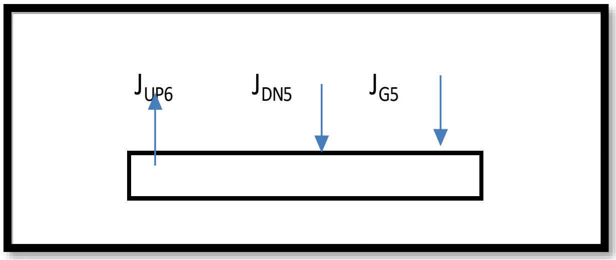


Figure 12: Input in Layer 6

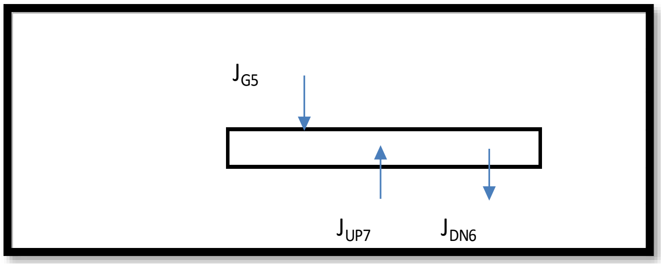


Figure 13: Output from Layer 6

Input: $J_{UP6} – J_{DN5} – J_{G5}$

Output: $J_{UP7} – J_{G6} – J_{DN6}$

Since the input must be equal to the output, it yields to:

$J_{UP7} – J_{G6} – J_{DN6} - J_{UP6} + J_{DN5} + J_{G5} = 0$

Which leads to $dC_I/dt = 0$

And, subsequently, $(1/H_L) \times (J_{UP7} – J_{G6} – J_{DN6} - J_{UP6} + J_{DN5} + J_{G5}) = 0$

A summary of the particle mass balances through the layers of the settler is depicted in Figure 14.

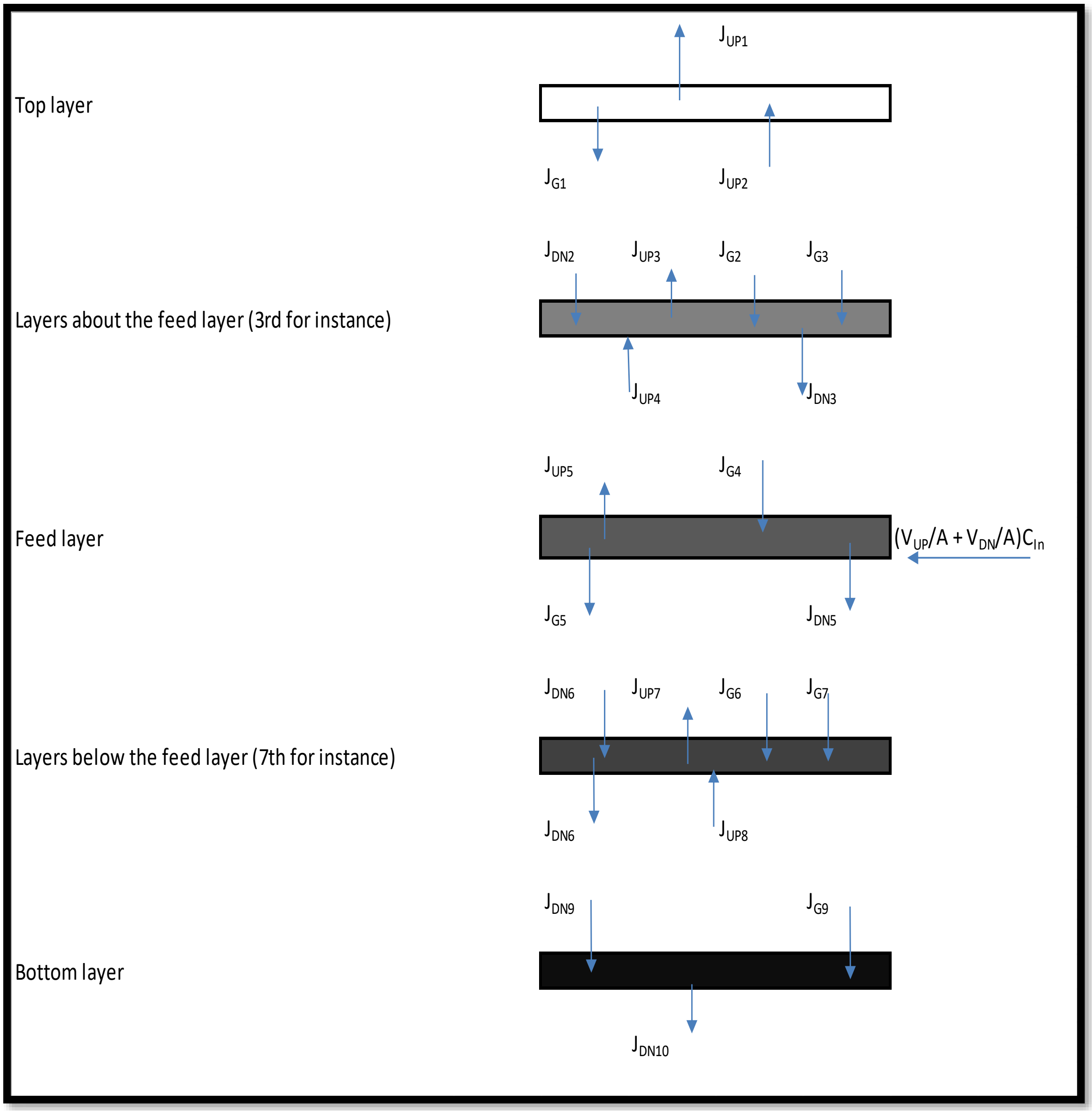


Figure 14: Particles Balance throughout all the Layers and Adapted from Takacs et al. (1991)

4.3. The UCTPSU Model

The University of Cape Town Primary Separation Unit (UCTPSU) model has been developed using the same settling processes and particle mass balances described in Section 4.2. It is, however, modified to include the UPO, BPO as well as ISS, with the aim of generating a better fractionation of the TSS between primary sludge removed and settled wastewater characteristics entering the activated sludge unit processes.

4.3.1 Modification implemented in the UCTPSU Model

The key modification in the UCTPSU model consists of disaggregating the TSS into three sub-components that are UPO, BPO and ISS, as performed in the discrete particle settling model. This is particularly facilitated in the PWM_SA model components interface, since the UPO, BPO and ISS are defined as individual components, which can be experimentally measured (refer to Section 1.2). Each of these components is split in five settling velocity groups, to which settling velocities are assigned. The settling velocities, from the discrete settling particle model, are used as initial parameters in this model. Furthermore, the settling proportions of UPO, BPO and ISS, that were established from the steady state and dynamic calculations within the discrete settling particle model, are also used as initial settling proportions.

4.3.2 Coding Configuration

The UCTPSU model forms part of the larger integrated PWM_SA model within the simulation platform WEST®, and, therefore, shares the same model components for compatibility, and to track these components throughout the system (i.e., the supermodel approach of Jones & Takács, 2004 and Volcke *et al.* (2006) is used). The PWM_SA universal set of components is presented in Table 21, with the components of interest highlighted (X_U_Inf, X_B_Inf, and X_ISS) and discussed further down.

Table 21: PWM_SA Model Components

Notation	Definition
H2O	Water
S_H	Hydrogen ion
S_Na	Sodium
S_K	Potassium
S_Ca	Calcium
S_Mg	Magnesium
S_NH	Ammonium
S_Cl	Chloride
S_VFA	Acetate
S_Pr	Propionate
S_CO3	Carbonate
S_SO4	Sulphate
S_PO4	Phosphate

S_H2	Dissolved hydrogen
S_CH4	Dissolved methane
S_U	Unbiodegradable soluble organics
S_F	Fermentable biodegradable soluble organics
S_Glu	Glucose
S_NOx	Nitrate
X_U_Inf	**Unbiodegradable particulate organics (UPO)**
X_B_Org	Biodegradable particulate organics
X_PAO_PP	Polyphosphate
X_PAO_Stor	Poly-hydroxy-alkanoate
X_Glygogen	Glycogen
X_Str_NH4	Struvite
X_ACP	Calcium phosphate
X_Str_K	K-struvite
X_Cal	Calcite
X_Mag	Magnesite
X_Newb	Newberyite
X_OHO	Ordinary heterotrophic organisms
X_PAO	Phosphate accumulating organisms
X_AD	Acidogens
X_AC	Acetogens
X_AM	Acetoclastic methanogens
X_HM	Hydrogenotrophic methanogens
X_U_Org	Endogenous residue
X_B_Inf	**Primary sludge biodegradable particulate organics** (**BPO**)
X_ANO	Autotrophic nitrifying organisms
X_ISS	**Influent inorganic settleable solids (ISS)**
G_CH4	Methane
G_CO2	Carbon dioxide
G_N2	Nitrogen

A set of vectors and matrixes applied on components and layers have also been defined to translate the particle flux theory used for the settling processes. Component vectors include specific volume (which is used in WEST® to model the volumetric mass), velocity, mass, mass flux and concentration. Concentration, areal flux, mass and mass flux matrixes of components and layers, are also defined.

A set of new components is added to fractionate the ISS, UPO and BPO in different sub-components and, hence, assign settling proportions. Therefore, each of the components X_U_Inf (UPO) , X_B_Inf (BPO) and X_ISS (ISS), which make up the TSS, is sub-divided into five sub-components, with each set of {ISS, UPO, BPO} sub-components representing a settling velocity group, as shown in Table 22.

Table 22: TSS Sub-Components with Respective Settling Velocity Groups

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
TSS components	**TSS Sub-Components**				
X_ISS	X_ISS1	X_ISS2	X_ISS3	X_ISS4	X_ISS5
X_U_Inf	X_U_Inf1	X_U_Inf2	X_U_Inf3	X_U_Inf4	X_U_Inf5
X_B_Inf	X_B_Inf1	X_B_Inf2	X_B_Inf3	X_B_Inf4	X_B_Inf5

Thereafter, a set of settling proportions which were extracted from the discrete particle settling model, is inputted as parameters, as displayed in Table 23. However, the settling proportions of the fifth settling group are defined as variables and expressed in terms of the first four settling groups, to facilitate the data calibration process.

Table 23: Set of Settling Proportions Used as Parameters

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
TSS components	**Settling Proportions Set as Parameters**				
X_ISS	Alpha_I	Beta_I	Gamma_I	Lambda_I	Theta_I
X_U_Inf	Alpha_U	Beta_U	Gamma_U	Lambda_U	Theta_U
X_B_Inf	Alpha_B	Beta_B	Gamma_B	Lambda_B	Theta_B

As a result, the fluxes and concentrations of these sub-components are defined in terms of the settling proportions and initial fluxes and concentrations of the incoming UPO, BPO and ISS fluxes and concentrations.

4.4. Closure

The implementation of the discrete particle settling model towards developing the University of Cape Town Primary Sedimentation Unit (UCTPSU) model, in PWM_SA which is within WEST®, has been elaborated in this chapter. The modelling approach of Bachis *et al.* (2015) was thoroughly described since it served as a platform to include the modifications that allow the UCTPSU model to propose a realistic fractionation of the TSS in UPO, BPO and ISS. The settling processes, which were based on the settler model of Takacs *et al.* (1991), have been extensively described. The settler was divided in 10 layers and a particle mass balance was performed around each layer.

The modifications added to this model to develop the UCTPSU model were then discussed, in terms of the TSS fractionation in components of UPO, BPO and ISS. Each of these components was further sub-divided into five sub-components with respective settling proportions, to create five settling velocity groups. This chapter also expanded on the coding configuration of the UCTPSU model. The developed model will, therefore, be evaluated in the next chapter.

5. UCTPSU Model Evaluation

5.1. Introduction

The UCTPSU model, which was developed in Chapter 4, is evaluated in this section. It is worth noting that the proposed evaluation is limited to the verification stage, which includes sanity checks on the model, i.e. does it generate the correct expected results for extreme conditions? e.g. no primary sludge production if all the particles settled extremely slowly. Subsequently, a preliminary model integration is further proposed, with the model being implemented in a plant-wide context, to assess its response under specific conditions and demonstrate its application and impact towards downstream unit processes.

