University College London

Doctoral Thesis

Mathematical Modelling of Clean Water Treatment Works

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A thesis submitted in fulfillment of the requirements
for the degree of Doctor of Philosphy
in the

Centre for Process Systems Engineering
Department of Chemical Engineering

2017

I, Folashade Akinmolayan, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

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Signature

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Date

Acknowledgements

Through the years, I met so many wonderful people I am thankful for seeing me through this journey. Firstly, I would like the thank Professor Eva Sorensen for guiding a nervous student. You have played so many important roles in my life, initially a supervisor, a line manager, a friend and a constant shoulder to cry on. Thank you for correcting me when I was wrong (spelling and grammar especially), supporting me when I was right, and taking time out of your own life to ensure I did not procrastinate. You have help mould me into the woman I have become today and I am beyond grateful our paths crossed. I am grateful to my secondary supervisor Professor Nina Thornhill for all the interesting discussions and your eye for details.

To the close friends before this journey: Gurbinder, Saffie, Folake, Beverley, Mickal, Bianca, Sara, Nafisah, Belquis, "The Lous", Vidal and Carl.

To the friends I met along the way: Rema, Matt, Mithila, Ishanka, Chara, Noor, Matteo, George and Alex.

You have all played a crucial role in this chapter of my life.

To Eria and Vivien, thank you for the long distance encouragement and entertainment.

To my "lovely ladies" lunch club: Emanuela, Kate, and Elpida thank you for your continued words of wisdom and encouragement.

Vassilis and Asif, you both are my PPSE best friends who always kept me laughing. You both understood the pains and joys of computer modelling. Thank you for your continued support and random adventures.

Above all I wish to thank my parents, siblings and nephews for their faith in me, their unconditional love, their endless support and understanding throughout all these years. None of this would be possible without them and to them I am eternally grateful. Special mentions go to my dad and my brother Ore for taking care of me when I neglected to take care of myself, for the sweet treats when I craved them but mostly for being there to kill the spiders whenever I needed them no matter the time of night.

Dami - thank you for your constant love, motivation, encouragement, Thai food and patience at all times. We shared this PhD journey together and you always cheered me up, stood by me through the good, bad and the panic because I could not solve an "error" in my code.

Abstract

One of the biggest operational risks to water companies arises from their ability to control the day-to-day management of their water treatment plants. With increasing pressures to remain competitive, companies are looking for solutions to be able to make predictions on how their treatment processes can be improved. This work focuses on mathematical modelling and optimisation of clean water treatment processes. The main motivation is to provide tools which water companies can use to predict the performance of their plants to enable better control of risks and uncertainties.

Most modelling work within water operations has so far been based on empirical observations rather than on mathematically describable relationships of the process as will be considered in this work. Mathematical models are essential to describe, predict and control the complicated interactions between the different parts of the treatment process, a concept which is well understood within the process industry but not yet established within the water treatment industry. This work will also consider the level of modelling detail actually required to accurately represent a water treatment plant.

This thesis develops the conceptual understanding of clean water treatment processes utilising first principles modelling techniques. The main objective of this work is the consideration of a complete mathematical model of an entire water treatment plant, which enables a wider view on how changes in one processing unit will affect the treatment process as a whole. The performance of the process models are first verified individually and are then combined to enable the simulation of a complete water treatment work. By using detailed modelling (especially gPROMS utilised in this work) requires specialist software knowledge. Without knowledge of advanced simulation tools or having a background in process modelling, the detailed models developed in this work would not be fully utilised if implemented in the water industry, if utilised at all. A systematic framework is presented for the development of simpler surrogate models that can be used to predict the effluent suspended solids concentration, for a given number of independent variables. This approach can provide valuable guidance in clean water treatment process design and operation, thus providing a tool to achieve better day-to-day performance management.

My thesis in a drop.

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Roman Symbols

A Cross-sectional area (m^2)

c_e Equilibrium concentration of suspended solids captured into flocs (mg/L)

$c_{m,0}$ Concentration of organisms at time t = 0 (org/mL)

c_m Concentration of organisms at any time after t = 0 (org/mL)

c_{n0} Initial number concentration of primary particles (L^{-1})

c_n Number concentration of primary particles (L^{-1})

D Concentration of disinfectant (mg/L)

d Diameter (m)

D_∞ Bulk particle diffusion coefficient (m^2/s)

d_c Collector diameter (m)

d_{disp} Dispersion function (m^2/s)

d_p Particle diameter (m)

D_x Dispersion coefficient in water (m^2/s)

F (Convective) flux function (mg/m^2s)

f_{bk} Kynch batch flux density function ($mg/(m^2s)$)

f_i Decay function of i^{th} reactant in water ($mg/L.s$)

g Gravitational constant (m/s^2)

G Velocity gradient (s^{-1})

I Intensity of UV radiation (W/cm^2)

J Hydraulic gradient in the clogged filter bed (-)

k Rate constant (s^{-1})

k_1 Reaction rate $(mg/L)^{1-\gamma}s^{-1}$)

K_A Collision constant (-)

K_B Break-up constant (s)

k_c Kinetic constant, coefficient of specific lethality for chlorine dioxide (L/mg.s)

k_o Kinetic constant, coefficient of specific lethality for ozone (L/mg.s)

k_{UV} Kinetic constant, a function of transmittance (cm^2/W)

N Number of deposited particles per filter grain which acts as additional collectors

n Number concentration of particle (L^{-1})

N_0 Inital particle count at time t=0 (-)

N_c Number of collectors in filter grains (-)

N_t Total particle count at time t (-)

Q Volumetric flow rate (L/s)

r Parameter in equation for f_{bk} (L/mg)

T Absolute temperature (K)

u Superficial fluid velocity (m/s)

V Volume (L)

v_0 Settling velocity of a single particle in unbounded fluid (m/s)

v_{hs} Settling velocity of a single particle in unbounded fluid (m/s)

w Maximum number of size categories in Smouluchowski equation (-)

x_i Normalised input variables influencing predicted response Z for surrogate model (-)

x_j Normalised input variables influencing predicted response Z for surrogate model (-)

Y_i Current input variables influencing predicted normalised x for surrogate model (-)

Z Predicted response for surrogate model (-)

Dimensionless

N_G Dimensionless gravitational force number given by $(\rho_p - \rho)gd_p^2/18\mu u$

N_{LO} Dimensionless van der Waals number given by $4A/9\pi\mu d_p^2 u$

N_R Dimensionless ratio of particle to collector size given by d_p/d_c

Greek Symbols

α Particle/filter attachment coefficients (-)

α_p Particle/particle attachment coefficients (-)

β Inverse of compactness factor (-)

β_0 Constant cofficient for surrogate model (-)

β_{ii} Quadratic interaction coefficient for surrogate model (-)

β_{ij} Quadratic interaction coefficient for surrogate model (-)

β_i Linear interaction coefficient for surrogate model (-)

η Single collector removal efficiency (-)

η_0 Single collector contact efficiency in the clean filter bed (-)

η_p Single deposited particle contact efficiency (-)

γ Empirical parameter which is related to the flow rate (-)

λ Filtration equation coefficient (-)

ϕ Coefficient related to floc resistance (-)

ρ_p Suspended solid density (mg/L)

σ Specific deposit (mg/L)

σ_c Critical specific deposit (mg/L)

τ Contact time (s^{-1})

τ Residence time (s)

Υ Order of reaction (-)

ε Filter medium porosity (-)

ϖ Detachment coefficient (s^{-1})

ϖ_0 Constant for a particular filtration system (s^{-1})

Subscripts

z Depth in the z-axis

c Concentration

e Effluent

f Feed

i Particles

j Particles

k Particles

n0 Concentrations of primary particles at time t=0 (mg/L)

ni ith and mth number of flocculation chambers

nm mth number of flocculation chambers

s Suspended solid

u Underflow

Abbreviations

ANN Artifical Neutral Network

Bottom Depth of thickening zone (m)

CFD Computational Fluid Dynamics

DAEs Differential Algebraic Equations

DAF Dissolved Air Flotation

NOM Natural Organic Matter

ODEs Ordinary Differential Equations

PBT Population Balance Theory

PDEs Partial Differential Equations

PSE Process Systems Engineering

RSM Response Surface Modelling

SCC Single Collector Collision

SST Secondary Settling Tank

TOC Total Organic Carbon

Top Height of clarification zone (m)

UV Ultraviolet

WTW Water Treatment Work

WWT Wastewater Treatment

Chapter 1

General introduction

In this chapter, a general background of water quality and raw water sources are presented, along with a summary of the various processing units available in normal clean water treatment facilities. The motivation and objectives of this thesis are highlighted, followed by an outline of the thesis structure.

1.1 Scope

The availability of a reliable and clean supply of water is vital for our health and well-being, and for agriculture, fisheries, industry and transportation. A major challenge facing a sustainable global future is the ever increasing demand for clean water of adequate quality and quantity. Even though water is one of the world's most abundant resources, there are many regions that are in low supply of clean water (Veoila, 2014). A source of water that is deemed safe to drink or to use for preparation of food is known as clean water or drinking water. Figure 1.1 shows the globally available raw water that can be utilised as clean water sources. The figure highlights that most of the world's water is in the oceans and saline lakes; this water will be salty and will require desalination in order to make it usable for most purposes. Fresh water is approximately 3% of the planet's water, but most of that is in the form of snow or ice. A report by the United Nations warns that "overcoming the crisis in water is one of the greatest human development challenges of the early 21st century" (UNDP, 2006). In 2008, 6.74

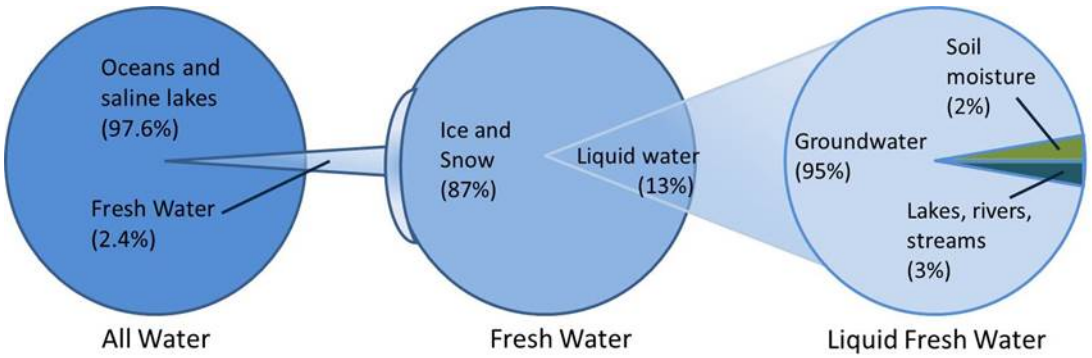


Figure 1.1: Breakdown of the water availability in the world.

billion people (about 85% of the global population) had access to a piped water supply through house connections, or to an improved water source through other means than via a house connection (DEFRA, 2014). Generally, the main challenges currently facing the water industry are (DEFRA, 2014):

- Population increase: The constant growth in global population leads to an increase in the demand for water.
- Climate change: Warmer climates, extreme weather events, and an unexpected increase in droughts can occur as a result of climate change. This decrease in water availability will lead to poorer water quality and develop a threat in sustaining economically important wildlife and species. With an expected decline in both leakage and the demand from individual households, the overall water demand is predicted to decrease; climate change will have an impact on the overall demand as more water is utilised in hotter conditions. Also, the push for a low carbon economy may increase water usage by industry.

In the UK, the problem of ensuring sufficient water supply that meets the stringent water regulations, will be intensified in the future by a combination of a rising population, climate change and the increased difficulty of building major new water infrastructure due to limitations in the amount of land accessible for new developments. Since the 1950s, household water demand has been increasing, due to changes in the use of water in the home and population growth; it is now more than half of all public water supply use, as shown in Figure 1.2 (DEFRA, 2014). It is estimated that the average water use in England is currently about 150 litres per person per day, equivalent to approximately one tonne of water per week.

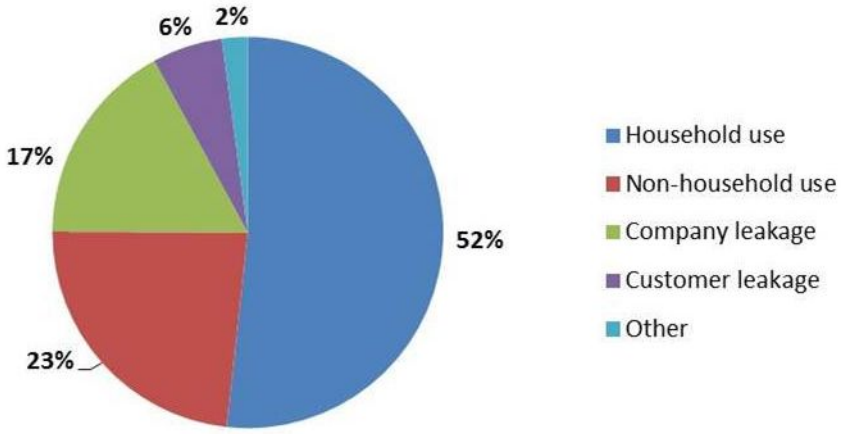


Figure 1.2: Public water supply for England and Wales (megalitres per day) (DEFRA, 2014).