5.2. Model Verification

Verification is important because it confirms that the model is internally consistent with all element masses of input components (i.e., COD, C, H, O, N, and P) accounted for, in a scientifically sound way. In this case, the verification consisted of checking the internal consistency with regards to the relevant UCTPSU model components, which are the unbiodegradable particulate organics (UPO), biodegradable particulate organics (BPO) and inorganic settleable solids (ISS), that make up the total suspended solids (TSS). This multiple-steps procedure was performed under steady state conditions and with respect to two scenarios: (i) checking for material mass balances over the UCTPSU model and particle mass balances around the layers that make up the model description, and (ii) checking, with specific loading conditions applied to the model, by varying the settling proportions assigned to the different settling velocity groups. For the latter scenario, the model was checked to see if it performed as expected, in terms of percentages of particles removal through primary sludge and percentages of particles exiting with the settled wastewater. The modification implemented in Section 4.3.1 was applied, and the wastewater characteristics (refer to Section 3.3), extracted from WRC (1984) and Ekama (2017), were used for these verification steps.

5.2.1. Mass Balances over the UCTPSU Model

The concentrations of all the components (Table 22) and sub-components (Table 23) of the influent raw wastewater were each set to 0.1 g/m^3 to initialize the simulations. The following settling velocities (expressed in m/d) and settling mass proportions in Table 24, were extracted from the discrete particle settling model calculation results (Table 11) and used as inputs into this verification step, as well as the influent data extracted from WRC (1984) and Ekama (2017).

Table 24: Settling Velocities and Proportions Used for the Initial Verification Process

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Settling Velocities (m/d)	127.2	88.8	50.4	21.6	5.5
Settling Proportions					
	Fs_1	**Fs_2**	**Fs_3**	**Fs_4**	**Fs_5**
UPO	47	20	17	12	4
BPO	12	15	20	25	28
ISS	37	25	18	15	5

Material mass balances in terms of ISS, UPO and BPO fluxes were performed over the UCTPSU model. The results are presented in Table 25 and 100% mass balances were obtained.

Table 25: Material Mass Balances over the UCTPSU model

Components	**UPO**	**BPO**	**ISS**
Influent Fluxes (kg/d)	1134.9	4390.1	720.0
Effluent Fluxes (kg/d)	62.9	1151.5	49.6
Underflow Fluxes (kg/d)	1072.0	3238.6	670.4
Mass Balances (%)	100.0	100.0	100.0

5.2.2. Mass Balances around the UCTPSU Model Layers

It was established, from Chapter 4, that a mass balance for a particle class and around a n^{th} layer is obtained when the concentration of the particles in the model, and over a long simulation time, remains constant. Therefore, the purpose of this verification step, in terms of the particle mass balances around the layers, is to confirm that the model is consistent with regards to removals of UPO, BPO and ISS. All the layers were checked with regards to the particle mass balances of UPO, BPO and ISS, and for all the settling velocity groups. The 3rd layer in the UCTPSU model is taken as a sample layer and the concentrations (labelled C_s) of the five settling velocity groups for UPO, BPO and ISS, respectively, are displayed in Figure 15, Figure 16 and Figure 17. For notation clarity:

- PST.C_s (X_ISS3) (3) refers to the ISS concentration of the 3rd settling velocity group, in the 3rd layer.

- PST.C_s (X_U_Inf2) (3) refers to the UPO concentration of the 2nd settling velocity group, in the 3rd layer.
- PST.C_s (X_B_Inf5) (3) refers to the BPO concentration of the 5th settling velocity group, in the 3rd layer.

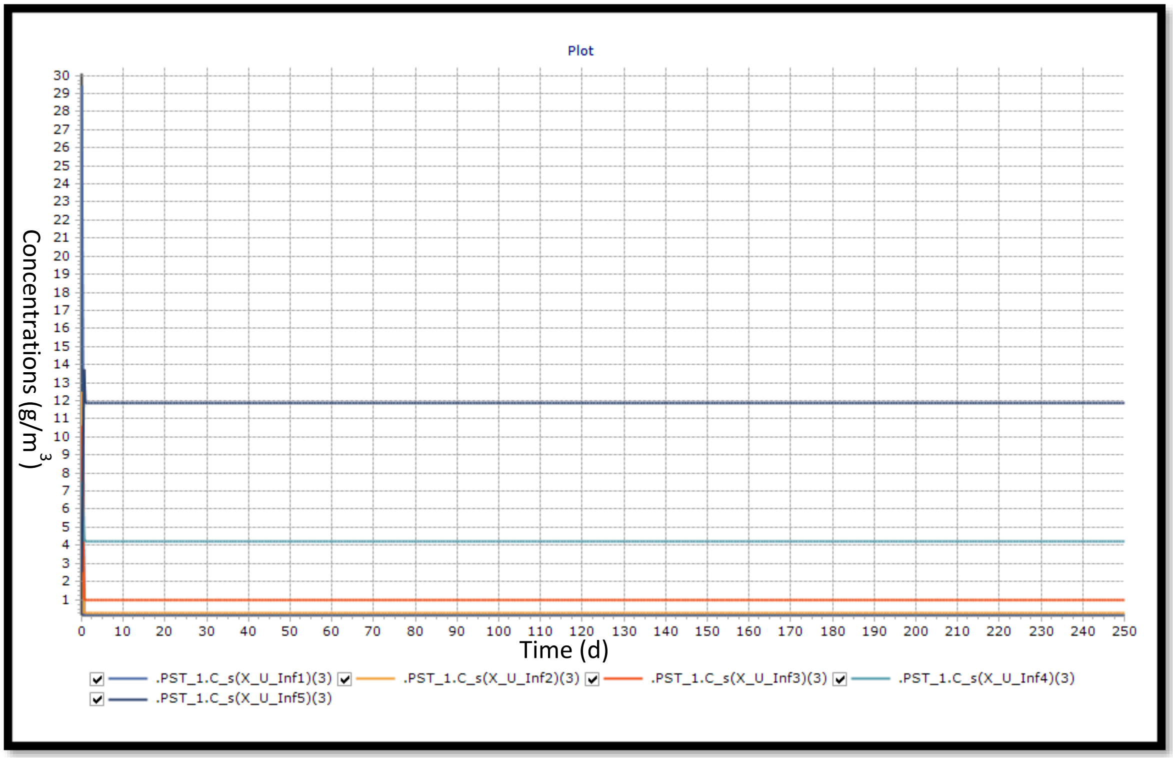


Figure 15: UPO Concentrations Profile in the 3rd Layer

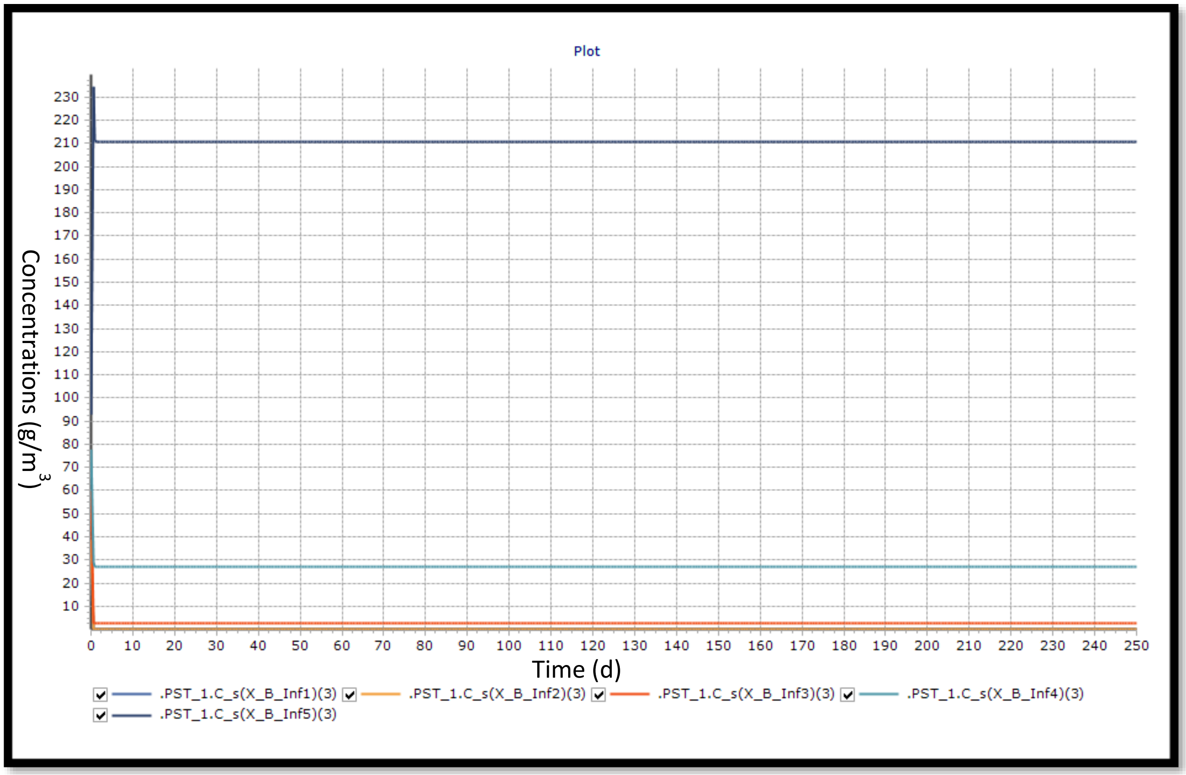


Figure 16: BPO Concentrations Profile in the 3rd Layer

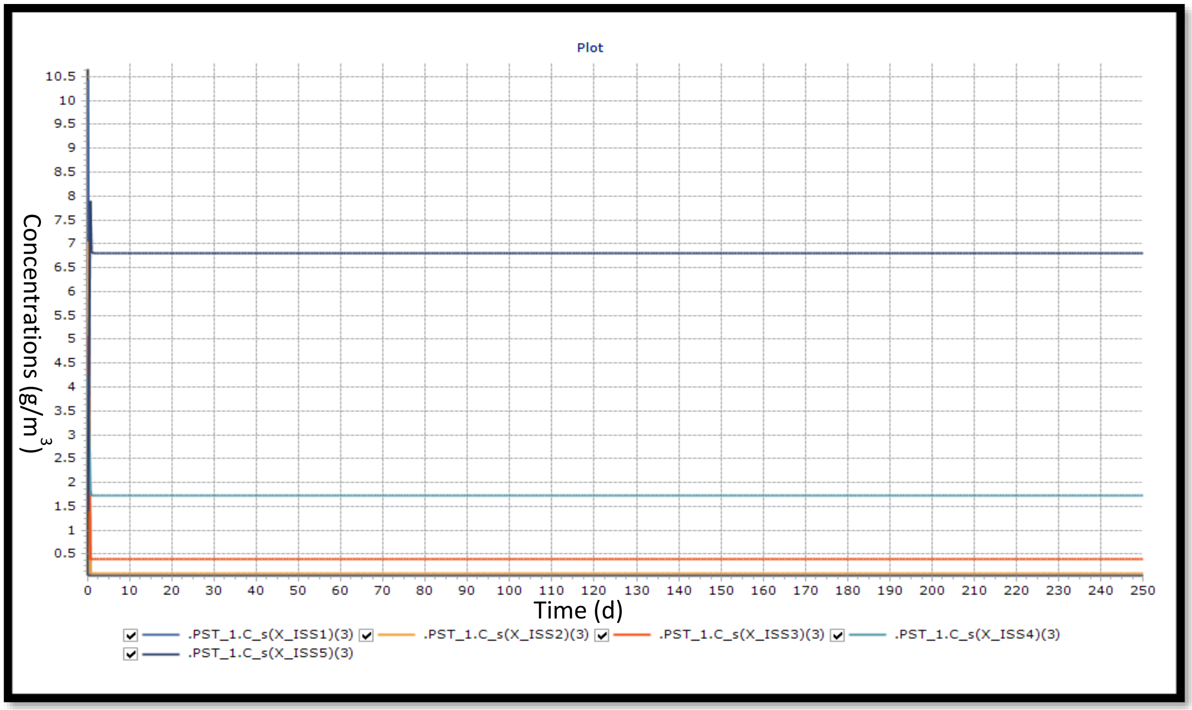


Figure 17: ISS Concentrations Profile in the 3rd Layer

The concentration profiles in the 3rd layer are constant and confirm that mass balances are maintained around that layer and, subsequently, the other layers. Since high velocities were assigned to the first settling velocity groups and low velocities towards the last settling velocity groups (see Table 24), particles get removed rapidly in these first groups and slowly in the last groups, across the 3rd layer. As such, the concentration of particles increases across the 5 settling velocity groups, from the fastest settling velocity group (the first group) to the slowest settling velocity group (the last group) (refer to Figure 15, Figure 16, and Figure 17). These patterns in the concentration profiles are, therefore, consistent and justified. It is worth mentioning that since the 3rd layer is above the feed layer from the UCTPSU model configuration (refer to Figure 14 showing the virtual distribution of settleable particles in a primary settling tank - PST), particle concentrations are expected to be low, as opposed to the 8th or 9th layer, which are below the feed layer and where concentrations will be expected to be much higher. This is because settleable particles are settling towards the bottom of the tank.

5.2.3. Specific Loading Conditions

After successfully checking that material mass balances were obtained over the UCTPSU model, and around the layers within it, by using WRC (1984) and Ekama (2017) data, as well as the set of settling proportions and velocities obtained from the discrete particle settling model, other specific loading conditions were applied to the model to confirm its internal consistency. These cases, simulated in WEST® (Vanhooren et al., 2003) were chosen in such a way that predictions generated are expected. It includes:

- Assigning very low settling velocities to all the settling velocity groups and checking that each settling velocity group could individually carry the removals, if allocated all the particles
- Assigning very high settling velocities to all the settling velocity groups, and checking that each settling velocity group could also, individually, carry the removals if allocated all the particles
- Assigning very high velocities to some settling velocity groups and very low velocities to others and verifying that the model is predicting the effluent and the underflow in expected proportions of the settling proportions allocated.

5.2.3.1. Very Low Settling Velocities Only

Settling velocities of 0.0 m/d (i.e. no settling) were applied in this scenario, to all the settling velocity groups. The removals were solely dictated by the bulk liquid velocities (V_{UP} and/or V_{DN}). Each settling velocity group was, therefore, assigned all the particles by allocating the value of 1 to the settling proportions in that settling velocity group and 0 to all the settling proportions of the other settling velocity groups.

First Settling Velocity Group

By assigning all the particles (UPO, BPO and ISS) to the first settling velocity group and knowing that the settling velocity is 0.0 m/d, as well as the underflow recycle which is set at 0.5% of the influent flow rate (see Section 3.3), it is expected that 99.5% of the particles exit through the effluent flow rate and the remaining portion, equivalent to 0.5%, is removed via the underflow rate. These residual particles removed through the underflow are due to the bulk liquid velocities. The results of this assignment are presented in Table 26, Table 27 and Table 28.

Table 26: UPO Mass Balances for Very Low Velocities

Components	UPO				
Settling Velocity Groups	1	2	3	4	5
Influent Fluxes (kg/d)	1134.9	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	1129.2	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	5.7	0.0	0.0	0.0	0.0
% Effluent	99.5	0.0	0.0	0.0	0.0
% Underflow	0.5	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

Table 27: BPO Mass Balances for Very Low Velocities

Components	BPO				
Settling Velocity Groups	1	2	3	4	5
Influent Fluxes (kg/d)	4390.1	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	4368.1	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	22.0	0.0	0.0	0.0	0.0
% Effluent	99.5	0.0	0.0	0.0	0.0
% Underflow	0.5	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

Table 28: ISS Mass Balances for Very Low Velocities

Components	ISS				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	720.0	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	716.4	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	3.6	0.0	0.0	0.0	0.0
% Effluent	99.5	0.0	0.0	0.0	0.0
% Underflow	0.5	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

These results are, therefore, in accordance with the expected removals.

Second to Fifth Settling Velocity Group

The same results obtained for the first settling velocity group were also obtained when the remaining settling velocity groups were tested. This is true because:

- The same settling velocities were assigned to the settling velocity groups (0.0 m/d)
- The particles were all assigned to one settling velocity group at the time and nothing else is removed by the other settling velocity groups
- All the other conditions remained unchanged.

5.2.3.2. Very High Settling Velocities Only

In this scenario, a very high settling velocity of 150.0 m/d (or 6.3 m/h) was distinctly applied to all the settling velocity groups and the same procedure, as described in the previous scenario, was followed. This settling velocity was selected to make sure complete removals take place when assigned to the settling velocity groups.

First Settling Velocity Group

By assigning the particles to the first settling velocity group, and knowing that the settling velocity is very high, it is expected that all the particles (UPO, BPO and ISS) get removed by the underflow recycle and into the primary sludge. However, some extremely low to no (the value is equal to zero) residual particle concentrations could, be found in the effluent of the raw wastewater, owing to the upwards bulk liquid velocity (V_{UP}). For this assignment, the residual particle concentrations are equal to zero. The results of the assignment are therefore presented in Table 29, Table 30 and Table 31 and all conform to the expected predictions.

Table 29: UPO Mass Balances for Very High Velocities

Components	**UPO**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	1134.9	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	0.0	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	1134.9	0.0	0.0	0.0	0.0
% Effluent	0.0	0.0	0.0	0.0	0.0
% Underflow	100.0	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

Table 30: BPO Mass Balances for Very High Velocities

Components	**BPO**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	4390.1	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	0.3	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	4389.8	0.0	0.0	0.0	0.0
% Effluent	0.0	0.0	0.0	0.0	0.0
% Underflow	100.0	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

Table 31: ISS Mass Balances for Very High Velocities

Components	**ISS**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	720.0	0.0	0.0	0.0	0.0
Effluent Fluxes (kg/d)	0.0	0.0	0.0	0.0	0.0
Underflow Fluxes (kg/d)	720.0	0.0	0.0	0.0	0.0
% Effluent	0.0	0.0	0.0	0.0	0.0
% Underflow	100.0	0.0	0.0	0.0	0.0
Mass Balances (%)	100.0				

These results are also in accordance with the expected removals.

Second to Fifth Settling Velocity Group

Similar to the case discussed for the very low settling velocities in Section 5.2.3.1, the same results predicted for the first settling velocity group were the same from the second to the fifth settling velocity group. It could be validated because the same velocities (150.0 m/d) were assigned to the respective settling velocity groups, the same assignment procedure was followed, and all other conditions did not change.

5.2.3.3. Very High and Low Settling Velocities Combination

For this third case scenario, the settling velocities and proportions across all the settling velocity groups were split as laid out in Table 32.

Table 32: Settling Velocities and Proportions for Very High and Low Velocities Combination

Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Settling Velocities (m/d)	150.0	150.0	0.0	0.0	0.0
Settling Proportions					
UPO	25	25	30	10	10
BPO	40	30	10	10	10
ISS	20	20	20	20	20

From the conclusions in Sections 5.2.3.1 and 5.2.3.2, the model is expected to behave as follows, concerning the underflow and effluent compositions and in terms of UPO, BPO and ISS:

- The underflow will comprise of particles (UPO, BPO and ISS) completely removed from the first two settling velocity groups and the proportion of particles (UPO, BPO and ISS) removed by the underflow recycle (set at 0.5% of the influent flowrate - see Section 3.3) in the last three settling velocity groups. The percentage removals from the first two settling velocity groups (which have been assigned very high settling velocities) are obtained by summing their assigned settling proportions. This is because the particles in these two groups settle out completely in the primary sludge. The percentage removals from the last three settling velocity groups (which have been assigned very low settling velocities) are calculated by multiplying the underflow recycle value with the corresponding settling proportions in these groups.
- As a result, the remaining particles, not removed through the underflow, will exit via the effluent.

Table 33 provides a quantitative summary of these predictions.

Table 33: Quantitative Summary of the Predictions

Particles	UPO	BPO	ISS
% Removed in the Underflow for the 1st Settling Velocity Group	25	40	20
% Removed in the Underflow for the 2nd Settling Velocity Group	25	30	20
% Removed in the Underflow for the 3rd Settling Velocity Group	0.2	0.1	0.1
% Removed in the Underflow for the 4th Settling Velocity Group	0.1	0.1	0.1
% Removed in the Underflow for the 5th Settling Velocity Group	0.1	0.1	0.1
Total % Removed in the Underflow	50.2	70.1	40.3
Total % Removed in the Effluent	49.8	29.9	59.7

After simulations in WEST®, the results of this test are presented in Table 34, Table 35 and Table 36.

Table 34: UPO Mass Balances for Very High and Low Velocities Combination

Components	**UPO**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	283.7	283.7	340.5	113.5	113.5
Effluent Fluxes (kg/d)	0.0	0.0	338.8	112.9	112.9
Underflow Fluxes (kg/d)	283.7	283.7	1.7	0.6	0.6
% Effluent per Group	0.0	0.0	99.5	99.5	99.5
% Underflow per Group	100.0	100.0	0.5	0.5	0.5
% Overall Effluent	49.8				
% Overall Underflow	50.2				
Mass Balances (%)	100.0				

Table 35: BPO Mass Balances for Very High and Low Velocities Combination

Components	**BPO**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	1756.0	1317.0	439.0	439.0	439.0
Effluent Fluxes (kg/d)	0.1	0.1	436.8	436.8	436.8
Underflow Fluxes (kg/d)	1755.9	1316.9	2.2	2.2	2.2
% Effluent per Group	0.0	0.0	99.5	99.5	99.5
% Underflow per Group	100.0	100.0	0.5	0.5	0.5
% Overall Effluent	29.9				
% Overall Underflow	70.1				
Mass Balances (%)	100.0				

Table 36: ISS Mass Balances for Very High and Low Velocities Combination

Components	**ISS**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**
Influent Fluxes (kg/d)	144.0	144.0	144.0	144.0	144.0
Effluent Fluxes (kg/d)	0.0	0.0	143.3	143.3	143.3
Underflow Fluxes (kg/d)	144.0	144.0	0.7	0.7	0.7
% Effluent per Group	0.0	0.0	99.5	99.5	99.5
% Underflow per Group	100.0	100.0	0.5	0.5	0.5
% Overall Effluent	59.7				
% Overall Underflow	40.3				
Mass Balances (%)	100.0				

The percentages expected have been obtained and confirmed that the UCTPSU model is internally consistent with respect to material mass balances. Furthermore, dynamic mass balance checks were also performed and can be found in Appendices 8.3.

5.3. Preliminary UCTPSU Model Plant-Wide Model Integration

Initial steady state simulations have been performed for a typical wastewater treatment plant, treating 15Ml/d of settled wastewater, with the typical wastewater characteristics obtained from values used in previous studies (WRC, 1984 ; Ekama, 2017). This was done to initiate a process of quantitative evaluation on the predictive capacity of the UCTPSU model, by assessing its application and its impact in a plant-wide context. The WEST ® platform (Vanhooren et al., 2003) was again used as the simulation environment which connects the UCTPSU to the activated sludge (AS) and anaerobic digestion (AD) systems within the PWM_SA (Ikumi *et al.*, 2014) plant-wide modelling framework.

5.3.1. Experimental Set Up

A wastewater treatment plant (WWTP) has been modelled in WEST®, which incorporated the UCTPSU model. Unit operations of the modelled WWTP included the UCTPSU, two gravity thickeners (GT) with one each to thicken the primary sludge (PS) from the UCTPSU, and waste activated sludge (WAS) from the AS system, three AS units (anaerobic, anoxic and aerobic), two ADs systems, each digesting PS and WAS separately, and one secondary settling tank (SST). The AS system is modelled under the UCT process configuration that caters for both biological nitrogen and phosphorus removal. Figure 18 displays the plant-wide virtual experimental set up in WEST®.