Within the EU, comparisons between country water usage are not always straightforward, although it seems many other countries are using significantly less than England (Figure 1.3). These current levels of water usage are unsustainable and recent efforts to address this usage have led to the development of new purification processes and improved water management techniques; however, over the next 20 years, behavioural changes and technological innovation will be needed to find a balance between the supply and demand of water (IChemE, 2007). One change currently being explored is the use of advanced computational tools in the management of technological risk, for example, arising from process uncertainty, innovation and early design decisions. Innovation is essential for any business to establish and maintain a competitive advantage, and involves making decisions in the absence of complete information, and this inevitably leads to risks. Computational tools, in this instance, can involve the use of mathematical models for: (a) the effective quantification of the technological risks associated with model-based decisions and (b) the optimisation of process design and operation through comprehensive studies into the alternatives. With successful implementation, tools will be able to predict the effects of design and operating decisions on key performance indicators within the accuracy necessary to achieve business objectives. Within the water industry, utilising computational tools will support decisions that account for both the treatment process and the impact of these decisions on the other parts of the business.

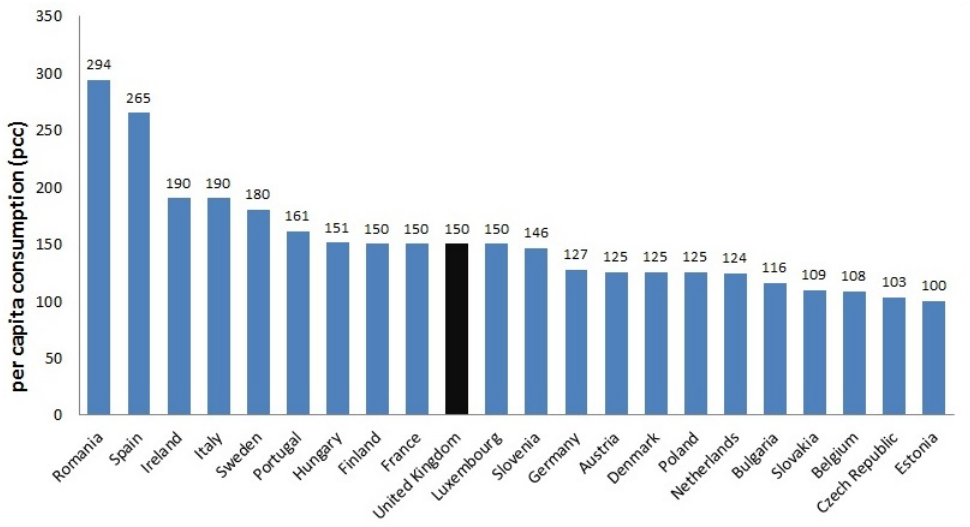


Figure 1.3: EU per capita water consumption (DEFRA, 2014).

1.2 Water Industry: raw water

Water quality regulations

The European Directive (Directive, 1998) on the quality of water intended for human consumption prescribes standards for the quality of drinking water, water offered for sale in bottles or containers, and water for use in food production undertakings. The requirements have been incorporated into the Water Supply Regulations 2000 in England and Wales (Directive, 1998). The main objective of the water quality standards is to protect human health from adverse effects resulting from excessive concentrations of potentially health-damaging substances in drinking water. The presence of microbiological and chemical contaminants in drinking water can lead to acute or chronic health effects, making the removal of these a primary concern for water treatment. The directive distinguishes between different contaminants by dividing them into two types: mandatory (these cannot exceed a specific parameter value) and non-mandatory (the specific parameter value can be used as an indicator) (Binnie and Kimber, 2009). The mandatory standards covers 28 microbiological and chemical parameters that are essential to be removed, whilst the non-mandatory standards covers 20 further microbiological, chemical and physical parameters that are prescribed for monitoring purposes (a table with all the parameters can be found in Appendix A). Microbes are

the primary contaminants of concern particularly Giardia[1] and Cryptosporidium[2], as they have adverse effects on our health. A specific regulation on the treatment of both Giardia and Cryptosporidium has been set to less than one oocyst[3], which are about five thousandths of a millimetre in diameter - is less than one-tenth the thickness of a human hair (Centers for Disease Control and Prevention, 2015a,b). The physical parameters include indicators such as turbidity[4], which is an important measure of discoloured water. Turbidity is often used as the main indication for the presence of suspended solids in the water (and will be discussed in more detail later).

1.2.1 Raw water sources

The type of raw water entering a clean water treatment plant will have an impact on the degree of removal efficiency for suspended solids throughout the system. Rational selection of raw water sources requires a review of the alternative sources available and their respective characteristics. The raw water that is used for drinking water treatment plants are categorised based on their source as upland water, lowland water, and a mixture of water that can be held in a reservoir. Upland water (surface water) can be from moorland springs and rivers, which have higher suspended solids concentration due to the fact they have contact with mineral deposits in the soil. Lowland waters (groundwater) are fed from upland lakes and groundwater springs and these have a lower suspended solids concentration as these waters are found in underground aquifers. This means many of the microorganisms and suspended solids have to pass through solids and rocks which act as a filter. The organic content of these waters can vary significantly from season to season especially following the first winter rains.

Groundwater

Any water that is underground can be classified as groundwater. Although groundwater is generally considered to be less likely to be contaminated than surface water, it may still require contaminant removal. Some surface water sinks into the ground, passing

[1]Giardia is a microscopic parasite that is considered one of the most common sources of waterborne illnesses (Centers for Disease Control and Prevention, 2015b). It is an intestinal infection identified by abdominal cramps, bloating, nausea and periods of watery diarrhoea.

[2]Cryptosporidium is a protozoan parasite that can infect the gut, thus causing an infection which leads to diarrhoea (Centers for Disease Control and Prevention, 2015a).

[3]An egg-like state of microscopic parasites that can be found in clean water (Centers for Disease Control and Prevention, 2015a).

[4]Turbidity is a key measurement of water quality and can be defined as the cloudiness in the fluid caused by suspended solids that are generally invisible to the naked eye (Binnie and Kimber, 2009).

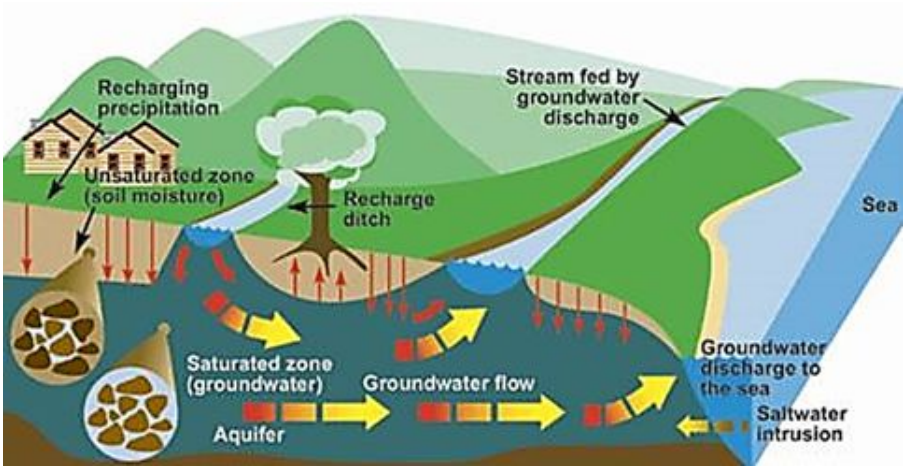


Figure 1.4: Illustration to show how water enters the unsaturated zone (soil moisture) and the saturated zone (groundwater) (Environment and Climate Change Canada, 2013).

through layers of sand, clay, rock, and gravel which clean the water (as can be seen in Figure 1.4). The water that sinks into the groundwater occurs in two different zones: unsaturated zone and saturated zone. In the unsaturated zone, pore spaces contain air; therefore, groundwater can not be easily taken from this zone. Usable groundwater occurs in the saturated zone, where pore spaces are completely filled with water. Even though groundwater will not be exposed to the same contaminants that surface water is subjected to, contaminants can nevertheless still be introduced; for instance, by rain washing fertilisers and insecticides into the soil where they will sink into the groundwater. The groundwater zones are contained and situated within aquifers and springs.

Aquifers can be classified by two types: confined and unconfined. Confined aquifers may be shallow or deep (Binnie and Kimber, 2009), and are characterised by being separated from the surface by an impermeable layer that confines the groundwater above and below it (Figure 1.5). An unconfined aquifer is often shallow, and it primarily contains permeable material. The top of the aquifer is called the water table although it does not have a flat surface, but has high areas and low areas.

Surface Water

Surface water is classified as water that collects on the ground or in streams, rivers, lakes or wetlands. The majority of these waters are exposed to contaminants due to the water being open to the atmosphere. Common contaminant sources can stem from untreated sewage and runoff from fertilised fields, parking lots, or unprotected

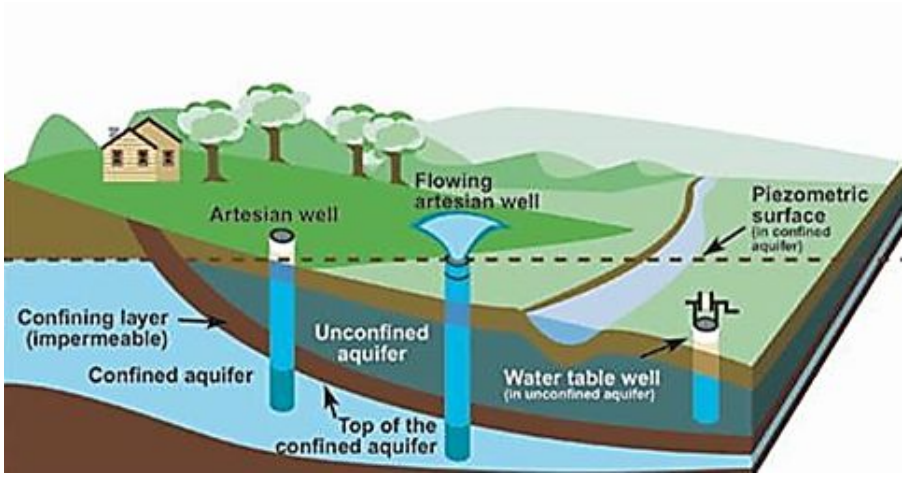


Figure 1.5: Illustration to show an artesian well, which has been drilled into a confined aquifer, and a water table well. The brown layer represents an "impermeable layer" (Environment and Climate Change Canada, 2013).

watersheds. Precipitation is the natural process to refill surface water, while the water can naturally be lost through discharge by evaporation and seeping into the ground.

Some public water systems, primarily those that utilise groundwater wells, can deliver untreated water directly to the customers' taps (Peavey et al., 1985; APEC Water, 2011). In the UK, most water tends to originate from either surface water or a blend of surface and groundwater. With many large public water systems drawing their raw water from surface sources such as lakes, streams, and rivers, which are vulnerable to many types of contamination (Viessman Jr and Hammer, 1985; APEC Water, 2011), in order to achieve clean water that adheres to the drinking water standards, a multi-stage clean water treatment approach involving a sequence of processes is needed.

1.3 Clean water treatment process

Clean water treatment is based on a wide range of unit operations, each contributing to some degree of removal or inactivation of contaminants from the raw water. These contaminants, or impurities, range in size from millimetres (grit and leaves) down to microns (colloids[5], viruses[6] and protozoa[7]). The actual treatment process is selected

[5]A colloid is a mixture in which one substance of microscopically dispersed insoluble particles is suspended throughout another substance.

[6]A virus is an infective agent that cannot grow or reproduce without a living cell.

[7]A protozoa is a parasitic single-celled organism that can divide only within a host organism.

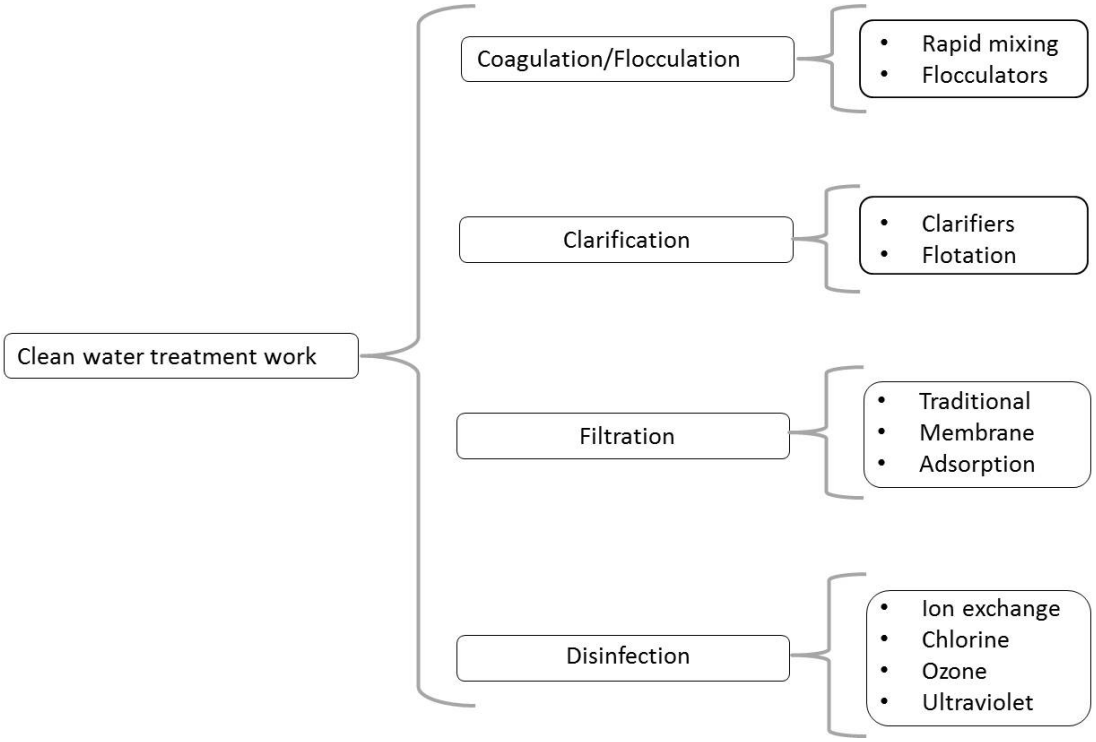


Figure 1.6: Main technologies available for water treatment processes.

based on various factors; the most critical being the nature of the water source and the intended use of the treated water.