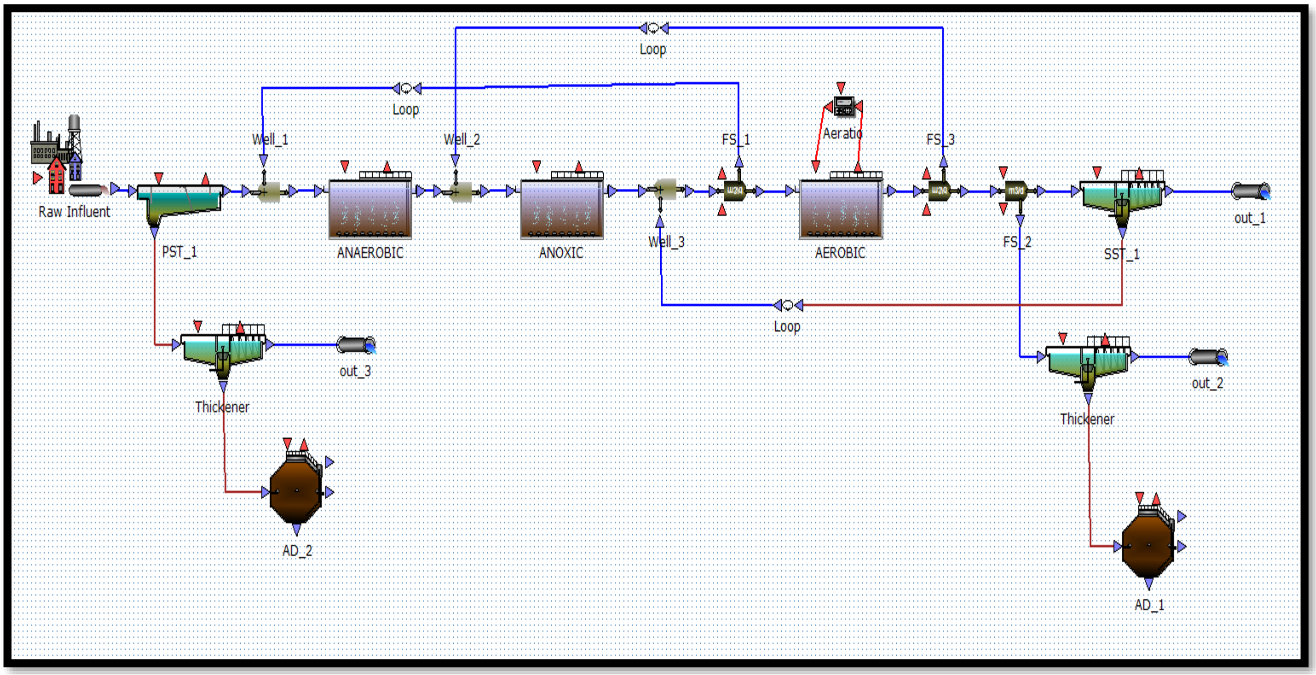


Figure 18: WWTP Configuration Used to Simulate the UCTPSU Model

The system operations parameters are given in Table 37. The raw wastewater characteristics were given in Section 3.3.

Table 37: Key Parameters of the Experimental Set Up

Parameter	Value
Wastewater temperature (°C)	20
PST area (m^2)	650
SST area (m^2)	1500
Anaerobic volume (m^3)	713
Anoxic volume (m^3)	3027
Aerobic volume (m^3)	3385
a-recycle	4
r-recycle	1
s-recycle	1
Sludge age of the AS system (d)	15
Sludge age of the AD system (d)	25

To simulate the application and demonstrate the impact of the UCTPSU model, two removal scenarios were applied:

- Scenario 1 consisted of removing the ISS, UPO and BPO at 50% each, as modelled in the PST configuration (point settler) of the Benchmark Simulation Model No 2 for Phosphorus (Solon et al., 2017).
- Scenario 2 removed these components in realistic proportions (refer to Section 2.3.2 and see Table 39), as experimentally observed in Wentzel *et al.* (2006) and Ikumi *et al.* (2014).

5.3.2. Settling Proportions Selection

Different settling proportions were tested by trial and error in the UCTPSU model, to achieve the removal percentages of the two scenarios in the primary sludge. These results are summarized in Table 38 and Table 39.

Table 38: Settling Proportions Corresponding to Scenarios 1 and 2

Components	**Scenario 1**					**Scenario 2**				
Settling Velocity Groups	**1**	**2**	**3**	**4**	**5**	**1**	**2**	**3**	**4**	**5**
UPO	5	10	10	13	62	30	22	17	12	19
BPO	7	9	10	11	63	5	8	10	10	67
ISS	5	10	10	13	62	20	25	18	15	22

Table 39: Removal Percentages Achieved in the Primary Sludge for Both Scenarios

Components	**Scenario 1 Removal Percentages**	**Scenario 2 Removal Percentages**
UPO	50%	83%
BPO	50%	47%
ISS	50%	80%

5.3.1. Impact Assessment

The impact of the UCTPSU model was assessed by comparing the output compositions of some downstream unit processes, when simulating different settling proportions of UPO, BPO and ISS to vary the removal percentages. The proposed analysis is limited to a theoretical comparison between the two scenarios elaborated on in Section 5.3.2. It seeks to compare the outputs of Scenario 1 (when incorrect proportions are used with regards to UPO, BPO and ISS (Solon et al., 2017) against the output compositions of Scenario 2 (when realistic proportions of UPO, BPO and ISS are estimated in the primary sludge (Wentzel *et al.,* 2006; Ikumi *et al.*, 2014). Therefore, this comparison of the two scenarios includes the settled wastewater composition, the capacity of the activated sludge system (reactor TSS concentration and volume, SST area optimization), the effluent quality in terms of N and P mainly, and the energy consumption by aeration of the activated sludge system, as well as the energy generated via combustion of biogas produced in the anaerobic digestion of the primary sludge.

In comparing the proposed results, statistical tests were incorporated to test whether differences were significant. In this regard, the Chi-square (χ^2) test of homogeneity was used to check if there was any statistically significant difference in the results of the two scenarios Scenario 1 and Scenario 2, obtained for the different downstream processes outputs: settled wastewater (settled WW) composition, AS system capacity, effluent quality, energy consumption and generation, anaerobic digestion of the PS concentrations, anaerobic digestion of the WAS concentrations. For the settled WW composition, the results of each scenario were also compared with the data set values from WRC (1984) and Ekama (2017).

The general form of the null (H_0) and alternative hypothesis (H_A) for the χ^2 test of homogeneity as applied in this dissertation are:

- H_0: The results of the scenarios are homogenous, i.e. there is no statistically significant difference in the results
- H_1: The results of the scenarios are not homogenous, i.e. there is a statistically significant difference in the results

Therefore, a 5% statistical significance level (α) was chosen for rejecting the null hypothesis i.e. the null hypothesis is rejected for a $p\text{-value} < 0.05$. The results of the χ^2 test of homogeneity are summarized in Appendices 8.4. However, the result for each evaluation are discussed in the relevant subsection.

5.3.1.1. Settled Wastewater Composition

The predicted settled wastewater characteristics for Scenarios 1 and 2 are compared with the data set values (WRC, 1984; Ekama, 2017) in Table 40. The soluble components concentrations are not changing, since a 100% water balance is assumed throughout.

Table 40: Summary of the Predicted Settled WW Characteristics of Scenarios 1 and 2, in Comparison with Data Set Values from WRC (1984) and Ekama (2017)

WW Characteristics	Scenario 1	Scenario 2	Data Set Values in WRC (1984) and Ekama (2017)
$f_{S'up}$	0.118	0.042	0.040
UPO (mgCOD/l)	55.64	18.97	18.00
BPO (mgCOD/l)	215.23	232.72	233.00
ISS (mgISS/l)	23.90	9.53	9.50
COD (mgCOD/l)	470.10	450.92	450.00
TKN (mgN/l)	54.60	52.33	52.70
TP (mgP/l)	15.14	14.64	14.63

The difference in the results of Scenarios 1 and 2 is statistically significant, since the p-value (0.0006) obtained from the χ^2 test, was less than 0.05. Scenario 2 predicted settled WW characteristics that are very close to those of the data set, since UPO,BPO and ISS, in both cases, were removed in realistic proportions, as experimentally observed by Wentzel *et al.* (2006) and Ikumi *et al.* (2014). This was further confirmed by the p-value of 1.0000, which meant that the difference in the results of Scenario 2 and the data set values is not statistically significant. On the other hand, Scenario 1 predictions were not close to the data set since the p-value (0.0003) was less than 0.05. Therefore, the difference in the results of Scenario 1 and the data set values is statistically significant It is also worth noting that the low removals in the primary sludge of UPO and ISS, in Scenario 1, yielded a very high content in the settled WW characteristics predicted and, subsequently, a much higher unbiodegradable COD particulate fraction ($f_{S'up}$) value.

5.3.1.2. Activated Sludge System Capacity

The AS system capacity focused on the reactor TSS concentration and its impact on the reactor volume, as well as the SST capacity. The difference in the results of Scenarios 1 and 2 is statistically significant, due to the p-value of 0.0025, obtained from the χ^2 test. Owing to the high removals of UPO and ISS in Scenario 2, compared to Scenario 1, the organic load on the AS reactor is much less in Scenario 2. Hence, a significant decrease of 12% in reactor volume. Subsequently, the optimized SST surface area is also reduced by 7% in Scenario 1, compared to Scenario 2. Incorrect PST predictions can, therefore, lead to incorrect plant capacity estimation in terms of AS reactor volume and SST surface area.

However, it was found that the TSS concentration of the AS reactor in Scenario 2 is less than the TSS concentration of Scenario 1. This could be explained by the lower $f_{S'up}$ value obtained in Scenario 2. These results are summarized in Figure 19.

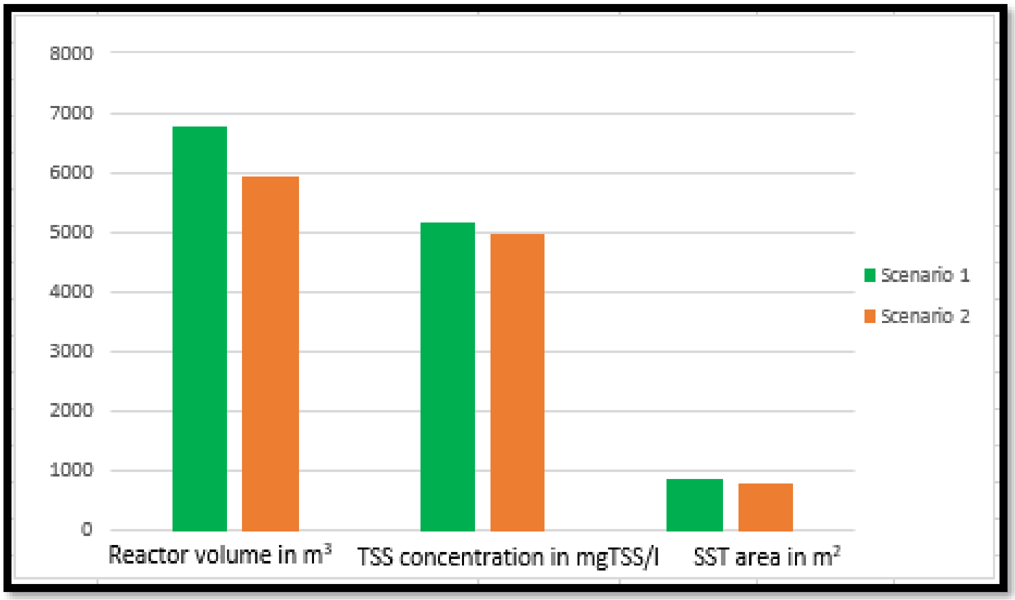


Figure 19: Comparison of the AS System Capacity Estimation between Scenario 1 and 2

5.3.1.3. Effluent Quality

The effluent concentrations extracted from both scenarios were not significantly different in values. In fact, the difference in the results of Scenarios 1 and 2 is not statistically significant, due to the p-value of 0.2446 obtained from the χ2 test. This can be explained from the fact that the BPO proportions of the settled WW (50% in Scenario 1 compared to 53% for Scenario 2) are not far apart. The increase in FSA (6%) in Scenario 1, compared to Scenario 2, could be explained by the breakdown of the organically bound nitrogen in the BPO, which is released in the ammonia pool of the AS system as FSA, for biomass production (sludge) and then nitrification. Since there is more BPO in the settled WW of Scenario 2, more FSA is, therefore, expected. Furthermore, there is no difference between the OP of both scenarios because the organically bound phosphorus in the BPO is very small. These results are summarized in Table 41.

Table 41: Effluent Quality Summary

Variables	Scenario 1	Scenario 2
FSA (mgN/l)	1.17	1.25
NO3 (mgN/l)	6.83	6.59
OP (mgP/l)	11.36	11.34
Soluble COD (mgCOD/l)	54.85	54.88

5.3.1.4. Energy Consumption and Generation

One of the downstream objectives of including the UCTPSU model in a plant-wide context, is to be able to investigate the energy aspect in the system by analyzing the energy utilized in the activated sludge system and the generation of energy through anaerobic digestion.

Energy Consumption in the Activated Sludge System

If more BPO overflow with the settled WW of the AS, then more oxygen will be required for aeration towards the breakdown of organics, as well as the endogenous respiration of the dead biomass. However, because the BPO proportions of the settled WW, for both scenarios, are very close (50% in Scenario 1 compared to 53% for Scenario 2), the quantitative impact in terms of the oxygen utilization (OU), as well as the oxygen utilization rate (OUR), was not clearly demarcated. Hence, the OU was 2% more in Scenario 1, compared to Scenario 2. Furthermore, the difference in the results of Scenarios 1 and 2 is not statistically significant, due to the p-value of 0.2640 obtained from the $\chi2$ test. As expected, more oxygen is required for organics breakdown and endogenous respiration in Scenario 2. Should further incorrect assumptions (from realistic proportions) be made with regards to Scenario 1, the inaccuracies in the energy estimations will increase as well.

Energy Generation through Anaerobic Digestion

With regard to the AD output, the main variable of interest is the methane gas production, which depends on the proportion of BPO that is available. It was established that Scenario 2 yielded 47% of BPO, compared to 50% in Scenario 1, through PS production. As such, the predicted methane gas generated has decreased from 6% in Scenario 1, compared to Scenario 2. Concerning the AD of the WAS, an increase of 2% in methane production was noted, in Scenario 1, compared to Scenario 2. This decrease is due to the higher BPO content of the WAS in Scenario 2, compared to Scenario 1, which is derived from the higher BPO content of the settled WW which, therefore, produces more active biomass. Furthermore, the difference in the results of Scenarios 1 and 2 is not statistically significant, due to the p-value of 0.2640 obtained from the $\chi2$ test.

5.3.1.5. Other Anaerobic Digestion Considerations

Wastewater characteristics such as COD, TKN, TP, TSS, VSS and ISS were also compared for the anaerobic digestion of the PS and the WAS, for both scenarios. With regards to the PS AD, the COD, TKN, TP, TSS, VSS and ISS contents of the AD system liquor were, respectively, 31%, 25%, 17%, 33%, 32% and 35% less in Scenario 1, compared to Scenario 2. Furthermore, the difference in the results of Scenarios 1 and 2 is statistically significant, due to the p-value of 0.0000 obtained from the $\chi2$ test. This is making sense because of the higher proportion of UPO (which greatly contributes to the particulate COD, TKN and TP) and ISS found in the PS of Scenario 2, compared to Scenario 1. These results are depicted in Figure 20.

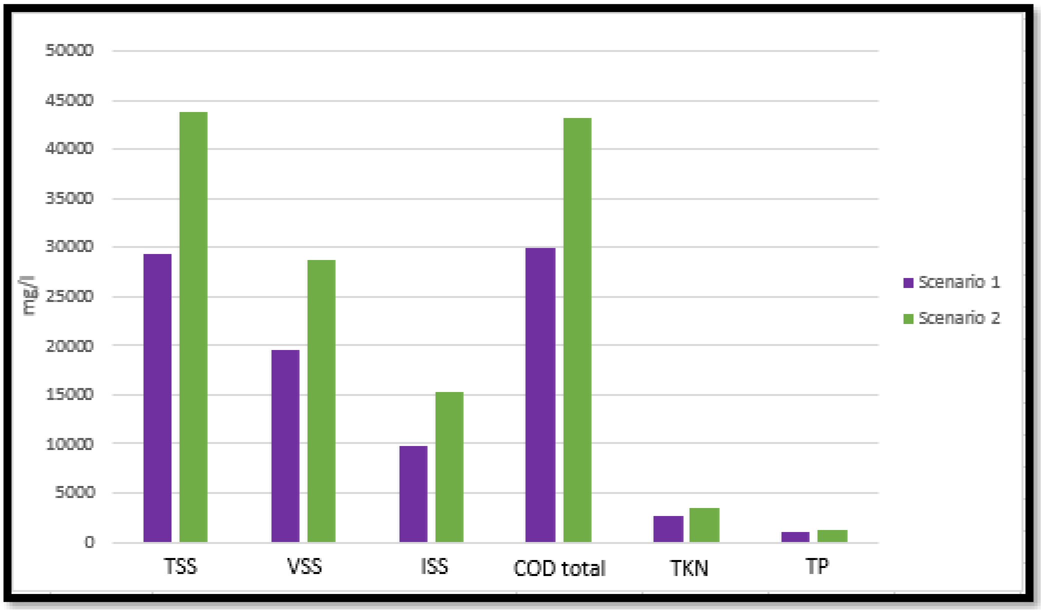


Figure 20: Comparison between the Anaerobic Digestion of the PS of Scenarios 1 and 2

Furthermore, the higher removal of UPO and ISS in Scenario 2 is very good for the AS reactor because it diverts inert material to the AD system where it is “retained” at a high concentration and, therefore, occupies a low volume and away from the AS reactor, where it would be retained at low concentration and occupy a large volume. Clearly, current PST models, which remove 50% UPO, BPO and ISS, get this split of inert material between the AS and AD systems wrong, which results in significantly larger AS reactors.

As far as the WAS AD is concerned, since the UPO and ISS contents of the WAS of Scenario 1 are mostly higher than those of Scenario 2, it follows that the COD, TKN and TP (because of the particulate COD, TKN and TP contributions), as well as the TSS, VSS and ISS contents of the AD system liquor, are respectively 31%, 23%, 19%, 37%, 32%, and 57% more, in Scenario 1, compared to Scenario 2. Furthermore, the difference in the results of Scenarios 1 and 2 is statistically significant, due to the p-value of 0.0000 obtained from the χ2 test. The results of the AD of WAS are displayed in Figure 21.

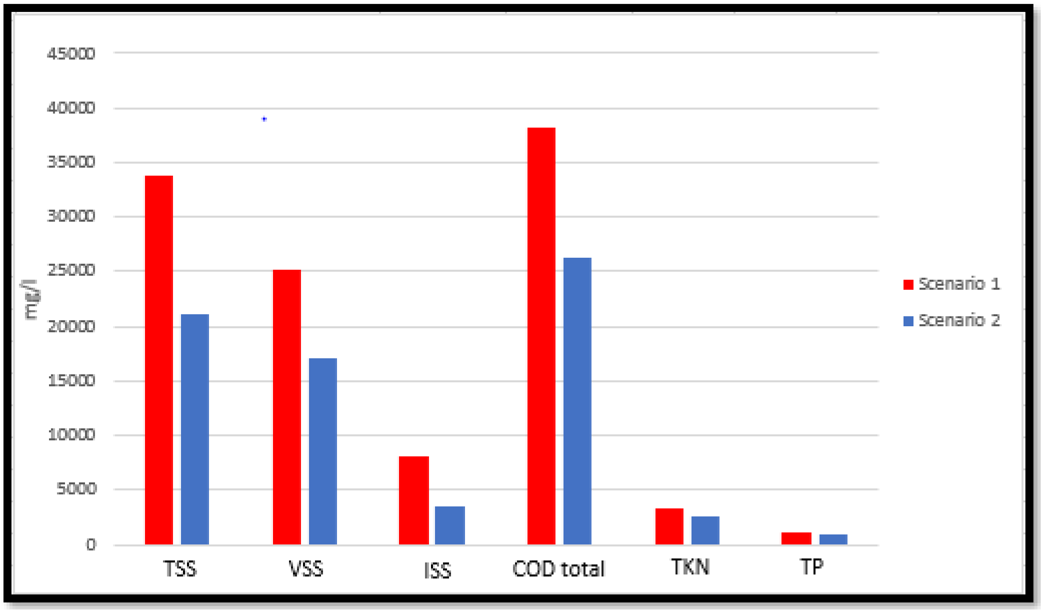


Figure 21: Comparison between the Anaerobic Digestion of the WAS of Scenarios 1 and 2

5.3.1.6. Impact Assessment Summary

A summary of the comparisons of both scenarios towards assessing the impact of the UCTPSU model predictions, is presented in Table 42.

Table 42: Comparative Assessment of Scenarios 1 and 2

Components	Scenario 1	Scenario 2
AS System Capacity Estimation		
Reactor volume (m^3)	6781	5948
SST surface area (m^2)	861	798
TSS concentration (mgTSS/l)	5175.00	4975.00
Primary Sludge Concentrations		
COD (mgCOD/l)	55456.23	60264.10
TKN (mgN/l)	1371.06	1834.12
TP (mgP/l)	515.48	623.68
TSS (mgTSS/l)	41841.09	47974.67
VSS (mgVSS/l)	36997.37	40270.58
ISS (mgISS/l)	4844.72	7703.15
Settled Wastewater Concentrations		
COD (mgCOD/l)	470.10	450.92
TKN (mgN/l)	54.60	52.33
TP (mgP/l)	15.14	14.64
TSS (mgTSS/l)	208.59	177.77
VSS (mgVSS/l)	184.70	168.24
ISS (mgISS/l)	23.90	9.53
Energy Consumption and Generation		
OUR in the AS (g/m^3.d)	1183	1203
OU in the AS (g/d)	4004024	4071784
Total CH4 from PS and WAS AD (m^3 /d)	1370	1308
Anaerobic Digestion of the PS Concentrations		
COD (mgCOD/l)	29920.54	43269.75
TKN (mgN/l)	2560.93	3437.08
FSA (mgN/l)	579.26	549.51
TP (mgP/l)	966.57	1170.09
OP (mgP/l)	559.02	436.46
TSS (mgTSS/l)	29339.40	43788.63

VSS (mgVSS/l)	19670.96	28727.32
ISS (mgISS/l)	9876.74	15257.53
Anaerobic Digestion of the WAS Concentrations		
COD (mgCOD/l)	38153.92	26292.70
TKN (mgN/l)	3364.14	2580.08
FSA (mgN/l)	822.38	841.69
TP (mgP/l)	1057.50	859.69
OP (mgP/l)	356.06	359.17
TSS (mgTSS/l)	33805.52	21143.73
VSS (mgVSS/l)	25083.19	17069.25
ISS (mgISS/l)	8559.34	3523.59
Effluent Quality		
FSA (mgN/l)	1.17	1.25
NO3 (mgN/l)	6.83	6.59
OP (mgP/l)	11.36	11.34
Soluble COD (mgCOD/l)	54.85	54.88

The above plant-wide simulations results have shown the impact of correctly predicting the proportions of UPO, BPO and ISS in the downstream processes of a treatment plant. Incorrect assumptions can lead to subsequent incorrect predictions and compromise an accurate tracking of different components through the system, as well as tactical decisions making to optimize the whole plant. Hence, the need to develop a realistic PST model, that can account for these predictions, by allowing measurements of key parameters, such as particle settling velocities and the unbiodegradable particulate fraction of the COD ($f_{S'up}$).

However, it must be highlighted the scope of works of this research is limited to a model development and verification procedure, with a basic statistical analysis as presented in this section. Towards a robust evaluation of the model, a rigorous sensitivity analysis has been performed in subsequent work (reference Joshua), using the Biomath protocol (reference needed from Newman and David). Therefore, this sensitivity analysis and model calibration will be thoroughly developed in (reference Joshua).

5.4. Closure

This chapter presented the evaluation of the University of Cape Town Primary Sedimentation Unit (UCTPSU) model. The model was verified using a multiple-steps procedure, under steady state conditions and using WRC (1984) and Ekama (2017) data. Material mass balances were performed over the UCTPSU model and around all the layers within the model, for the set of settling velocities and settling proportions obtained from the discrete particle settling model. Further verification steps were also performed by applying specific scenarios to which predictions could be directly expected, in terms of the percentages of removals in the primary sludge and the percentages exiting through the settled wastewater. It included assigning, respectively, very low velocities and very high velocities to each settling velocity group and ensuring material mass balances. The last scenario consisted of setting up a combination of very high and very low velocities from the first to the fifth settling velocity group and assigning specific settling proportions to UPO, BPO and ISS classes. All the material mass balances from the different checks were achieved and confirmed that the model was internally consistent.

The UCTPSU model was, thereafter, integrated in a plant-wide context to assess its predictive capability, by comparing the outputs of two scenarios where settling proportions were varied to achieve different removal percentages. The steady state simulations on these scenarios have shown the model application and demonstrated that incorrect assumptions, in terms of UPO, BPO and ISS removal predictions, can lead to incorrect predictions towards outputs generated by downstream processes.