There are a variety of unit operations that can be utilised for clean water treatment, which may vary slightly depending on different locations, the technology of the plant and the water it needs to process; however, the basic principles are largely the same. Figure 1.6 shows the hierarchical organisation of a typical water treatment work, where each main process (e.g. coagulation/flocculation) can have a variety of unit operations that can be selected to fulfil the requirements of that process (rapid mixing or flocculators). Table 1.1 explains in more detail the various unit operations and their typical applications.

Water treatment can be classified into clean water and wastewater treatment. The main difference between the two types of water treatment are the sources of water. For clean water treatment plants, generally the type of water that comes in is taken from surface water, groundwater or rainwater which is cleaned and distributed for human consumption; however, wastewater treatment plants collect sewerage and other wastewaters from various sites (such as from houses, industry etc.), cleans it and releases it back to the environment at a safe level for humans, fish and plants to be around. For these two types of treatment, the units can be broadly categorised into chemical and

Table 1.1: A description of typical unit processes used for the treatment of water (Crittenden et al., 2012).

Process	Unit operations	Description	Typical Application in Water treatment
Coagulation	*Rapid Mixing*	Process of destabilising colloidal particles so that particle growth can occur during flocculation. Mixing and blending two or more soluble solutions through input of energy.	Addition of chemicals (soluble solutions) such as ferric chloride, alum, and polymers to destabilise particles found in water.
Flocculation	*Flocculator*	Aggregation of particles that have been chemically destabilised through coagulation.	Used to create larger particles that can subsequently be more readily removed by other processes such as gravity settling or filtration.
Clarification	*Clarifier*	Removal of solids by gravity settling.	Used to remove particles greater than 0.5 mm in diameter, generally following coagulation and flocculation.
	Flotation	Removal of fine particles and flocculated particles with specific gravity less than water or with very low settling velocities so they float to the top of the fluid.	Removal of particles following coagulation and flocculation for high quality raw waters that are low in turbidity, colour and/or total organic carbon.
Filtration	*Traditional (Rapid gravity)*	The removal of particles by passing water through a bed of granular material; particles are removed by transport and attachment to the filter media.	Removal of solids following coagulation and flocculation, gravity sedimentation or flotation.
	Membrane	The removal of particles by passing water through a porous membrane material; particles are removed by size exclusion because the particles are larger than the pores.	Used to remove colour (turbidity), viruses, bacteria, and protozoa such as Gardia and Cryptosporidium.
Disinfection	*Chemical disinfection*	Addition of oxidising chemical agents to inactivate pathogenic organisms in water.	Disinfection of water with chlorine, chlorine compounds, or ozone.
	UV light oxidation	Use of UV light to oxidise complex organic molecules and compounds by disrupting the DNA structure of microorganisms.	Used for oxidation of organic molecules, such as in bacteria.

physical processing units. In chemical units, a chemical is added to induce a response; for instance, chlorine is added to inactivate bacterial microorganisms in the disinfection stage. The unit operations in physical processing units cause a physical change to the treated water; for instance, the impeller in the flocculation unit promotes growth of small colloidal particles after the addition of a chemical additive.

The raw water feed into clean water treatment processes often contain colloidal particles that cause the water to appear cloudy. The raw water is initially passed through mechanical mesh screens to remove large debris, after which it enters the coagulation unit. Chemical coagulants, such as aluminium sulphate, are then added to the raw water to destabilise the colloidal particles and this encourages the rapid formation of small particles, or agglomerates, through flocculation[8]. Solid-water separation processes, such as sedimentation, are used to reduce the floc concentration in the treated water; these unit types are broadly called clarification units, and they are important as they ensure the subsequent treatment process (usually filtration) can be operated more easily and cost-effectively to produce quality water. The process of filtration consists of passing water through a porous medium such as a bed of anthracite sand or other suitable material to retain solid matter whilst allowing the water to pass through. In order to achieve the required quality of filtered water, the filtration system has to retain particles larger than the pores and allow a flow of water to pass through the bed of media at a low speed. This will ensure the media retains most solid matter while permitting the water to pass to a final disinfection stage. The disinfection units are used to target the removal of microorganisms through the use of chemicals such as chlorine, UV dosing and ozonation.

1.4 Motivation

With a growing population and the impact of climate change, as well as reduced space available for new infrastructure, there are increasing pressures on the water industry. There is a greater need for more efficient water treatment works, whether it is to increase throughput, minimise capital expenditure or reduce operational costs. A better understanding of the fundamental knowledge of the individual treatment units and their interactions, including an understanding of the dynamic behaviour of the works, is needed in order to mitigate risks, such as reduced levels of water purity in distribution

[8]Flocculation is the promotion of floc growth through collision either in a slow mixing unit or using movement through baffled chambers.

due to an unexpected change in the earlier treatment processing steps. Although drinking water treatment works have been functioning for more than a century, in the last few decades the operation has become more and more complex (Trussell, 2000), which makes efficient management more challenging.

The operation of drinking water treatment works has traditionally been based on experience. Current raw water quality and flow can be different from what the treatment processes were originally designed to handle. Due to more stringent regulations (DEFRA, 2009), plants have to produce water of an increasingly higher quality, which requires intensive quality monitoring of the source, the product, and of the treatment work operation. Raw water quality is subject to changes, and these can be seasonal effects (e.g. temperature, turbidity), which affect long-term trends (e.g. salt content) or short-term trends (e.g. sudden heavy rain fall). The management of a treatment work can therefore be challenging, but the works are not currently controlled to the same level as, for instance, a chemical plant.

The IChemE technical strategy road-map (IChemE, 2007) indicates that technological advances are needed to secure sustainable water supplies, and research priorities should include water purification, water treatment, and sewage sludge disposal. The technologies utilised in water treatment can be energy intensive and the energy footprint in water can be substantial. In the UK, approximately 3% of the total national electricity consumption is utilised by the water industry. Over the past 20 years, the energy use has increased significantly, with power costs making up 13% of total production costs, and only 10% of power originating from renewable sources (Rothausen and Conway, 2011).

The challenge of meeting water demands is a complex one, demanding a difficult mix of political intervention, new technology, improved water conservation and distribution, increased technical and engineering skills. According to Rosen (2000) and Trussell (2000), by 2050 a drinking water treatment work will be entirely controlled from a central control centre, where dedicated integral control programmes incorporating advanced process and control models will control the treatment processes and mitigate risk. The development of detailed mathematical model representations of each water treatment process is therefore essential in order to meet this objective. Mathematical models are descriptions of real world systems, which can help enhance the understanding of the behaviour of complex systems. Many industries, such as chemicals, pharmaceuticals and food, are already making extensive use of mathematical modelling and optimisation tools as a way of enhancing their processes (Barakat and Sørensen, 2008; Klatt and

Marquardt, 2009; Bennamoun et al., 2009; Wang et al., 2013). Models used for these purposes, and to simulate the operation of a drinking water treatment work, must be accurate and must capture the main behaviour of the process, but must also be valid under changing process conditions.

Currently, research available in literature tends to narrow its focus to modelling specific aspects of each processing unit as opposed to focusing on the treatment work as a whole. For example, the mechanism for the removal of colloidal particles suspended in water has been extensively researched and modelled for the coagulation, flocculation and sedimentation unit operations individually (Holthoff et al., 1996; Edzwald and Van Benschoten, 1990; Edzwald, 1993; Saritha et al., 2015) but not how their interactions can be effectively utilised. A plant-wide modelling approach will allow for effective risk mitigation as the ability to see the cause and effect of changes through simulation is a powerful tool. Within the water industry, most modelling work tends to be empirical[9] rather than mechanistic[10]. The empirical approach is not rigorous and use of such models is limited to only specific applications and conditions, which is time consuming when trying to create varying scenarios. Mechanistic models are more robust and develop a more detailed understanding of the fundamentals occurring within unit operations. There are some existing models that are heavily reliant on mechanistic models based on experimental data. Many flocculation 'models' are data-driven (Thomas et al., 1999; Heddam et al., 2012) and are therefore difficult to generalise or extend to other treatment works. Other treatment processes, such clarification and filtration, have been more widely studied and the models incorporate more phenomenological occurrences so the models are on a sounder basis. A mathematical model that can provide a description of the connections between the individual units will be an important step in the direction of controlling a water treatment work via a central control centre.

In a process systems engineering approach, mathematical models are mainly derived from first principles utilising fundamental knowledge of the phenomena occurring. These models can, however, be quite complex, and simpler "surrogate" models can be derived from these models which will still be able to predict trends but at a fraction of the computational power. A system based on surrogate models would be an advantage (in comparison to a time consuming detailed model) to a central control centre, leading to monitoring of the water treatment works in real time. As the water industry aims

[9]Empirical modelling is based on empirical observations rather than on mathematically describable relaitonships of the system modelled.

[10]Mechanistic modelling is based on fundamental chemical and physical relationships which can be mathematically described, such as, diffusion.

to gain a competitive advantage, the implementation of a simpler surrogate model as an optimisation tool utilising fundamental knowledge would be beneficial as it can be applied to any site, with a change in the conditions.

1.5 Objectives and contributions of this thesis

Current research in the area of modelling clean water treatment works is young when considering the long history of the water treatment industry. As stated earlier, fundamental research so far has mainly focused on gaining an understanding of the individual units. To the best of the author's knowledge, currently no full mathematical model based on first principles which describes an entire conventional clean water treatment work is available in the open literature. The primary aim of this thesis is therefore to draw upon previous work in the literature to develop a first principles mathematical model of an entire conventional clean water treatment work.

The main deliverables from this work are:

1. A critical assessment of the current state-of-art in mathematical modelling in the clean water treatment industry, focusing on detailed mathematical models and optimisation techniques.
2. Development and validation of mathematical models for each of the main unit operation in a conventional clean water treatment works.
3. Development of a complete mathematical model of conventional clean water treatment works that can accurately describe the water treatment process mechanisms, and the connections between individual units.
4. Development of surrogate models for incorporation into a systematic method for the synthesis of clean water treatment works. These surrogate models should be able to accurately predict the mechanistic trends of the corresponding detailed mathematical model.

1.6 Organisation of this thesis

An introduction to the relevance of developing mathematical models of clean water treatment processing units has been given, and the general aim of the work has been set

out. The rest of the thesis is divided into six chapters. Chapter 2 provides an extensive literature review of current work related to modelling of processing units utilised in the water industry. An overview of the different methods, models and techniques currently available are analysed to comprehensively evaluate the applicability of these mathematical modelling tools.

Chapter 3 examines the development of mathematical models of clean water treatment unit operations based on first principles followed by model validation based on data from literature. The mathematical models considered are the three physical processing units in the conventional clean water treatment process: coagulation/flocculation, clarification and filtration. This chapter highlights that the knowledge and understanding of the individual clean water processing units can be advantageous through varying case studies and will lead to robust complete water treatment work models.

Chapter 4 considers the development and application of a complete water treatment work model. A first principles modelling based approach for linking individual clean water processing units, which are commonly studied in isolation, is proposed. Use of the model can include process development for design purposes, or as a training tool for work operators. The main advantages in the use of modelling can be realised when computational tools can be used as risk mitigation by simulating feedback responses to proposed changes in the work.

Chapter 5 addresses the need for computationally efficient mathematical models within the water industry, and explores the use of surrogate modelling techniques for optimisation or control purposes. The use of complex mathematical models will result in excessively detailed treatment work models and this could prove difficult to validate with a real world clean water treatment works. In addition to this, operators will need to be trained in order interact with the advanced computational tools used for detailed modelling whilst the simpler surrogate models can be simulated on Microsoft Excel which is more user friendly. The use of surrogate models will also reduce the computational time demand and this is an advantage in an industry that is trying to move away from, reactive to proactive approaches in its operation.

Finally, Chapter 6 concludes with the major findings of this work and with conclusions from each part of the project. A number of areas for future work are discussed. The chapter focuses in particular on the broader implications for the use of fundamental models of processing units in the water industry.

Chapter 2

Literature review

This chapter is divided into sections which present a detailed literature review on various processes in clean water treatment that motivate the objectives of this work, as outlined in chapter 1. The chapter begins by assessing the current state-of-the-art surrounding the use of mathematical models in the water industry, which is followed by how application of various methods utilised by process systems engineering can prove propitious to the clean water treatment processes.