6. Conclusions and Recommendations

6.1. Introduction

This research project aimed at developing a mathematical model of a primary settling tank (PST), which can account for a realistic representation of PST removal of settleable particulates in municipal sewage, in correct proportions of biodegradable particulate organics (BPO), unbiodegradable particulate organics (UPO) and inorganic settleable solids (ISS). This TSS fractionation method was selected because these parameters can be easily measured through experiments. Therefore, the model was expected to predict the composition of the primary sludge (PS) that is treated in the anaerobic digestion (AD) system and the composition of the settled wastewater (settled WW) that is going to the activated sludge unit processes.

To fulfill this aim, a discrete particle settling model was developed, and the results obtained from calculations in this model were used to feed into the development of a current total suspended solids (TSS) based dynamic model. The dynamic model was successfully achieved through a rigorous verification procedure and using data from previous studies (WRC, 1984; Ekama, 2017). Thereafter, a preliminary plant-wide integration was presented to demonstrate the application and potential impact of the model. As such, this chapter summarizes the conclusions drawn, as well as other key points that arose during the development of the proposed realistic PST.

6.2. Discrete Particle Settling Model Development

Removals under discrete conditions were modelled in Microsoft Excel. These were performed for steady state and dynamic calculations and were aimed at mimicking correct removal proportions of UPO, BPO and ISS (Wentzel *et al.,* 2006; Ikumi *et al.*, 2014), using raw wastewater (raw WW) and settled WW characteristics from WRC (1984) and Ekama (2017). The particle settling velocity distribution (PSVD) concept of Bachis *et al.* (2015) was adapted to this discrete particle settling model. As such, the influent raw TSS was divided into five fractions, and each fraction was attributed to a distinct settling velocity group. The TSS fraction, contained in each settling velocity group, was further split into UPO, BPO and ISS settling proportions and descending settling velocities were assigned to the different settling velocity groups. It was found that to match the modelling predictions at both steady state and dynamic calculations:

- The UPO and ISS were removed in greater proportions in the fastest settling velocity groups and, subsequently, decreased towards the slowest settling velocity groups.
- On the other hand, the BPO proportions were removed in low proportions in the fastest settling velocity groups and progressively increased towards the slowest settling velocity groups.

As such, the discrete particle settling modelling approach could be implemented in a dynamic PST framework, to develop a realistic PST model.

6.3. UCTPSU Model Development and Evaluation

Based on the results obtained from the steady state and dynamic calculation outputs of the discrete particle settling model, the University of Cape Town Primary Sedimentation Unit (UCTPSU) was developed in the simulation program WEST® (Vanhooren *et al.,* 2003). The developed model is an improvement of a current TSS-based model (Bachis *et al.*, 2015). The dynamic settling configurations were based on the work done by Takacs *et al.* (1991) in which the settler is divided into several layers, and a dynamic particle mass balance is performed around each layer, for each particle component. The same fractionation of the TSS into UPO, BPO and ISS, as described in the discrete particle settling model, was also implemented.

The model was subjected to a rigorous verification process where material mass balances were first performed over the UCTPSU model, and around all the layers within the model, for the set of settling velocities and settling fractions obtained from the discrete particle settling model settler model. Specific loading conditions were then applied to the model to check that expected predictions were satisfied in terms of the percentages of removals in the primary sludge (PS) and the percentages exiting through the settled WW, with strict material mass balance checks at each stage. These conditions were defined as follow:

i. Assigning all the particulates to each settling group, respectively, and successively applying very high and very low velocities
ii. Assigning a combination of high and low velocities to the five settling velocity groups and assigning different settling fractions to the UPO, BPO and ISS.

The UCTPSU model was, subsequently, integrated in a plant-wide context and steady state simulations were performed by mimicking non-realistic proportions and realistic percentage removals of UPO, BPO and ISS components. This was done to assess the predictive capability of the UCTPSU model and assess the impact that such a model can have at a plant-wide level. The impact assessment compared the results obtained from the settled WW compositions, the activated sludge (AS) system capacity, the effluent quality, as well as the energy consumption and generation from the AS system and the anaerobic digestion (AD) unit. It was shown that incorrect assumptions, in terms of proportions of UPO, BPO and ISS removed, can lead to incorrect predictions towards generated outputs from the downstream unit processes.

6.4. Measurements of Wastewater Characteristics

This investigation has been conducted for municipal wastewater only and has highlighted the need to measure key parameters in a wastewater treatment plant. The UCTPSU model development has shown that measuring particle settling velocities is critical in realistically predicting PST removals. Furthermore, in order to be able to estimate realistic proportions of UPO, BPO and ISS, the unbiodegradable particulate COD fraction will have to be measured. This fraction will assist in fractionating the VSS into UPO and BPO and, subsequently, the ISS fraction can be determined from the TSS.

6.5. Closure

The UCTPSU model, which is an improved model from a current TSS based model (Bachis *et al.,* 2015), has been developed in two phases. First, discrete settling conditions were applied to describe removals with steady state and dynamic calculations, in terms of correct proportions of UPO, BPO and ISS components, as experimentally determined by Wentzel *et al.* (2006) and Ikumi *et al.* (2014). Thereafter, the UCTPSU model was developed to predict steady state and dynamic conditions, by using key insights obtained from the discrete particle settling model. The UCTPSU model has been developed in such a way that it can be integrated to run plant wide model simulations. It is expected that further modelling enhancement will permit better plant wide model predictions.

6.6. Recommendations and Prospective Work

A realistic PST (the UCTPSU) model that takes into consideration the fractionation of TSS into UPO, BPO and ISS, has been presented and the potential for integration into a plant wide context, for better optimization and tactical decision making, has also been shown. However, for better modelling predictions and to also evaluate the robustness of the proposed model, the following areas would require further investigation.

6.6.1. Experimental Campaign

The development of the UCTPSU model requires the input of experimental data that will assist towards a rigorous calibration and achieving a much more realistic model. The extensive review of literature in Chapter 2 (see Section 2.1.1.6) has shown the potential of using a tool, such as the settleometers (Poinapen *et al.,* 2009). This tool can allow a clear demarcation of particle settling velocities and biodegradability tests can be further performed on the primary sludge samples from the different columns, to determine the settleability fractions in terms of UPO, BPO and ISS. It is expected that the data collection will provide realistic ranges of settleable fractions of the TSS components towards the model calibration.

Therefore, it is important to design a robust experimental protocol to collect comprehensive data sets (settling velocities and settling mass fractions) and analyze their biodegradability content, with which the model can be calibrated on. Furthermore, it would be useful for the data sets to incorporate dry and wet weather flows, as investigated by Lessard & Beck (1988) and Bachis *et al.* (2015), to assess the experiment responses to these scenarios.

6.6.2. Extensive Model Evaluation

The model evaluation of the UCTPSU has been limited to a verification process, as well as preliminary steady state plant-wide simulations, to demonstrate the model potential impact and its application. The data collection inputs will be used to proceed to a rigorous calibration process towards a complete model evaluation. This includes:

- Conducting a sensitivity analysis procedure. Sensitivity analysis is a crucial step towards confidently evaluating a model. As such, this process will assist in selecting model parameters that can be accurately determined with a set of measurements, and further determining the parameters that are of minimal effect or insensitive towards model outputs (Takács, 2008).
- Calibrating the model against the experimental data. The process will be useful in estimating model parameters, based on measurements used as inputs, and analyze how well the model is replicating that set of measured data.
- Validating the model with another set of full-plant scale data. This stage is meant to assess how well the model replicates another set of data, with no changes in model parameters estimated after calibration.
- Proposing a complete model integration in a plant-wide context, with the model calibrated and validated, to give a holistic perspective of the model application and its usefulness.

6.6.3. CEPT Investigation

Primary sedimentation can be improved by chemical dosing through chemically enhanced primary treatment (CEPT). Similarly to Bachis *et al.* (2015) CEPT investigation, it would be useful to investigate the impact of adding chemicals to improve the removals of solids and what impact it has on the model developed, when it comes to predictions in a plant-wide context. However, it is worth noting that the model is based on discrete settling, and not flocculation settling which is more significant in CEPT scenarios. Therefore, modifications to the model may need to be made to accommodate flocculation settling for realistic results in CEPT scenarios.

6.6.4. Biological Processes and Kinetics

With reference to Section 2.5.4, it would be useful to extend the UCTPSU model by inclusion of specific biological processes and kinetics, such as fermentation and hydrolysis. Depending on the retention time that a PST is subjected to, COD removal can take place through flocculation of colloidal particles or metabolic uptake (Lessard & Beck, 1988). Hydrolysis can also occur, since Gernaey *et al.* (2001) found that there was a variation of COD concentrations from the influent to the effluent in the PST. These inclusions could lead to further PST applications, as well as a much more holistic integration in a plant-wide context.

7. References

Amerlinck, Y. (2015). *Model refinements in view of wastewater treatment plant optimization: improving the balance in sub-model detail* (Vol. 1). PhD Thesis, Ghent University, Belgium.

Bachis, G., Maruéjouls, T., Tik, S., Amerlinck, Y., Melcer, H., Nopens, I., … Vanrolleghem, P. A. (2015). Modelling and characterization of primary settlers in view of whole plant and resource recovery modelling. *Water Science and Technology*, *72*(12), 2251–2261. https://doi.org/10.2166/wst.2015.455

Botha, R. F., & Ekama, G. A. (2015). *Characterization of organics for anaerobic digestion by modelling augmented biochemical methane potential test results* (Masters Thesis, University of Cape Town). Retrieved from https://open.uct.ac.za/bitstream/handle/11427/13557/thesis_ebe_2015_botha_rf.pdf?sequence=

Chagnon, F., & Harleman, D. R. F. (1992). *An Introduction to Chemically Enhanced Primary Treatment Efficiency of CEPT*. 1–5.

Chebbo, G., & Gromaire, M. C. (2009). VICAS-An Operating Protocol to Measure the Distributions of Suspended Solid Settling Velocities within Urban Drainage Samples. *Journal of Environmental Engineering-Asce*, *135*(9), 768–775. https://doi.org/10.1061/(asce)0733-9372(2009)135:9(768)

Cheremisinoff, N. P. (2002). Handbook of water and wastewater treatment technologies. In *Handbook of Water and Wastewater Treatment Technologies*. https://doi.org/10.1016/B978-075067498-0/50000-0

Christoulas, D. G., Yannakopoulos, P. H., & Andreadakis, A. D. (1998). An empirical model for primary sedimentation of sewage. *Environment International*, *24*(8), 925–934. https://doi.org/10.1016/S0160-4120(98)00076-2

Davis, M. L. (2011). Water and wastewater engineering: Design principles and practice. In *Water and wastewater engineering*. Retrieved from http://bases.bireme.br/cgi-bin/wxislind.exe/iah/online/?IsisScript=iah/iah.xis&src=google&base=REPIDISCA&lang=p&nextAction=lnk&exprSearch=166852&indexSearch=ID%5Cnhttp://onlinelibrary.wiley.com/doi/10.1002/ep.10602/abstract

Ekama, G. (2018). *Integrated plant wide design of wastewater treatment plants (CIV5050Z) - Design Project*. Retrieved from https://vula.uct.ac.za/access/content/group/e244c138-3adb-4dee-ac5d-34c1efb8eac5/CIV5050Z2018DesignProjectBrief.pdf

Ekama, G A. (2009). Using bioprocess stoichiometry to build a plant-wide mass balance based steady-state WWTP model. *Water Research*, *43*(8), 2101–2120. https://doi.org/10.1016/j.watres.2009.01.036

Ekama, George A. (2017). Optimizing water and resource recovery facilities (WRRF) for energy generation without compromising effluent quality. *IWA Conference on Sustainable Wastewater Treatment and Resource Recovery: Research, Planning, Design and Operation*, 1–14.

Ekama, George A, & Wentzel, M. C. (2008). Nitrogen Removal. In *Biological wastewater treatment: Principles, modelling and design* (Vol. 2).

Gernaey, K., Vanrolleghem, P. A., & Lessard, P. (2001). Modeling of a reactive primary clarifier. *Water Science and Technology*, *43*(7), 73–81.

Gori, R., Giaccherini, F., Jiang, L.-M., Sobhani, R., & Rosso, D. (2013). Role of primary sedimentation on plant-wide energy recovery and carbon footprint. *Water Science and Technology*, 870–878. https://doi.org/10.2166/wst.2013.270

Harleman, D., & Murcott, S. (2001). An innovative approach to urban wastewater treatment in the developing world. *WATER 21*, 44–48.