2.1 Introduction

Water companies have resource management plans which look 25 years ahead to show projections of future demand for water and how the companies aim to meet this demand (Davies and Daykin, 2011). Every day, the UK water industry collects, treats and supplies more than 17 billion litres of purified water for domestic and commercial use, whilst simultaneously collecting and treating over 16 billion litres of the resulting wastewater to return to the environment (Binnie and Kimber, 2009).

To treat a particular water source, there are a number of key treatment processing steps that are generally used, most commonly coagulation, flocculation, clarification, filtration and disinfection, and each main step has a number of variations. The actual

treatment process route is selected based on various factors (Binnie and Kimber, 2009) as stated earlier, the most critical being the nature of the water source and the intended use of the treated water.

Traditionally, the water industry has been sitting within the civil engineering domain rather than the chemical engineering domain; however, due to the increasing pressure for companies to remain competitive in the national or global marketplace, the search for efficient methodologies for operational management and mitigation of risk has led some to consider the use of Process Systems Engineering (PSE) methods, in particular, detailed modelling from first principles, which have been highly successful within the chemical industries. The use of PSE methods for design and control within water treatment has been shown to lead to better water quality, cost reduction and to a greater stability performance of the plant as well as to an increased understanding of the individual treatment processing steps (Brouwer and De Blois, 2008; Rietveld et al., 2009). Modelling of the individual steps in clean water treatment has received some attention in terms of design and operation; however, very little has been considered in terms of the integration of the individual steps to create a representation of the overall plant performance which can be used for operational management.

The first part of this chapter will define what is meant by Process Systems Engineering (PSE) in a water treatment context, and will outline how this area has led to significant advances within other industries which are related, or similar, to clean water treatment (Klatt and Marquardt, 2009; Stephanopoulos and Reklaitis, 2011; Gernaey et al., 2012). At the core of any Process Systems Engineering (PSE) methodology is a detailed mathematical model of the process under investigation, and the second part of this chapter will focus on assessing the current state-of-the-art on the models available for the different clean water treatment processing steps, both as individual units and as a complete plant. These models can be incorporated into a wider PSE approach within clean water treatment with the aim to achieve better plant designs or retrofits as well as vastly improved operational management.

2.2 What is Process Systems Engineering (PSE)?

Process Systems Engineering (PSE) is an established area within chemical engineering with roots dating back to between the 1950s (Klatt and Marquardt, 2009) and the 1960s (Grossmann and Westerberg, 2000), with its progression closely linked to the

developments within computing. PSE involves the understanding and use of systematic and model-based solutions for the design and operation of chemical process systems (Ponton, 1995). There are numerous fields of PSE that have been considered in the past, are currently under investigation or are anticipated to be of high relevance to industry in the future. Grossmann and Westerberg (2000) provided a condensed summary of the main fields within the headings of process and product design, process control, process operation, and supporting tools. A few examples of how PSE methodologies have been applied in other industries are given in Table 2.1 to illustrate typical usage and advantages.

2.2.1 Fundamentals and methodologies of PSE

At the heart of any PSE method lays a mathematical model. A mathematical model is a description of a system in terms of equations that has been formulated to describe how the system behaves and to predict the physical and/or chemical behaviour of the system under different conditions. A simulation solves the equation set and shows either the conditions of the system at steady state or how the system behaves over time from a given initial condition (dynamic). The benefit of the simulation depends to a large extent on the accuracy of the model, i.e. whether the equations accurately describing the process in terms of its physical and/or chemical behaviour, and whether the parameter values used are accurate, i.e. statistically significant.

There are two main approaches to developing mathematical models: empirical modelling and mechanistic modelling. Empirical models are based on direct observation, measurement and extensive data records. These models depend on the availability of representative data for model building and validation with a "trial and error" approach is often adopted. Mechanistic models are based on a fundamental understanding of the chemistry and physics governing the behaviour of the system. They do not require much data for model development beyond that required for determining model parameters. The term "mechanistic model" is broad as it covers a variety of model types such as sets of ordinary differential equations (ODEs), differential algebraic equations (DAEs), and partial differential equations (PDEs).

Most modelling work within water operations has so far been based on empirical observations or hydraulic modelling[1] rather than mathematically describable relationships

[1]A hydraulic model is a mathematical model of a fluid introduced into a water/wastewater sewer/storm sewer system at various rates and pressures. These models can be used to analyse system hydraulic behaviour under variable conditions (Novak et al., 2010).

Table 2.1: Examples of uses of process systems engineering (PSE) principles in other industries.

Industry	Research area	Numerical techniques	Advantages	Author(s)
Chemicals	Heat exchanger and distillation network synthesis.	One, two and three dimensional finite element, finite difference and finite volume methods. Network optimisation using linear and non-linear programming.	By optimising design and operating conditions, more consistent and better product quality can be achieved. Improves competitiveness and increases profitability of their core business.	(Klatt and Marquardt, 2009; Barakat and Sørensen, 2008; Klemeš and Kravanja, 2013; Ochoa-Estopier et al., 2014)
Drying	Direct drying systems (i.e. flash dryers, spray dryers. etc).	Computational fluid dynamics (CFD).	Better understanding and design of drying equipment with less cost and effort than laboratory testing. Techniques have been successfully adapted to simulate the thermal processes of industrial dryers. These techniques have been routinely used owing to the availability of user-friendly commercial packages.	(Bennamoun et al., 2009; Jamaleddine and Ray, 2010)
Food	Heating and cooling processes	One, two and three dimensional finite element, finite difference and finite volume methods.	Deeper understanding of food processing means it is possible to evaluate design alternatives quickly and start commercial production at a faster rate. Models have the potential for integration with other models, such as biochemical and microbial reactions.	(Wang et al., 2013)

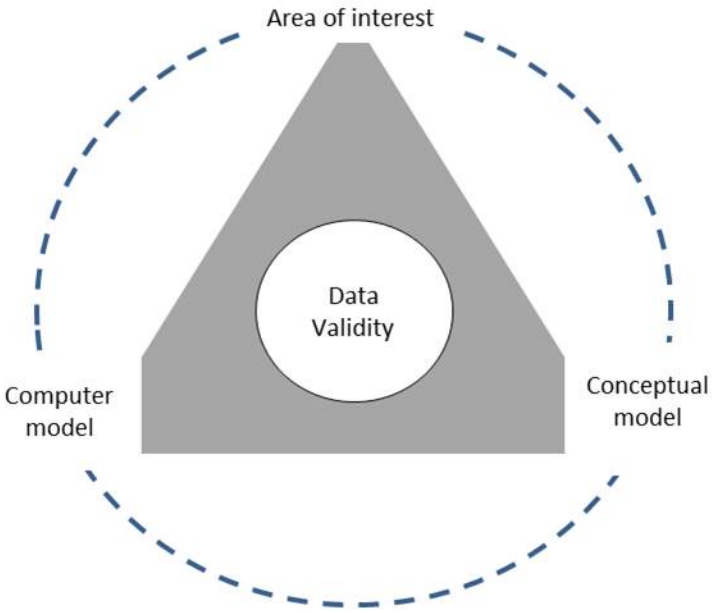


Figure 2.1: Graphical representation of the modelling process. Adapted with permissions from Sargent (2005).

of the process through mechanistic modelling. As mentioned earlier, the empirical approach to modelling is not rigorous and use of such models is limited to the specific conditions used in the development of the model. Mechanistic models, however, can be used for other applications of a similar type, and to some extent under other conditions, and are therefore far more powerful. For example, a mechanistic model developed for a distillation column in a refinery can be used to model a distillation column on other process plants, subject to varying conditions.

Roger Sargent, widely accepted as the Father of PSE, introduced a paradigm that relates model verification and validation to the model development process as illustrated in Figure 2.1 (Sargent, 2005). The real or proposed process to be modelled can be broadly labelled as the *"area of interest"*. The *"conceptual model"* is used to narrow down the area of interest to a specific study domain, e.g. an individual process unit, which will be the focus of the mathematical representation. At this stage, the theories and assumptions underlying the conceptual model are considered, checked and it is decided if the model will be fit for purpose, e.g. are the right parts of the process considered and under the right operating conditions. The representation is then implemented as a mathematical equation set within a *"computer model"*. The validity of the computer model has to be verified. Here, verification is defined as ensuring that both the equation set and the implementation of the model are accurate. The operational validation determines if the model's output has obtained a sufficient accuracy for the intended purpose, and this is

done through a series of computational experiments or simulation runs, under different scenarios or conditions. At the centre of the modelling process lies data validity, which is defined as ensuring that the necessary data for model building, validation and testing are all adequate and accurate to the required degree of accuracy. This data is usually obtained either from plant data or from separate experiments.

Modelling and simulation offer an efficient and powerful tool for system analysis which is as applicable to the clean water industry as it is to the chemical industries. Although the use of mathematical modelling is still limited within the clean water treatment industry, the use of mathematical modelling within the wastewater treatment industry, for instance, has become increasingly popular since its introduction in the mid-1990s (Dupont and Sinkjaer, 1994). Simulations using verified and accurate models can be used to obtained valuable information about a process far quicker than experiments and with minimal cost, and will lead to better water quality, reduction in capital expenditure, and more stable performance of a plant due to the increased understanding of the phenomena occurring.

2.2.2 Enterprise-wide optimisation

Enterprise wide modelling and optimisation is an area of research that lies in the interface between chemical engineering and operations research (Grossmann, 2005). There have been several papers that have reviewed enterprise-wide optimisation in terms of supply chain management in addition to process modelling and control (Larsson and Skogestad, 2000; Shah, 2005; Charpentier, 2005; Varma et al., 2007); however, as with all emerging technologies, EWO has challenges it has to face before it can be fully functional. One of the challenges highlighted by Grossmann (2005) states a major issue is integration of novel mathematical programming to capture the complexity of the various process operations.

One of the key features in the incorporation of a mathematical model of a full WTW is the integration of information and decision making amongst functions that comprise the process control region. According to Trussell (2000), Rosen (2000) and Grossmann (2005), within the next 30 years, a clean water treatment plant will be controlled from a central control centre where the dedicated integral control programmes which incorporate advanced process and control models will control the entire process.

Figure 2.2 represents an integrated framework for the application of a PSE method into the water industry. The collection of data in the water industry is by Supervisory

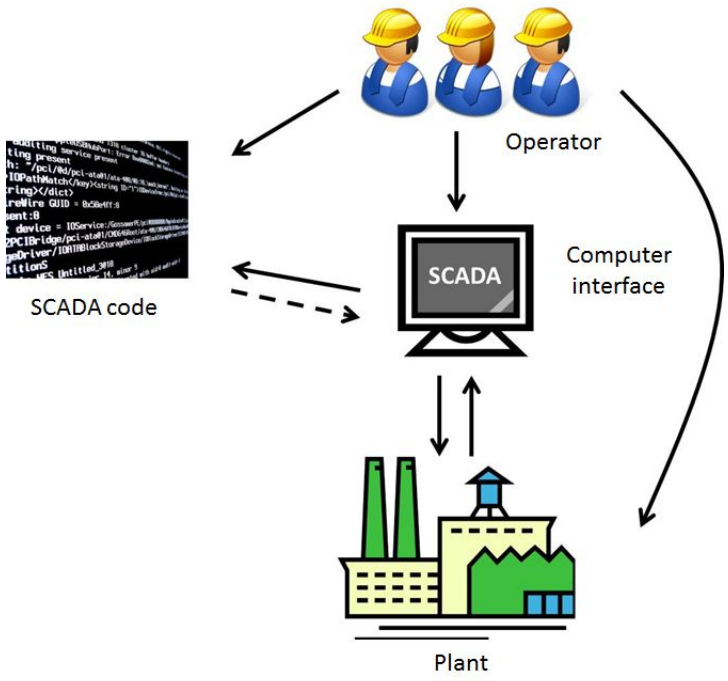


Figure 2.2: Integrated framework for PSE in a clean water treatment plant.

Control and Data Acquisition (SCADA) which can be used to monitor and control a plant or equipment. This control system may be automatic, or begin by operator commands. Ideally, the complete WTW mathematical model should be able to receive data from the SCADA screen to be able to predict how an imminent change in one unit will affect the quality of the water at a later stage in order to be able to mitigate the disturbance. The benefits of having a system like this in place will allow for information to be fed back, monitored and altered as needed, whether it is fully automated or user-controlled.