Ikumi, D. S., Harding, T., Brouckaert, C., & Ekama, G. A. (2014). *Plant wide integrated biological, chemical and physical bioprocesses modelling of wastewater treatment plants in three phases (aqueous-gas-solid)*.

Ikumi, D. S., Harding, T. H., & Ekama, G. A. (2014). Biodegradability of wastewater and activated sludge organics in anaerobic digestion. *Water Research*, *56*, 267–279. https://doi.org/10.1016/j.watres.2014.02.008

Jones, R., & Takács, I. (2004). Modeling the Impact of Anaerobic Digestion on the Overall Performance of Biological Nutrient Removal Wastewater Treatment Plants. *Proc., 77th Annual WEFTEC, Water Environment Federation, Alexandria, VA, Session 24*, 244–257. https://doi.org/10.2175/193864703784641207

Lessard, P., & Beck, M. B. (1988). Dynamic modeling of primary sedimentation. *Journal of Environmental Engineering*, *114*(4), 753–769. https://doi.org/10.1061/(ASCE)0733-9372(1988)114:4(753)

Lessard, P., & Beck, M. B. (1991). Dynamic simulation of storm tanks. *Water Research*, *25*(4), 375–391. https://doi.org/10.1016/0043-1354(91)90074-Z

Maruejouls, T., Vanrolleghem, P. A., Pelletier, G., & Lessard, P. (2012). A phenomenological retention tank model using settling velocity distributions. *Water Research*, *46*(20), 6857–6867. https://doi.org/10.1016/j.watres.2011.11.067

Maruéjouls, T., Vanrolleghem, P. A., Pelletier, G., & Lessard, P. (2013). Characterisation of retention tank water quality: Particle settling velocity distribution and retention time. *Water Quality Research Journal of Canada*, *48*(4), 321–332. https://doi.org/10.2166/wqrjc.2013.046

Matko, T., Fawcett, N., Sharp, A., & Stephenson, T. (1996). Recent progress in the numerical modelling of wastewater sedimentation tanks. *Trans IChemE*, *74*(B), 245–258. https://doi.org/10.1205/095758296528590

Metcalf, E., & Eddy, H. (2003). Wastewater engineering: treatment and reuse. In *Tata McGraw-Hill Publishing Company Limited, 4th edition. New Delhi, India*. https://doi.org/10.1016/0309-1708(80)90067-6

Moody, L., Burns, R., Wu-Haan, W., & Spajić, R. (2009). Use of biochemical methane potential (BMP) assays for predicting and enhancing anaerobic digester performance. *Proceedings of The 4th International and 44th Croatian Symposium of Agriculture*, 930–934. Retrieved from http://lib.dr.iastate.edu/abe_eng_conf

Nowak, O. (2015). Benchmarks for the energy demand of nutrient removal plants. *Water Science and Technology*, *47*(February 2003), 123–132. https://doi.org/10.2166/wst.2003.0637

Otterpohl, R., & Freund, M. (1992). Dynamic-models for clarifiers of activated-sludge plants with dry and wet weather flows. *Water Science and Technology*, *26*(5), 1391–1400. Retrieved from http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=28&SID=R1jjyKeshc9OWY1kv5W&page=1&doc=1%5Cnhttp://www.iwaponline.com/wst/02605/wst026051391.htm

Piro, P., Carbone, M., Penna, N., & Marsalek, J. (2011). Characterization of the settling process for wastewater from a combined sewer system. *Water Research*, *45*(20), 6615–6624. https://doi.org/10.1016/j.watres.2011.09.034

Poinapen, J., Ekama, G. A., & Wentzel, M. C. (2009). Biological sulphate reduction with primary sewage sludge in an upflow anaerobic sludge bed (uasb) reactor -part 4: Bed settling characteristics. *Water SA*, *35*(5), 553–560. https://doi.org/10.4314/wsa.v35i5.49181

Rashed, I. G. A.-A., Afify, H. A., Ahmed, A. E.-M., & Ayoub, M. A. E.-S. (2013). Optimization of chemical precipitation to improve the primary treatment of wastewater. *Desalination and Water Treatment*, *51*(37–39), 7048–7056. https://doi.org/10.1080/19443994.2013.792147

Solon, K., Flores-Alsina, X., Kazadi Mbamba, C., Ikumi, D., Volcke, E. I. P., Vaneeckhaute, C., … Jeppsson, U. (2017). Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies. *Water Research*, *113*, 97–110. https://doi.org/10.1016/j.watres.2017.02.007

Sötemann, S. W., Ristow, N. W., Wentzel, M. C., & Ekama, G. A. (2005). A steady state model for anaerobic digestion of sewage sludges. *WaterSA*, Vol. 31, pp. 511–527. https://doi.org/10.4314/wsa.v31i4.5143

Takács, I. (2008). EXPERIMENTS IN ACTIVATED SLUDGE. Retrieved from https://library.wur.nl/WebQuery/hydrotheek/1868878

Takacs, I., Patry, G. G., & Nolasco, D. (1991). A dynamic model of the clarification-tickening process. *Water Research*, *25*(10), 1263–1271.

Tik, B. S., Maruéjouls, T., Bachis, G., Vallet, B., & Lessard, P. (2014). *Using particle settling velocity distributions to better model the fate of stormwater TSS throughout the integrated urban wastewater system*. 48–52. Retrieved from http://modeleau.fsg.ulaval.ca/fileadmin/modeleau/documents/Publications/pvr1175.pdf

Vallet, B. (2011). Modélisation d ' un bassin d ' orage en vue de l ' amélioration de la qualité des rivières par la gestion en temps réel Sommaire Mise en contexte Mise en contexte. *PhD Thesis*, 1–19.

Vallet, B., Muschalla, D., Lessard, P., & Vanrolleghem, P. A. (2014). A new dynamic water quality model for stormwater basins as a tool for urban runoff management: Concept and validation. *Urban Water Journal*, *11*(3), 211–220. https://doi.org/10.1080/1573062X.2013.775313

Vanhooren, H., Meirlaen, J., Amerlinck, Y., Claeys, F., Vangheluwe, H., & Vanrolleghem, P. A. (2003). WEST : modelling biological wastewater treatment. *Journal of Hydroinformatics*, 27–50.

Volcke, E. I. P., van Loosdrecht, M. C. M., & Vanrolleghem, P. A. (2006). Continuity-based model interfacing for plant-wide simulation: A general approach. *Water Research*, *40*(15), 2817–2828. https://doi.org/10.1016/j.watres.2006.05.011

Wentzel, M. C., Ekama, G. A., & Sötemann, S. W. (2006). Mass balance-based plant-wide wastewater treatment plant models - Part 1: Biodegradability of wastewater organics under anaerobic conditions. *Water SA*, *32*(3), 269–275. https://doi.org/10.4314/wsa.v32i3.5261

Wentzel, Mark C, Ekama, G. A., & Sötemann, S. W. (2006). Mass balance-based plant-wide wastewater treatment plant models – Part 1: Biodegradability of wastewater organics under anaerobic conditions. *Water SA*, *32*(1), 287–296. https://doi.org/10.4314/wsa.v32i3.5273

WRC. (1984). *Theory, design and operation of nutrient removal activated sludge processes*. *(Chs 4-6)*(Ed. Wiechers HNS, Water Research Commission, TT16/84 , ISBN 0 908356 13 7).

8. Appendices

Appendices 1: Wastewater Characteristics

Appendices 2: Discrete Particle Settling Model Calculation Results

Appendices 3: UCTPSU Model Implementation (Dynamic Mass Balances Checks)

Appendices 4: Statistical Tests Results Summary

8.1. Wastewater Characteristics

The wastewater characteristics have been fractionated in raw wastewater (raw WW), settled wastewater (settled WW) and primary sludge (PS) compositions, using appropriate mass ratios (WRC, 1984; Ekama, 2017).

Table 43: Raw WW COD

		COD	
		750.00	
Dissolved	VFA	FBSO	USO
199.00	36.00	110.00	53.00
Non-settleable		BPO	UPO
251.00		233.00	18.00
Settleable		BPO	UPO
300.00		206.00	94.00

Table 44: Raw WW TKN

			TKN	
			61.66	
Dissolved	FSA	VFA	FBSO	USO
48.53	45.00	0.00	1.70	1.83
Non-settleable			BPO	UPO
4.17			2.95	1.22
Settleable			BPO	UPO
8.96			2.61	6.35

Table 45: Raw WW TP

			TP	
			17.59	
Dissolved	OP	VFA	FBSO	USO
12.78	11.46	0.00	1.32	0.00
Non-settleable			BPO	UPO
1.86			1.55	0.30
Settleable			BPO	UPO
2.96			1.37	1.59

Table 46: Raw WW C

		C	
		256.51	
Dissolved	VFA	FBSO	USO
68.08	13.50	36.41	18.18
Non-settleable		BPO	UPO
85.52		79.22	6.30
Settleable		BPO	UPO
102.92		70.04	32.88

Table 47: Settled WW COD

		COD	
		450.00	
Dissolved	VFA	FBSO	USO
199.00	36.00	110.00	53.00
Non-settleable		BPO	UPO
251.00		233.00	18.00
Settleable		BPO	UPO
0.00		0.00	0.00

Table 48: Settled WW TKN

			TKN	
			52.70	
Dissolved	FSA	VFA	FBSO	USO
48.53	45.00	0.00	1.70	1.83
Non-settleable			BPO	UPO
4.17			2.95	1.22
Settleable			BPO	UPO
0.00			0.00	0.00

Table 49: Settled WW TP

			TP	
			14.63	
Dissolved	OP	VFA	FBSO	USO
12.78	11.46	0.00	1.32	0.00
Non-settleable			BPO	UPO
1.86			1.55	0.30
Settleable			BPO	UPO
0.00			0.00	0.00

Table 50: Settled WW C

		C	
		153.60	
Dissolved	VFA	FBSO	USO
68.08	13.50	36.41	18.18
Non-settleable		BPO	UPO
85.52		79.22	6.30
Settleable		BPO	UPO
0.00		0.00	0.00

Table 51: PS COD

		COD	
		60450.00	
Dissolved	VFA	FBSO	USO
199.00	36.00	110.00	53.00
Non-settleable		BPO	UPO
251.00		233.00	18.00
Settleable		BPO	UPO
60000.00		41200.00	18800.00

Table 52: PS TKN

			TKN	
			1843.98	
Dissolved	FSA	VFA	FBSO	USO
48.53	45.00	0.00	1.70	1.83
Non-settleable			BPO	UPO
4.17			2.95	1.22
Settleable			BPO	UPO
1791.28			521.87	1269.41

Table 53: PS TP

			TP	
			606.65	
Dissolved	OP	VFA	FBSO	USO
12.78	11.46	0.00	1.32	0.00
Non-settleable			BPO	UPO
1.86			1.55	0.30
Settleable			BPO	UPO
592.02			274.67	317.35

Table 54: PS C

		C	
		20737.15	
Dissolved	VFA	FBSO	USO
68.08	13.50	36.41	18.18
Non-settleable		BPO	UPO
85.52		79.22	6.30
Settleable		BPO	UPO
20583.56		14008.00	6575.56

Table 55: Flows and Loadings for Raw WW

Time dt (h)	Flow (m^3/h)	Flow (Ml/d)	Total COD (mgCOD/l)	VFA (mgCOD/l)	FBSO (mgCOD/l)	USO (mgCOD/l)	Settleable BPO (mgCOD/l)	Non-Settleable BPO (mgCOD/l)	Settleable UPO (mgCOD/l)	Non-Settleable UPO (mgCOD/l)	FSA (mgN/l)	TKN (mgN/l)
06H00	225.0	5.4	289.12	0.00	56.67	20.05	79.37	89.86	36.23	6.95	17.97	24.38
08H00	315.6	7.6	292.56	0.00	57.34	20.28	80.31	90.93	36.66	7.03	27.15	33.64
10H00	937.5	22.5	550.70	0.00	107.94	38.18	151.18	171.17	69.01	13.23	42.19	54.40
12H00	1075.0	25.8	757.22	0.00	148.41	52.50	207.87	235.35	94.88	18.19	49.23	66.01
14H00	906.3	21.8	853.59	0.00	167.30	59.18	234.33	265.31	106.96	20.51	54.70	73.62
16H00	731.3	17.6	874.24	0.00	171.35	60.61	240.00	271.73	109.55	21.01	58.60	77.98
18H00	637.5	15.3	963.73	0.00	188.89	66.82	264.57	299.54	120.76	23.16	48.84	70.20
20H00	725.0	17.4	894.89	0.00	175.40	62.05	245.67	278.14	112.14	21.50	44.93	64.77
22H00	662.5	15.9	826.06	0.00	161.91	57.27	226.77	256.75	103.51	19.85	40.24	58.55
00H00	606.3	14.6	791.64	0.00	155.16	54.89	217.32	246.05	99.20	19.02	31.25	48.80
02H00	425.0	10.2	722.80	0.00	141.67	50.11	198.42	224.65	90.57	17.37	29.30	45.32
04H00	275.0	6.6	481.87	0.00	94.45	33.41	132.28	149.77	60.38	11.58	23.83	34.51
06H00	225.0	5.4	289.12	0.00	56.67	20.05	79.37	89.86	36.23	6.95	17.97	24.38
Mean	625.0	15.0	688.38	0.00	134.92	47.73	188.98	213.96	86.26	16.54	39.07	54.33
FWA	625.0	15.0	750.00	0.00	147.00	52.00	205.89	233.11	93.98	18.02	43.40	60.03