2.3 Mathematical modelling - clean water industry

Fundamental research within modelling of clean water treatment has so far mainly been focused on gaining an understanding of the individual treatment units or processing steps, and has (to a large extent) either considered very simple models or models focusing only on certain aspect of the unit. These models therefore do not provide a process unit description which is required if a full-plant model is to be considered and thus, the development of models to simulate an entire clean water treatment process would be extremely beneficial. These models would enable the ability to mitigate risks

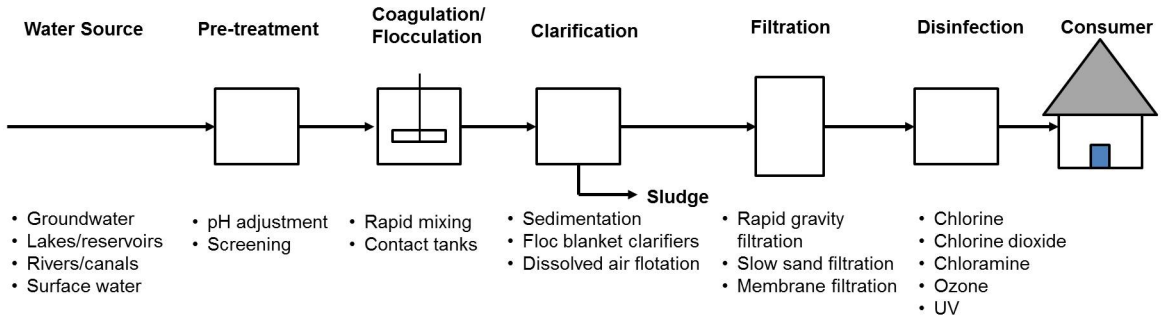


Figure 2.3: Typical process diagram for clean water treatment plant (with examples of variations).

by simulating feedback responses to proposed changes in the work. Use of such models can improve process development for design purposes, or as a training tool for work operators.

The processing steps or units used in clean water treatment plants generally vary depending on the source of raw water and the intended use of the treated water. In addition, the performance of one treatment unit affects the performance of the later units in the treatment process; hence, the evaluation of the performance of an overall clean water treatment plant becomes a highly complex problem.

Figure 2.3 presents a general schematic of conventional treatment processes for clean water, including examples of variations depending on the source water characteristics for pre-treatment stages (which are pH adjustment controls and mechanical units, such as, screens), coagulation (rapid mix), flocculation (contact tanks), clarification (sedimentation, floc blanket clarifiers, dissolved air flotation), filtration (rapid gravity, slow sand and membrane filtration) and chemical disinfection (chlorine, chlorine dioxide, chloramine, ozone and ultraviolet light). The physical process of each processing step can be studied and modelled in a variety of ways, which will lead to the enhanced fundamental knowledge; however, research tends to narrow its focus on specific aspects for each unit. The rest of this chapter is divided as follows: sub-section 2.3.1 considers the current debate between a correlation between turbidity and suspended solids concentration, which is an important consideration as suspended solids concentration is the usual variable in the mechanistic mathematical models whilst turbidity is the real world monitor for suspended solids concentration. Then sub-sections 2.3.2 to 2.3.5 review the available mathematical models for different aspects within the coagulation and flocculation, clarification, filtration and disinfection treatment processes. These sub-sections evaluate the available models focusing on comparisons and similarities

between mathematical models available in the clean water industry and within the water industry in general. Section 2.4 focuses on drawing from literature some answers to common questions. For example, why fundamental knowledge is based on particle concentration whilst real world application utilises turbidity, and whether a correlation can be found? Based on knowledge of the background chemistry, how can this information be incorporated to formulate process models? What are the current findings from the use of models in wastewater treatment and can these be applied to the clean water industry? Finally, Section 2.6 concludes with the major findings and conclusions from each part of the sections.

2.3.1 Turbidity vs. Suspended solids concentration

Particles present in water, such as suspended solids and dissolved coloured material, reduce water clarity by creating an opaque appearance. The number of particles and their size distribution should be taken into account in order to accurately describe the behaviour of the treatment process using a mathematical model. Turbidity is the cloudiness of a fluid caused by a large number of particles, which individually are invisible to the naked eye, and it is used as a measure by treatment plants of how much suspended solids are present in the water. The turbidity of water is measured based on the amount of light scattered by the suspended solid particles in the water (Perlman, 2004). The more suspended solid particles present then more light will be scattered. As such, turbidity can be related to the number of suspended solids particles through particle concentration and particle size distribution, both strongly influencing the scattering of the light (Kleizen et al., 1995). Turbidity is not a direct measurement of the total suspended materials in the water, but instead serves as a measure of the relative clarity of the water. Turbidity is often used to indicate changes in the total suspended solids concentration in the water but without providing an exact measure of the quantity of the suspended solids (Kemker, 2014).

Much research has been devoted to improving the understanding of turbidity in water treatment processes (Edzwald and Van Benschoten, 1990; Thompson et al., 2003; Hannouche et al., 2011), for example, it has been shown that for most surface waters, coagulant doses should be determined by the concentration of natural organic matter (NOM) rather than by turbidity (Edzwald and Van Benschoten, 1990), and this is a practice that is still used today. There is still considerable work to be done in finding a predictive correlation between turbidity and particle concentration in order to use

plant data based on turbidity in a mathematical model which considers a concentration of suspended solids. It is often assumed that turbidity provides a direct measure of suspended solids concentration and that there is a formula or set of conversion factors with which suspended solids concentration can be calculated from Nephelometric Turbidity Unit (NTUs). Hannouche et al. (2011) confirm the existence of a strong linear relationship between turbidity and suspended solids concentration; however, their relationship has limitations depending on dry and wet weather conditions. It can be concluded that a greater understanding of suspended solids suspensions and their predictive relationship with turbidity is needed in order to adequately model and verify with a clean water treatment plant.

2.3.2 Coagulation and flocculation

In a clean water treatment work, water from reservoirs and rivers containing colloidal and small particles of algae, grit and gravel pass through a preliminary treatment stage consisting of screens to physically remove the larger solids, and other debris before the water passes to the main treatment process. The first main step of the clean water treatment process is usually coagulation and flocculation. This step is in fact a three stage process, consisting of rapid mixing, coagulation of colloidal particles and then flocculation. Coagulation and flocculation happen in quick succession, and are therefore often considered as one overall process. Coagulation is a quick destabilisation and initial coalescing of colloidal particles, specifically hydrophobic colloids, including clay and non-hydrated metal oxides. Flocculation is the slow stirring or gentle agitation to aggregate the destabilised particles, forming a rapid settling floc. This gentle mixing increases the collisions between the particles and helps them to agglomerate. The agglomeration of the particles occurs over a longer time period and causes a precipitate to form in the water, which can be removed using simple physical methods, such as liquid-solid separation methods, e.g. for dissolved air flotation, scraping is utilised.

Key to coagulation and flocculation is destabilisation, and this phenomena must be accurately described in a predictive model. Destabilisation is the process in which the particles in a stable suspension are modified to order to increase their inclination to attach to one another. For the aggregation of particles in suspension, there is a need for them to be transported towards one another, and for this, unit operations such as rapid mixing are utilised.

Depending on the type of colloidal suspension that should undergo coagulation, different

chemical destabilisation mechanisms can be employed. There are generally four main mechanisms that can occur to achieve destabilising of colloidal systems: double layer compression, charge neutralisation, entrapment in a precipitate (sweep flocculation), and particle bridging (Gregory, 2005). Charge neutralisation and entrapment in a precipitate (sweep flocculation) are the two primary destabilisation mechanisms in drinking water treatment, and past authors have studied these mechanisms extensively (Amirtharajah and Mills, 1982; Edzwald and Van Benschoten, 1990):

- *Charge Neutralisation:* Positively charged metal coagulant is attracted to the negatively charged colloids via electrostatic interaction. This makes agglomeration easier by reducing the electrical forces keeping the particles apart. This method of destabilisation will need a coagulant dose proportional to the quantity of colloidal material present. If the dose is not proportional, a charge reversal can occur where the colloids will not be destabilised and this can be caused by overdosing.
- *Entrapment in a precipitate:* Precipitation as hydroxide flocs may occur with the addition of aluminium or iron salts. If colloids are present, then the precipitation occurs around them. This is due to the concept that at high colloid concentrations, the colloidal particles act as nuclei onto which the coagulant precipitates.

The mechanism utilised is dependent upon the coagulant dose. Most clean water treatment plants operate using entrapment in a precipitate (sweep flocculation), which requires a higher dose of coagulant, rather than charge neutralisation. A detailed description of the chemistry behind coagulation and flocculation can be found in the works of Gregory (2005); Post et al. (2011) and Crittenden et al. (2012). They state that the hydrolysis reactions between the coagulant and particles are complex, and insoluble precipitates are formed that destabilise particles by neutralising the charge on fine particles. These reactions take place between coagulants and natural organic matter (NOM) molecules, and on the surfaces of the suspended solid particles. In general, NOM molecules are large and contain many functional groups that affect their chemical behaviour (Croue et al., 1999).

An important aspect of coagulation and flocculation is mixing. There is some literature available that questions if rapid mixing is a necessary step (Edzwald, 2014; Allerdings et al., 2015) which adds an interesting question about the length of time for which rapid mixing should occur. The common understanding is that due to the fragile nature of the flocs created, intense mixing will encourage the desegregation of flocs, which is

the opposite of what is intended (Gregory, 2005; Post et al., 2011; Crittenden et al., 2012). However, Letterman and Yiacoumi (2010) argue that evidence is limited which prove mixing at high intensity for too long can be damaging to subsequent process performance; this could be due to aggregates that are eroded or broken having a reduced tendency to reform with time due to changes in surface chemical or physical properties. A mathematical model which accurately captures the aggregation and disaggregation of particles can be used to consider different scenarios, involving different coagulants and operation at a variety of high intensity mixing speeds in order to determine the best operating conditions. From researching the state of art in the area of coagulation and flocculation, there are three key areas that can be developed in order to achieve the goal of an accurate mathematical model: hydrodynamic forces between particles, particle size distribution and coagulant dosing. Equations used to describe these phenomena are discussed later in this section.

Hydrodynamic forces between particles

There are two research areas current developments for the modelling of the hydrodynamic forces between colliding particles are developing, both of which contribute to an enhanced definition of aggregate structure: (1) the drag upon the aggregates, and (2) the collision trajectory shadow. This is an area which is associated with the paths the aggregates take as they approach one another. Aggregates formed by flocculation usually do not have a spherical shape, but rather a more irregular structure. Fractal geometry was firstly introduced to quantitatively describe objects and phenomena that were previously considered to be too complex and disordered (Mandelbrot, 1987). It is now mainly used as a way to describe the structure of particle aggregates. Experiments have shown that aggregates formed by shear coagulation (Brownian motion in a laminar shear flow) are usually fractal-like (Oles, 1992; Chakraborti et al., 2003).

Kinetic hydrodynamic forces in flocculation have been extensively studied and the earlier models are based on an assumption that inter-particle interactions are negligible until the point of contact, where the adhesion takes place with complete efficiency. Argaman and Kaufman (1970) developed a model in which aggregation and break-up are the main phenomena considered. Following from this, it was assumed that the net flocculation in a turbulent environment depends upon the balance of the opposing processes of aggregation and floc breakup (Parker et al., 1972; Oles, 1992; Spicer and Pratsinis, 1996).

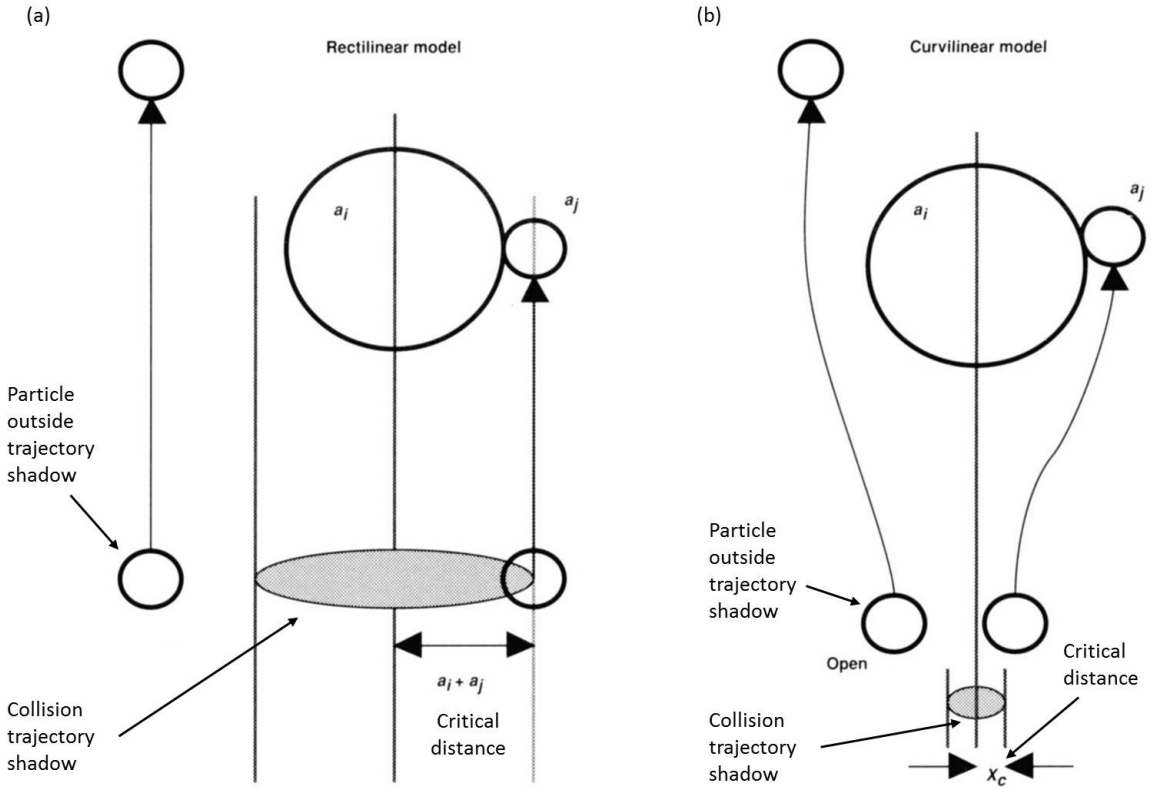


Figure 2.4: Possible particle collision trajectories. (a) Rectilinear model. (b) Curvilinear model. Adapted with permissions from Han and Lawler (1992).