Table 56: Flows and Loadings for Raw WW (Continued)

Time dt (h)	OP (mgP/l)	TP (mgP/l)	Settleable and Non-Settleable ISS (mgISS/l)	Settleable and Non-Settleable TSS (mgTSS/l)	Settleable and Non-Settleable VSS (mgVSS/l)	Settleable ISS (mgISS/l)	Settleable TSS (mgTSS/l)	Settleable VSS (mgVSS/l)	Settleable TSS (ml/l)
06H00	2.89	5.14	15.16	157.14	141.97	12.13	89.51	77.38	3.40
08H00	2.55	4.84	24.91	168.57	143.66	19.93	98.22	78.30	3.73
10H00	5.92	10.22	34.66	305.08	270.43	27.73	175.11	147.38	6.66
12H00	8.51	14.42	51.99	423.82	371.84	41.59	244.24	202.65	9.29
14H00	9.40	16.06	56.32	475.48	419.16	45.05	273.50	228.44	10.40
16H00	9.84	16.66	60.65	489.95	429.30	48.52	282.49	233.97	10.74
18H00	10.88	18.40	64.98	538.23	473.25	51.99	309.90	257.92	11.78
20H00	9.62	16.60	56.32	495.76	439.44	45.05	284.55	239.49	10.82
22H00	8.80	15.25	47.65	453.29	405.64	38.12	259.19	221.07	9.86
00H00	8.06	14.24	43.32	432.06	388.74	34.66	246.52	211.86	9.37
02H00	7.77	13.41	38.99	393.92	354.93	31.19	224.63	193.44	8.54
04H00	5.18	8.94	23.83	260.45	236.62	19.06	148.02	128.96	5.63
06H00	2.89	5.14	15.16	157.14	141.97	12.13	89.51	77.38	3.40
Mean	7.40	12.77	43.32	381.35	338.03	34.66	218.88	184.23	8.32
FWA	8.15	14.00	48.00	416.29	368.29	38.40	239.12	200.72	9.09

8.2. Discrete Particle Settling Model Calculation Results

This section presents checks of mass balances for the WRC (1984) and Ekama (2017) data set, as well as mass balances for the steady state and dynamic calculations.

8.2.1. Mass Balances for the WRC (1984) and Ekama (2017) Data Set

Table 57: Mass Balances for the Data Set

Raw Wastewater			**Settled Wastewater**		**Primary Sludge**		
Flow (Ml/d)	15.0		14.9		0.1		
	Fluxes (kg/d)	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Mass Balances (%)**
TSS	6244.4	416.29	2641.5	176.99	3602.8	48037.78	100.0
VSS	5524.4	368.29	2499.8	167.49	3024.6	40328.28	100.0
ISS	720.0	48.00	141.8	9.50	578.2	7709.50	100.0
UPO	1134.4	75.62	181.4	12.15	953.0	12706.28	100.0
BPO	4390.0	292.67	2318.4	155.33	2071.7	27622.00	100.0
COD	11250.0	750.00	6716.3	450.00	4533.8	60450.00	100.0
OrgN	924.8	61.66	786.5	52.70	138.3	1843.98	100.0
OrgP	263.9	17.59	218.4	14.63	45.5	606.65	100.0
OrgC	3847.7	256.51	2292.4	153.60	1555.3	20737.15	100.0

8.2.2. Steady State Calculations Mass Balances

Table 58: Mass Balances for Calculations under Steady State Conditions

Raw Wastewater			**Settled Wastewater**		**Primary Sludge**			
Flow (Ml/d)	15.0		14.9		0.1		**Mass Balances (%)**	
	Fluxes (kg/d)	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Model consistency**	**Model accuracy**
TSS	6244.4	416.29	2650.0	177.55	3594.4	47925.36	100.0	99.9
VSS	5524.4	368.29	2508.2	168.05	3016.2	40215.60	100.0	99.9
ISS	720.0	48.00	141.8	9.50	578.2	7709.76	100.0	100.0
UPO	1134.4	75.62	181.5	12.16	952.9	12704.93	100.0	100.0
BPO	4390.0	292.67	2326.7	155.89	2063.3	27510.67	100.0	99.8
COD	11250.0	750.00	6743.9	451.85	4506.2	60082.00	100.0	99.8
OrgN	924.8	61.66	790.4	52.96	134.5	1793.20	100.0	99.6
OrgP	263.9	17.59	219.5	14.70	44.5	592.73	100.0	99.6
OrgC	3847.7	256.51	2301.9	154.23	1545.9	20611.59	100.0	99.8

8.2.3. Dynamic Calculations Mass Balances

Table 59: Mass Balances for Calculations under Dynamic Conditions

Raw Wastewater			Settled Wastewater		Primary Sludge			
Flow (Ml/d)	15.0		14.9		0.1		**Mass Balances (%)**	
	Fluxes (kg/d)	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Fluxes (kg/d)**	**Concs (mg/l)**	**Model consistency**	**Model accuracy**
TSS	6244.4	416.29	2642.0	177.02	3602.4	48032.02	100.0	100.0
VSS	5524.4	368.29	2500.4	167.53	3024.0	40319.69	100.0	100.0
ISS	720.0	48.00	141.6	9.49	578.4	7712.34	100.0	100.0
UPO	1134.4	75.62	181.1	12.13	953.3	12710.71	100.0	100.0
BPO	4390.0	292.67	2319.3	155.40	2070.7	27608.97	100.0	100.0
COD	11250.0	750.00	6732.2	451.07	4517.9	60238.03	100.0	99.9
OrgN	924.8	61.66	790.2	52.94	134.7	1795.64	100.0	99.6
OrgP	263.9	17.59	219.4	14.70	44.5	593.86	100.0	99.6
OrgC	3847.7	256.51	2297.9	153.96	1549.9	20664.73	100.0	99.9

8.3. UCTPSU Model Implementation (Dynamic Mass Balances Checks)

The checks on mass balances were performed using the data set from WRC (1984) and Ekama (2017). A very high settling velocity scenario (see Section 5.2.3.2 of Chapter 5) was used for these mass balance checks. The ISS component was used as a sample calculation, for a period of 6 hours. Since the simulations are dynamic, there is a change in the concentrations and, hence, masses of particles in the UCTPSU model. That change in mass is no more constant than in the case of steady state simulations and, therefore, needs to be accounted for. As such, the mass balances are expressed as follow:

Mass entering the UCTPSU = Mass exiting via the UCTPSU overflow + Mass exiting via the UCTPSU underflow

+ Mass in the layers within the UCTPSU

To perform the mass balances, the concentration distribution of the ISS sub-components are extracted, from the 1st to the 10th layer. That distribution is summarized in Table 60.

Table 60: Concentration Distribution of ISS within the UCTPSU Layers for the Period of Simulation (6 hours)

Concentrations (g/m^3)	Value
C_s(X_ISS1)(1)	0.00
C_s(X_ISS2)(1)	0.00
C_s(X_ISS3)(1)	0.00
C_s(X_ISS4)(1)	0.00
C_s(X_ISS5)(1)	0.00
C_s(X_ISS1)(2)	0.00
C_s(X_ISS2)(2)	0.00
C_s(X_ISS3)(2)	0.00
C_s(X_ISS4)(2)	0.00
C_s(X_ISS5)(2)	0.00
C_s(X_ISS1)(3)	0.00
C_s(X_ISS2)(3)	0.00
C_s(X_ISS3)(3)	0.00
C_s(X_ISS4)(3)	0.00
C_s(X_ISS5)(3)	0.00
C_s(X_ISS1)(4)	0.06

C_s(X_ISS2)(4)	0.00
C_s(X_ISS3)(4)	0.00
C_s(X_ISS4)(4)	0.00
C_s(X_ISS5)(4)	0.00
C_s(X_ISS1)(5)	0.99
C_s(X_ISS2)(5)	0.00
C_s(X_ISS3)(5)	0.00
C_s(X_ISS4)(5)	0.00
C_s(X_ISS5)(5)	0.00
C_s(X_ISS1)(6)	0.99
C_s(X_ISS2)(6)	0.00
C_s(X_ISS3)(6)	0.00
C_s(X_ISS4)(6)	0.00
C_s(X_ISS5)(6)	0.00
C_s(X_ISS1)(7)	0.99
C_s(X_ISS2)(7)	0.00
C_s(X_ISS3)(7)	0.00
C_s(X_ISS4)(7)	0.00
C_s(X_ISS5)(7)	0.00
C_s(X_ISS1)(8)	0.99
C_s(X_ISS2)(8)	0.00
C_s(X_ISS3)(8)	0.00
C_s(X_ISS4)(8)	0.00
C_s(X_ISS5)(8)	0.00
C_s(X_ISS1)(9)	0.99
C_s(X_ISS2)(9)	0.00
C_s(X_ISS3)(9)	0.00
C_s(X_ISS4)(9)	0.00
C_s(X_ISS5)(9)	0.00
C_s(X_ISS1)(10)	71.69
C_s(X_ISS2)(10)	0.00

C_s(X_ISS3)(10)	0.00
C_s(X_ISS4)(10)	0.00
C_s(X_ISS5)(10)	0.00

The total concentrations of ISS exiting the UCTPSU via the overflow (Conc_over) and the underflow (Conc_under) are calculated as the sums of the concentrations of the ISS sub-components in the 1st layer and the 10th layer, respectively. The masses in the overflow and underflow are, therefore, calculated by multiplying the concentrations by the respective flows. Furthermore, the mass changes within the layers are computed by multiplying the concentrations of each sub-component from the 1st to the 10th layer, with the volume of a layer (which is uniform throughout the UCTPSU model). These results are presented in Table 61.

Table 61: Dynamic Mass Balances Results

Parameters	**Value**
Q_in (m^3/d)	5400.0
Q_out (m^3/d)	75.0
Q_under (m^3/d)	5325.0
Variables	**Value**
Conc_over (g/m^3)	0.00
Conc_under (g/m^3)	71.70
Flux_in (g/d)	82080.0
Mass_in (g)	20520.0
Mass_overflow (g)	0.00
Mass_underflow (g)	672.1
Mass Change in the 1st layer	0.0
Mass Change from the 2nd to the 9th layer	1307.1
Mass Change in the 10th layer	18640.2
Total Mass Out (g)	20619.5
Mass Balances (%)	**100.5**

8.4. Statistical Tests Results Summary

Table 62: Summary of Results of χ^2 Test of Homogeneity

Downstream Processes Outputs		DoF	p-value
Settled Wastewater Composition	Scenario 1 vs Scenario 2	6	**0.0006**
	Scenario 1 vs Data Set	6	**0.0003**
	Scenario 2 vs Data Set	6	1.0000
AS System Capacity Estimation (Scenario 1 vs Scenario 2)		2	**0.0025**
Effluent Quality (Scenario 1 vs Scenario 2)		5	0.2446
Energy Consumption and Generation (Scenario 1 vs Scenario 2)		2	0.2640
Anaerobic Digestion of the PS Concentrations (Scenario 1 vs Scenario 2)		7	**0.0000**
Anaerobic Digestion of the WAS Concentrations (Scenario 1 vs Scenario 2)		7	**0.0000**

DoF = Degrees of Freedom

p-values (<0.05) in bold imply the null hypothesis should be rejected; the difference in the results of the scenarios are statistically significant.

p-values not in bold imply the null hypothesis should not be rejected; the difference in the results of the scenarios are not statistically significant.