In actual fact, the hydrodynamic forces impact substantially upon colliding particles, where the fluid within the space is extruded out. The traditional approach to modelling hydrodynamic forces assumes that the particles follow a straight line path, and inter-particle forces are not considered. This approach is known as *rectilinear*. There is, however, an alternative approach called *curvilinear*, where the approaching particles are forced to rotate slightly around one another due to the hydrodynamic force. The linear path (assumed by the traditional approach) is deviated from and the motion of the fluid causes the particles to rotate relative to one another. Figure 2.4 depicts the rectilinear and curvilinear approaches, where the collision trajectory shadow is a pseudo area where the a_j particle travelling within this area will strike the a_i particle. The a_j particle outside of the trajectory shadow will miss the larger a_i particle. The curvilinear collision model is believed to be more accurate than the rectilinear model in predicting particle coagulation rates (Jianjun, 2002).

Particle size distribution

In addition to particle coagulation, aggregation breakage plays an important role in regulating the size distribution of particles in a flocculation system. The basis of most of the current theories used to model changes in particle size distribution (PSD) in water by accounting for particle influx and coagulation dates back to work by Smoluchowski from 1917 (Gon Lee et al., 2000). In discrete form, Smoluchowski's equation can be written as:

$$\frac{dn_k}{dt} = \frac{1}{2}\alpha \sum_{i+j=k} \beta\left(i,j\right) n_i n_j - \alpha n_k \sum_{i=1}^{w} \beta\left(i,k\right) n_i \tag{2.3.1}$$

where w is the maximum number of size categories; n_i, n_j, and n_k are the number concentration of particle sizes i, j, and k, respectively; α is the collision efficiency factor; and $\beta(i, j)$ and $\beta(i, k)$ are the collision frequency function between particles. The first term of Equation 2.3.1 represents the formation of particle size k by collision of particles of size i and j. The second term represents the loss of particle size k by collision with all other particles. The ratio of 1/2 in front of the first term is needed to avoid double counting (Gon Lee et al., 2000). Much of the research to date within flocculation modelling has been directed towards establishing equations and specific values for the collision efficiency factor, a, and the collision frequency function, β,. There are two main interpretations of these two parameters: a) that they are independent of one another and b) that a could be considered as an experimental correction factor compensating for weaknesses in the theoretical representation of β (Thomas et al., 1999). To make the differential equations more manageable, Smoluchowski made a number of simplifying assumptions, as reported by Thomas et al. (1999):

1. The collision efficiency factor, α, is unity for all collisions.
2. Fluid motion undergoes laminar shear.
3. All particles are mono-dispersed (i.e. all of the same size).
4. No breakage of flocs occur.
5. All particles are spherical in shape and remain so after collision.
6. Collisions involve only two particles.

Based on these assumptions, Smoluchowski developed the following analytical expressions for the collision frequency for both perikinetic[2], orthokinetic flocculation[3] and differential sedimentation[4]:

$$\beta_{perikinetic} = \left({}^{2kT}/_{3\mu}\right)\left({}^{1}/_{d_i} + {}^{1}/_{d_j}\right)\left(d_i + d_j\right) \tag{2.3.2}$$

$$\beta_{orthokinetic} = \left({}^{1}/_{6}\right)\left({}^{du}/_{dy}\right)\left(d_i + d_j\right)^3 \tag{2.3.3}$$

$$\beta_{Sedimentation} = \left(\frac{\pi g}{72\mu}\right)\left(\rho_s - \rho_L\right)\left(d_i + d_j\right)^3\left(d_i - d_j\right) \tag{2.3.4}$$

where k is Boltzmann's constant, T is the absolute temperature of the fluid (K), μ is the fluid viscosity (Pa. s), and ${}^{du}/_{dy}$ is the velocity gradient of the fluid (s^{-1}), $d_{i,j}$ is the diameter of particles i and j (m), g is the gravitational constant (m/s^2) and $\rho_{s,L}$ is the density of the particles and water (kg/m^3). Smoluchowski produced solutions to the set of differential equations for both perikinetic and orthokinetic flocculation. The most commonly used solution is for orthokinetic flocculation and is given by:

$$N_t = N_0 exp\left({}^{4}/_{\pi}\right)\left({}^{du}/_{dy}\right)\phi t \tag{2.3.5}$$

where N_t is the total particle count at time t, N_0 is the initial particle at time t=0 count and ϕ is the volume fraction of the particles, which is assumed to be constant and given by $\phi = {}^{4}/_{3}\pi a^3 N_0$, a being the particle radius. Numerous researchers have attempted to model actual flocculation systems as summarised in Table 2.2, each addressing some of the constraints in the original Smoluchowski's equation.

The traditional diffusion approach of the Smoluchowski theory for coagulation of colloids has been extensively analysed and shown to be valid only in the particular case of coalescence of small particles with large particles (Veshchunov, 2011). Monte Carlo stochastic simulations have been attempted based on a single-particle method, as this method does not require any information on nearby particles but rather a fabricated coalescence partner with a given size is generated (Vikhansky and Kraft, 2005). Other

[2]Perikinetic collision occurs by brownian motion, which can also be explained as the erratic random movement of microscopic particles in a fluid as a result of continuous bombardment from molecules of the surrounding medium (Gon Lee et al., 2000).

[3]Orthokinetic flocculation occurs when contact or collisions of colloidal particles result from bulk fluid motion such as stirring (Gon Lee et al., 2000).

[4]Differential sedimentation occurs in heterogeneous suspensions during sedimentation, providing an additional mechanism for promoting flocculation due to gravitational forces, as the larger particles that are formed begin to settle. The difference in the particle size and/or density causes the particles to collide and flocculate (Gon Lee et al., 2000).

Table 2.2: Examples of previously published works conducted for coagulation/flocculation modelling.

Topic	Author(s)
Smoluchowski's coagulation equation	(Hendriks and Ziff, 1985; Gon Lee et al., 2000; Piskunov and Golubev, 2002)
Bulk flow patterns	(Bridgeman et al., 2009)
Population balance	(Vigil and Ziff, 1989; Kramer and Clark, 1999; Ducoste, 2002; Selomulya et al., 2003; Ding et al., 2006; Runkana et al., 2006; Vadasarukkai et al., 2011)
Computational Fluid Dynamics (CFD)	(Bridgeman et al., 2010; Samaras et al., 2010; Vadasarukkai et al., 2011; Militaru et al., 2013)
Monte Carlo simulation	(Spouge, 1985; Vikhansky and Kraft, 2004, 2005)

simulations involve the assumption of random coagulation (Spouge, 1985). Piskunov and Golubev (2002) use a "generalised functions" method to approximate the solutions of the Smoluchowski equation, which concludes that their method can be used most efficiently as a fast numerical method for computation within 3-D systems. Various authors from Table 2.2 show that mixed flocculators are more complex than a continuous stirred tank reactor and pose significant challenges to modellers.

Most of this early work captures the physical phenomena of coagulation but does not consider the overall coagulation process and where it takes place, which is interesting from a theoretical point of view. However, for practical application, studying these theories in isolation is not advantageous to companies wanting a competitive edge. Some early work have modelled flocculation occurring in a continuous stirred tank reactor (CSTR) taking into consideration floc break up (Parker et al., 1972; Haarhoff et al., 1997). Bridgeman et al. (2009) reports that there is a body of published work which considers the bulk flow patterns, primarily at laboratory scale, although little has been done in terms of multiphase modelling (the idea of colloidal particles and water). They also suggest that there is significant scope for the use of coupled population balance models and CFD to develop water treatment flocculation models (Vadasarukkai et al., 2011). Moreover, taking into account Smoluchowski's coagulation equation to determine

the maximum size which flocs are able to reach during the coagulation process, mixing in turbulent stirred tank reactors is considered in some studies, such as Hendriks and Ziff (1985) and Gon Lee et al. (2000).

Coagulant dosing

The conventional view of coagulation is that coagulant dosing is determined largely by the raw water turbidity or by colour for highly coloured waters (Edzwald and Laminski, 2007). Optimal coagulant dosages are critical for proper floc formation and filter performance. The conventional method of controlling coagulant dosage relies heavily on a manual method called *jar testing* (Binnie and Kimber, 2009).

Jar testing is a bench scale method which mimics coagulation/flocculation in the water treatment process and is used to determine the required concentration of coagulant dosage to destabilise any colloidal particles in the water treatment work. The method involves placing raw water samples in beakers and applying different quantities of coagulant at various mixing speeds to each sample. Based on the findings from a jar test, a recommended coagulant dosage is prescribed and the agreed value is introduced into the process. Jar tests are generally carried out periodically (monthly, weekly, daily or whenever a chemical is being changed) but there is no set requirement for how often jar testing should be conducted; however, the more it is done, the better the plant will operate. This means that the tests are reactive rather than proactive as the coagulant dosages are changed in response to the occurrence of water quality problems and subsequent jar testing. Due to the variable testing time, jar tests cannot be used to respond to rapid changes in raw water qualities and thus are not suitable for real-time control (Bin Robenson, 2008). In order to overcome this disadvantage, researchers are considering the use of models of the coagulation process in order to much more rapidly predict the required changes to the coagulant dosage (Valentin et al., 1999; Wu and Lo, 2008; Heddam et al., 2012).

A number of studies have reported on the application of empirical models for determining coagulant doses for treatment of drinking water. These models include the use of Artificial Neural Networks (ANN) to model poly aluminium chloride dosage (Valentin et al., 1999; Wu and Lo, 2008) and an investigation in the use of Adaptive Neuro-Fuzzy Inference System (ANFIS) (Heddam et al., 2012), also to model coagulant dose. It was found that the ANFIS coagulant dose method was better than the traditional ANN method when a direct comparison between the response time, economic costs

and applicability was made. Clark et al. (1993) suggested that the precipitation of aluminium hydroxide could be considered a rapid, competitive, consecutive chemical reaction, and they used this approach to study the effect of mixing on the formation of aluminium chloride solutions in base titration. It should be noted that these methods are empirical, and are therefore limited to the process units and process conditions for which the models were developed, i.e. cannot be extended to other units or conditions and therefore suffers from the same drawbacks as all non-mechanistic models.

Summary and outlook

Some PSE-based modelling methods have been successfully applied to the fundamentals of coagulation and flocculation in order to address various research challenges (Runkana et al., 2006; Bridgeman et al., 2009; Veshchunov, 2011). A model which incorporates inter-related hydrodynamic, physical and chemical processes would be of great use to the water industry in the development of a large scale water treatment plant model.

A review of the past literature reveals that the majority of the work published within this area mainly considers the microscopic aspects of the system, for example the chemistry behind the interaction of particles and chemical coagulants (Thomas et al., 1999), and that the models either deal with the chemical effects in a simplistic manner or neglect them. As a result, there is still a poor understanding of the interactions between the coagulant chemical and the primary suspended solid particles, and therefore also of what would be the most appropriate dose to use of the coagulant chemical depending on the raw water source and the operation.

There are many different solutions that can be utilised in order to improve the accuracy of existing models. Some examples are to evaluate the influence of Van Der Waals attraction and hydrodynamic forces (Krusters et al., 1991; Veerapanen and Wiesner, 1996; Wu and Lee, 1998; Thomas et al., 1999), in which there has been some substantial developments.

Following the research into the works of several authors in literature, there are two main conclusions. Firstly, the experimental results established by idealised particle suspensions are unlikely to provide accurate representation of the behaviour for real systems. Secondly, focusing on the microscopic behaviour of particles in an attempt to find correlations between process parameters (e.g. mixing intensity, coagulant dosage) and flocculation kinetics (e.g. collision efficiencies) would be extremely difficult. A

mathematical model that can draw upon the key aspects of the microscopic behaviour whilst integrating the hydrodynamic forces would be extremely beneficial in the development of a process model that is able to predict real system behaviour.

2.3.3 Clarification

To reduce the concentration of particles flowing into the filtration units, solid-water separation processes such as settling tanks and flotation are employed, usually following after flocculation. These clarification units are important as it ensures the filtration units can be operated easier and more cost-effectively to produce quality water. There are various types of clarification units: flocculation clarifiers (Gernaey et al., 2001; Burger et al., 2005; Edzwald and Laminski, 2007), electro-flocculation clarifiers (Cañizares et al., 2008), dispersed air flotation clarifiers (Puget et al., 2004; Haarhoff and Edzwald, 2004) and dissolved air flotation clarifiers (Leppinen et al., 2001; Haarhoff and Edzwald, 2004; Edzwald, 2010). Flocculation clarifiers work as a solid-liquid separation process in which particles settle under the force of gravity and the clear water rises to the top of the tank to be removed with the effluent flow whilst electro-flocculation is a process where flocculating metal ions are electrolytically added to the water at an anode, and gas micro bubbles are released at a cathode. The flocculating metal ions cling to particles in the water, increasing their size, and the gas micro bubbles capture the flocculated particles (flocs) and float them to the surface, from where they can be easily removed. Flotation (dispersed and dissolved) is the gravity separation process where gas bubbles attach to solid particles causing the detectable density of the bubble-solid agglomerates to be less than that of the water. This enables the solid particle to float. The use of flotation is an alternative form of clarification in the water treatment process even though flocculation clarifier (sedimentation) units are more commonly used. Table 2.3 shows the advantages and disadvantages of different clarification units for water treatment including a selection of authors who have modelled different aspects of these units. A detailed analysis of previous studies particularly related to clean water treatment is presented later on in this section.

In the water treatment process, flocculation clarifiers and dissolved air flotation are the most commonly used clarification treatment processes. For both these processes, one and two dimensional models developed in the literature have been explored and will be discussed in this section. The phenomena occurring in flocculation clarification

Table 2.3: Advantages and disadvantages of general flocculation clarifiers and flotation units, including typical usage and references for further information.

Process	Use	Advantages	Disadvantages	Author(s)
Flocculation clarifiers	Clean water and wastewater primary clarifier.	Allow for space reduction and decreased structural-mechanical costs. Provide reduced flow shear because of the direct passage of floc to clarification zone.	High flocculator energy input can produce currents in the clarification zone that upset sludge settling performance. Floc formation in the single-stage flocculation chamber is more difficult to control.	(Gernaey et al., 2001)
	Thickener clarifier.	Radial or peripheral weirs allow effective effluent draw from the clarifier surface area and develop predictable vertical flow patterns.	Sludge blanket control must be maintained to ensure that flocculated water exiting at the bottom of the flocculation chamber does not suspended solids from the sludge blanket.	(Burger et al., 2005)
Electro-flocculation	Wastewater treatment.	No turbulence is created. Suitable for small treatment plants.	Uses hydrogen which is very expensive.	(Cañizares et al., 2008)
Dispersed air flotation	Synthetic diary waste	**Not suitable for water treatment.**		(Puget et al., 2004)
Dissolved air flotation by vacuum	Clean water treatment (focussing on size of bubbles and particles)	High operation rate. Rapid start up.	Batch process. Requires sophisticated equipment to maintain vacuum. Air available is limited by vacuum.	(Leppinen et al., 2001; Haarhoff and Edzwald, 2004; Edzwald, 2010)
Dissolved airflotation by pressure	Clean water treatment	Rapid start up. Short residence time. Better treated water quality.	Requires careful control to achieve high quality output.	(Haarhoff and Edzwald, 2004; Edzwald and Laminski, 2007; Edzwald, 2010)

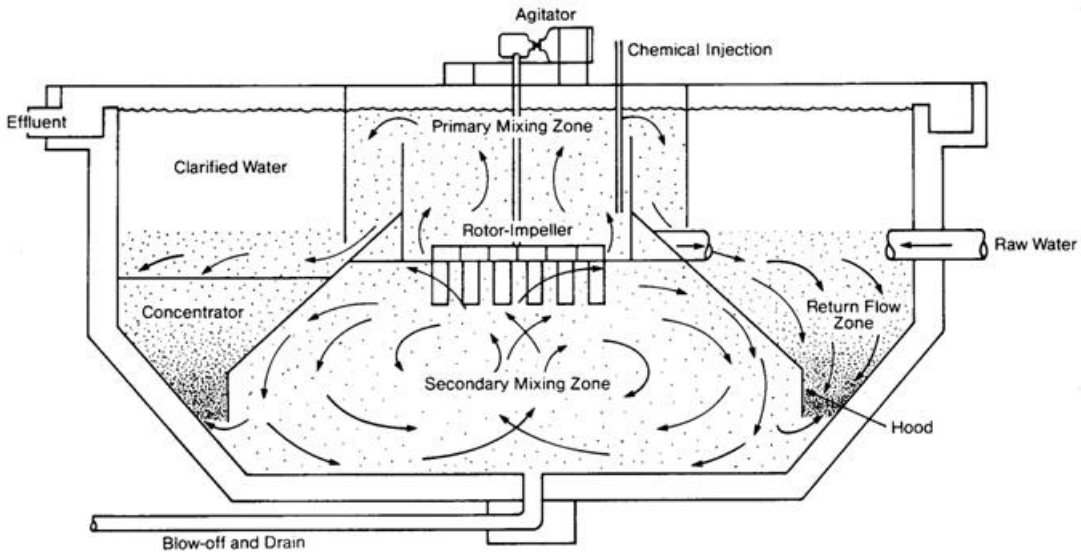


Figure 2.5: Cross-section of solid-contact clarifier (AWWA Committee Report, 1951).

units are utilised in both the clean water and wastewater treatment processes as shown in Table 2.3; and although mathematical modelling in wastewater treatment is more advanced than in clean water treatment, the various phenomena both industries have in common is discussed in this section.

Clarifier tank studies

In flocculation clarifiers, such as solid-contact clarifiers (as shown in Figure 2.5), raw water is brought into a primary mixing zone, where further coagulation and flocculation take place. Following this, a secondary mixing zone is used to promote particle collisions so that smaller particles are entrained in larger flocs. Water passes out of an inverted cone into the concentrator/return flow zone, where suspended solids settle to the bottom (due to gravity) and clarified water flows into a weir. In order for recirculation of the large flocs to occur, suspended solids are drawn back into the primary mixing zone. The concentration of solids in both mixing zones are controlled by continuous, or the occasional, removal of sludge. A sludge blanket clarifier is an enhanced design, which passes the water up from the bottom of the clarifier through a blanket of suspended solids that acts as a filter (which is not shown in the figure) (Burger et al., 2005; Gernaey et al., 2012).

A starting point for many sedimentation models is the model first proposed by Kynch in 1952 (Concha and Bustos, 1991). Kynch proposed a kinematic theory of sedimentation

based on concentration changes in a suspension, which is based on mass conservation of sediment particles settling through a control volume of fluid. The model assumes that a set of N different sized solid spheres that have the same density are settling in a volume filled with a fluid of known properties, with the only external force being applied to the sediment suspension being gravity and where no wall effects are present. Also, it is assumes that there are no compression effects present near the bottom layer as the particles are considered non-compressible. By letting v_i denote the hindered settling velocity of spherical particles of size class i and c_i be the mass concentration of these particles of size class i, then the mass balances of the solid particles for each size class i (where i = 1,2,... N and N is the total number of size classes) can be written as (Concha and Bustos, 1991):

$$\begin{array}{c} \frac{\partial c_i}{\partial t} + \frac{\partial f_{bk}}{\partial z} = 0, \qquad\qquad i = 1, 2...N \\ s.t.\, c_i(0, z) = c_i^0(z), \quad 0 \leq z \leq L,\ i = 1, 2...N \end{array} \tag{2.3.6}$$

where $f_{bk} = c_i.v_i$ is the mass flux of particles through a depth z at time t (mg/m^{2}s), z is the depth measured from the top of the unit (m), and $c_i^0(z)$ is the initial mass concentration profile over the depth z (mg/L). Equation 2.3.6 is a representation of the kinematic model of sedimentation for a poly-dispersed suspension of non-compressible particles based on Kynch's theory of sedimentation. If, however, flocculent suspensions form compressible sediments, then this kinematic model is no longer sufficient, and dynamic effects need to be taken into consideration.

Discretisation of Partial Differential Equations

One- and two-dimensional models are often derived as a set of Partial Differential Equations (PDEs). The classic approach to solving PDEs is using numerical methods, such as finite difference methods. Utilising this approach consists of transforming the continuous domain of the state variables by a network of discrete points. The PDE is converted into a set of finite difference equations that can be solved subject to the appropriate boundary conditions - this is also known as discretisation. Discretisation is a mathematical concept and relates to how the dimensions of the process unit has been split into sub-sections in order to numerically solve the equation set which forms the model, and this is an area which has been investigated, most notably, by Jeppsson and Diehl (1996) and Burger et al. (2011) for wastewater treatment. One important

difference between first- and second-order models is the way in which discretisation is considered, and thus the way dispersion is approximated (Burger et al., 2011).

Mathematical models of clarifier units that are based on both first- and second-order discretisation are available and have been studied by many authors, a detailed review of which has been provided by Li and Stenstrom (2014). Examples are clarification mathematical models proposed by Takacs et al. (1991) and the more recently suggested mathematical models by others (e.g.De Clercq et al. (2008); Plosz et al. (2012)), which are based on one-dimensional advection-dispersion PDEs. One-dimensional models are used to model dynamic conditions, such as settling, and to better represent effluent and underflow concentration changes and sludge mass shifts. The discretisation results in sections where it is assumed that the concentration is uniform.

One dimensional (1-D) clarifier unit modelling

There have been extensions made to Kynch's model in order to simulate continuous and batch sedimentation cylindrical volumes whereby variations through the depth of the water column is considered by one dimensional modelling (Concha and Bustos, 1991; Burger et al., 1999, 2000) and theories based on macroscopic balances have been utilised (Head et al., 1997). Bache (2010) reported that the development of theories based on macroscopic balances is made difficult by the lack of supporting information, and suggested that research should be aimed towards identifying aspects, such as blanket settling velocity and mass flux, of the floc blanket theory to gain a wider picture of the on-going processes within a clarifier. A useful framework for the simulation of batch and continuous thickening is provided by a series of papers on the phenomenological theory of sedimentation of flocculated suspensions by various researchers (Concha and Bustos, 1991; Burger and Concha, 1998; Burger et al., 1999), where they considered different parameters such as varying area and conical shape of the clarifier tanks. Burger et al. (2000) and Garrido et al. (2000) demonstrated the application of the method to several batch and continuous sedimentation processes.

Knowledge shared from the wastewater industry

Even though the wastewater treatment industry has a different purpose than the clean water industry, there are some unit operations that have similar purposes; for example, a sludge clarifier shares the same role as a secondary settling tank in wastewater. The

secondary settling tank is utilised after biological treatment of microorganisms in order to allow the microorganisms to settle. Models describing secondary settling clarifiers utilised in wastewater treatment can be used to represent sedimentation units in clean water treatment with some modifications and assumptions. The behaviour of sludge blanket clarifiers applied to secondary settling clarifiers in wastewater treatment has been successfully simulated, and this theory has been applied to modelling of clean water treatment by neglecting the biological matter (Head et al., 1997). Clarke et al. (1978) and Wilson et al. (1979) presented a similar, but more complex, analysis to Head et al. (1997) but it was found to be computationally time consuming and did not produce results that effectively resembled the performance encountered in real works.

For design and operation of secondary settling units, flux-based, one-dimensional clarifier models can be used (Jeppsson and Diehl, 1996; Burger et al., 2011). The hydrodynamic behaviour, when described in one-dimension, can be expressed as depth and the interaction between the flocs that are settling. The hydrodynamic behaviour and floc interaction are, however, also important aspects which must be considered in order to estimate the clarification and sludge thickening behaviour, as well as the solids inventory of clarifiers in plant-wide process prediction. However, effluent suspended solids prediction from one-dimensional models were not designed to fulfil this purpose and these models must therefore be used with care.

The one-dimensional model proposed by Burger et al. (2011) and De Clercq et al. (2008) considers a solid-liquid separation of activated sludge forced by gravity occurring in a secondary settling tank (SST). The particulate concentration depends on both space and time; c(z, t), where the z-axis points downwards (Figure 2.6). Considering the sludge, Burger et al. (2011) utilise idealising assumptions, such as:

1. There is no biological activity in the SST;
2. The sludge has flocculated prior to entering the SST and consists of suspended solid particles of the same size and shape;
3. Outside the SST (i.e. in the outlet and effluent pipes) the sludge and water have the same speed.

To capture the processes of gravity settling and compression, Kynch's hindered settling velocity assumptions, described earlier, can be used to provide a unique solution (Equation 2.3.6) (Kynch, 1952). With only dispersion effects taken into account, various

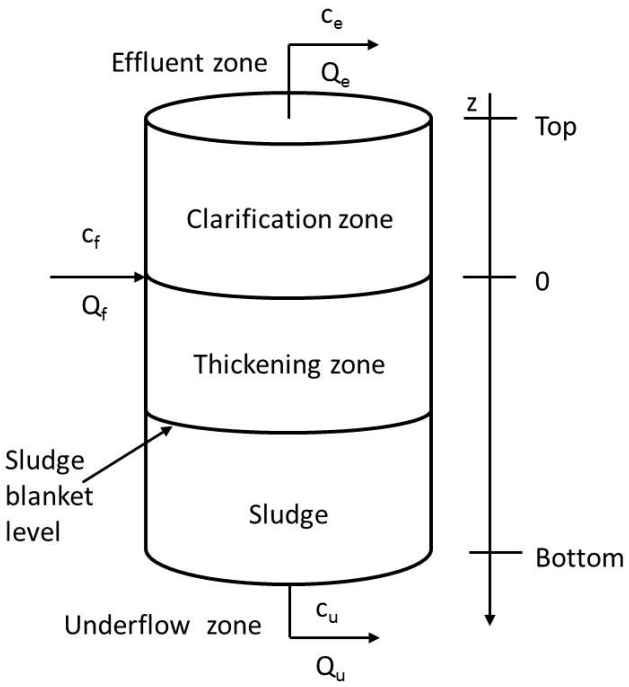


Figure 2.6: Schematic overview of an ideal one-dimensional clarifier. Adapted with permissions from Burger et al. (2011).

authors have demonstrated the validity of Kynch's concentration discontinuity theory (Concha and Bustos, 1991; Jeppsson and Diehl, 1996; Burger et al., 2003). The following constitutive relation assumes the downward settling velocity of the suspended solid particles in batch sedimentation can be written as:

$$v_i = \begin{cases} v_{hs}(c) & for\ 0 \leq c \leq c_C \\ v_{hs}(c)\left(1 - \frac{\rho_s \sigma_e'(c)}{cg\Delta\rho}\right)\frac{\partial c}{\partial z} & for\ c > c_C \end{cases} \tag{2.3.7}$$

$$v_{hs}(c) = v_0 c e^{-rc} \tag{2.3.8}$$

where the hindered settling velocity $v_{hs}(c)$ is a function of the local concentration only (Kynch, 1952), g is the gravity of acceleration, ρ_s is the density of the solids and $\Delta\rho$ is the density difference between the solids and the liquid. When concentrations are greater than the critical concentration c_C, a compression effect reduces the settling velocity when the concentration increases with depth. Inserting Equation 2.3.7 into Equation 2.3.6, the following degenerate parabolic PDE with one unknown variable, c is formed:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial z}\left(c v_{hs}(c)\right) = \frac{\partial}{\partial z}\left(d_{comp}(c)\frac{\partial c}{\partial z}\right) \tag{2.3.9}$$

where the compression function can be written as:

$$d_{comp}(c) = \begin{cases} 0 & for\ 0 \leq c \leq c_C \\ \frac{\rho_s}{g\Delta\rho} v_{hs}(c)\sigma_e^{'}(c) & for\ c > c_C \end{cases} \tag{2.3.10}$$

$$\sigma_e^{'}(c) = \alpha ln\left(\frac{c - c_c + \beta}{\beta}\right) \tag{2.3.11}$$

Consider a continuous sedimentation in the ideal 1-D secondary settling tank (as show in Figure 2.6) where *Top* is the height of the clarification zone and *Bottom* is the depth of the thickening zone, Q_e is the effluent volumetric flow rate, Q_u is the downward volumetric flow rate and Q_f is the feed volumetric flow rate. An assumption made is that there is either a downward (Q_u) volumetric flow or an upward (Q_e) at each point of the one-dimensional axis. This assumption is to hold true at all points except for where the feed is assumed to be situated. The one-dimensional assumption also neglects wall effects and implies that no horizontal effects are considered. For simplicity it has been assumed that it is a constant parameter, a. The higher and lower sludge concentration are mixed by turbulent currents, especially around the feed inlet due to its velocity field. The depth-concentration profile is smoothed by the hydrodynamic dispersion phenomenon. Another of the idealising assumptions is that the mixture follows the bulk flows in the outlet pipes. This means that once the mixture has left the secondary settling tank (SST) there will be no backflow, suggesting:

$$d_{disp}(z) = \begin{cases} 0 & for\ |z| \geq b \\ acos\left(\frac{\pi z}{2b}\right) & for\ |z| < b \end{cases} \tag{2.3.12}$$

$$d_{disp}(z) = 0 \quad for\, z < -Top \quad and\, z > Bottom \tag{2.3.13}$$

The conservation law of mass is used to derive an equation that captures this assumption (Burger et al., 2011). The increase of mass per time unit in an arbitrary interval (z_1, z_2) equals the flux in minus flux out plus the production inside the interval:

$$\frac{d}{dt}\int_{z_1}^{z_2} Ac(z,\, t)dz = A\left(\phi|_{z=z_1} - \phi|_{z=z_2}\right) + \int_{z_1}^{z_2} Q_f(t)c_f(t)\delta(z)dz \tag{2.3.14}$$

The last term contains the feed volumetric flow Q_f, the feed concentration c_f and the Dirac delta distribution δ as a source term. The flux ϕ contains all constitutive

functions:

$$\phi\left(c,\,\frac{\partial c}{\partial z},\,z,\,t\right) = F(c,\,z,\,t) - \left(\gamma(z)d_{comp}(c) + d_{disp}(z)\right)\frac{\partial c}{\partial z} \tag{2.3.15}$$

If the solution c(z, t) of Equation 2.3.14 is continuously differentiable, then Equation 2.3.14 is equivalent to the following convection-diffusion[5] PDE, can be derived and defined for all z:

$$\frac{\partial}{\partial t}\left[A(z)dz\,c\,(z,t)\right] = -\left[v_{hs}(c) + \frac{Q_e}{A_{(z+dz)}}\right]c\,A_{(z+dz)} + \left[v_{hs}(c) + \frac{Q_u}{A(z)}\right]c\,A(z)$$

$$+A(z+dz)\left(d_{comp}(c) + d_{disp}(z)\right)_{(z+dz)}\frac{\partial c}{\partial z}\,|_{z+dz} - A(z)\left(d_{comp}(c) + d_{disp}(z)\right)\frac{\partial c}{\partial z}\,|_{z}$$

$$\frac{\partial c}{\partial t} = -\left\{\frac{\left[c\left(v_{hs}A + Q_e\right)\right]_{z+dz} - \left[c\left(v_{hs}A + Q_u\right)\right]_z}{A(z)dz}\right\}$$
$$+\frac{\left[A(d_{comp}(c) + d_{disp}(z))\right]_{z+dz} - \left[A(d_{comp}(c) + d_{disp}(z))\right]_z}{A(z)dz}$$

With the area, A, being constant and the convective flux function, F, incorporating the three volumetric upward, downward and feed flows and the hindered settling velocity within the SST:

$$F(c,\,z,\,t) = \begin{cases} & -Q_e(z)c/A\ for\ Effluent\,zone(z < Top) \\ v_{hs}(c) & -Q_e(z)c/A\ for\ Clarification\,zone(Top < z < Feed) \\ v_{hs}(c) & -Q_f(z)c/A\ for\ Inlet\,zone(z = Feed) \\ v_{hs}(c) & +Q_u(z)c/A\ for\ Thickening\,zone(Feed < z < Bottom) \\ & +Q_u(z)c/A\ for\ Underflow\,zone(z > Bottom) \end{cases} \tag{2.3.16}$$

The mass conservation law is therefore applied around each section, thus generating a non-linear hyperbolic PDE (Takacs et al., 1991; Jeppsson and Diehl, 1996) by modelling the feed flux as a source point:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial z}F\left(c,\,z,\,t\right) = \frac{\partial}{\partial z}\left(\left(\gamma(z)d_{comp}(c) + d_{disp}(z)\right)\frac{\partial c}{\partial z}\right) + \frac{Q_f(t)c_f(t)}{A}\delta(z) \tag{2.3.17}$$

[5]Second- order derivative terms are often referred to as 'diffusion' terms, although they may model other phenomena.

The effects of suspended solids compression have also been added based on Kynch's theory (Fitch, 1983; Font, 1988), and has been found to be important as it improves the predictive power of the model (De Clercq et al., 2008; Ramin et al., 2014; Van Loosdrecht et al., 2015; Torfs et al., 2015; Burger et al., 2016). It should be noted that the increased complexity of the mathematical model in this instance will lead to longer computational times.

Two dimensional (2-D) clarifier unit modelling

There has been some work conducted to broaden from one dimensional to two dimensional modelling, incorporating radial variations, mainly utilising computational fluid dynamics (CFD) techniques. This approach results in the incorporation of hydraulic flow considerations, such as density currents, turbulence and secondary setting tank geometry. The main benefit of 2-D modelling is that it avoids many of the assumptions made by 1-D modelling as the 2-D models can capture more varied phenomena occurring; however, it is more time consuming. The most frequent application of 2-D models is towards the improvement of SST geometry design and to optimise performance. When considering sedimentation tanks where the suspended solids concentration is limited and suspended solid particles settle individually without interaction with neighbouring particles, Imam et al. (1983) applied a fixed settling velocity and used the mean particle velocity in their model to simulate floc interaction during clarification. Stamou et al. (1989) simulated the flow in a sedimentation tank using a 2-D model, where they solved the momentum and solid concentration equations; however, these equations where not connected to account for buoyancy. Adams and Rodi (1990) used the same model and extended the investigation to also consider the inlet flow arrangements and flow field calculations. Further advancement of this work accounted for flocculation where six different size classes with their respective velocities were considered by Lyn et al. (1992).

Larsen (1977) applied a simplified CFD model to several secondary clarifiers and demonstrated the presence of a "density waterfall". A density waterfall is described as a phenomenon that causes the incoming fluid to sink to the tank bottom not long after entering. This phenomenon has since been confirmed by various authors (Kim et al., 2005; Goula et al., 2008; Das et al., 2016). Other early work includes work by Shamber and Larock (1981) and by McCorquodale et al. (1991), who utilised finite volume methods to solve their clarifier models, with the latter also using finite difference methods for the boundary conditions, and Huang and Jin (2010) who provided a

numerical model for a type of circular sedimentation basin. Their model included an optimising element using the tank dimensions based on the sludge raking frequency and preferred removal efficiency. The blankets of floc formed that are held in steady state are complex and McCorquodale and Zhou (1993) investigated the effect of a variety of solids and hydraulic loads on circular clarifier performance, whilst Zhou et al. (1994) linked the energy equation with the Navier–Stokes equations to simulate the effect of neutral density and warm water into a clarifier model.

Much research has used CFD simulations in order to describe water flow and suspended solids removal in settling tanks for wastewater treatment. Even so, works in CFD modelling of sedimentation tanks for clean water treatment are limited in literature (Goula et al., 2008; Dufresne et al., 2009). Koltsaklis et al. (2013) stated that the physical characteristics of the flocs may not be as significant in the flow field of clarifiers for clean water due to the lower suspended solids concentration and larger particle size distributions than those encountered in wastewater treatment. Their work provides an insight into the flow patterns in a clean sedimentation tank which can be used to investigate novel designs or varying operating conditions, for instance temperature variation, for production-scale tanks.

2.3.3.1 Flotation tank studies

The final type of clarifiers which are considered in this work are flotation units. Flotation is the gravity separation process where gas bubbles attach to solid particles to cause the apparent density of the bubble-solid agglomerates to be less than that of the water, hence enabling the agglomerate to float. There are three main types of flotation systems (Reynolds and Richards, 1996): electrolytic flotation, dispersed air flotation and dissolved air flotation (DAF).

The rest of this sub-section will analyse the main one- and two-dimensional mathematical models developed in literature for dissolved air flotation, including Table 2.4 that investigates two key theories of DAF: single collectors collision theory and rise velocity equation in the separation modelling zone including details on the model bias.

One dimensional DAF modelling

As discussed earlier, dissolved air flotation (DAF) is the most viable as a water treatment floc separation method. Over the years, several conceptual models have been

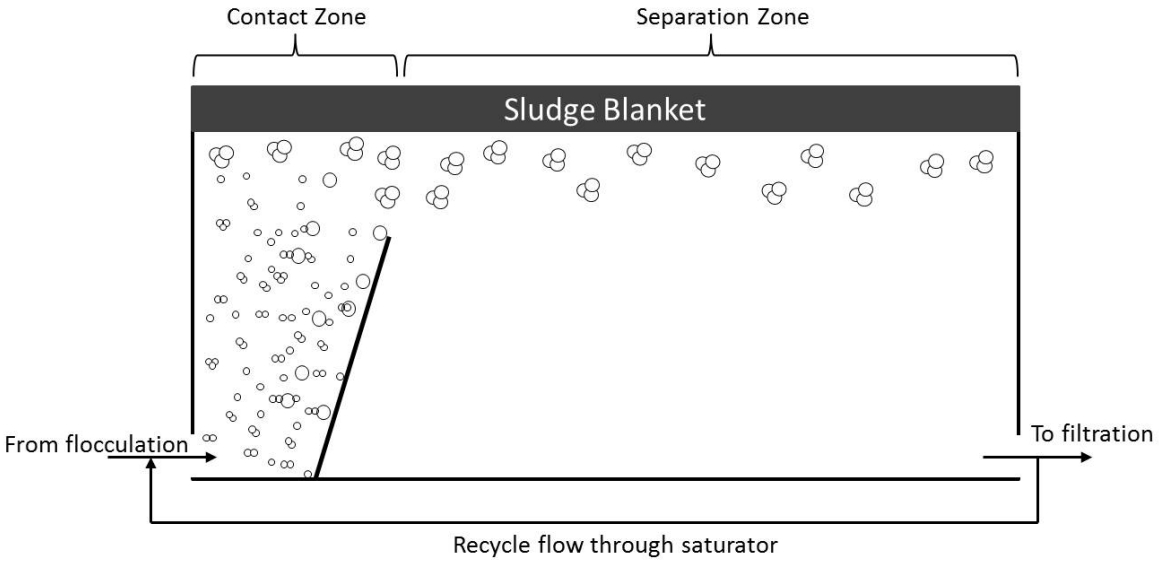


Figure 2.7: Schematic overview of a dissolved air flotation unit.

developed for DAF and can be classified into two groups: i) based on the single collector collision theory in laminar flow conditions (called SCC models); and ii) based on a kinetic model considering the population balance theory of bubbles and flocs in a turbulent flow condition (called PBT models). The SCC theory treats each bubble as a single collector of particles and considers them as "white water" blankets. The PBT approach depicts collisions between bubbles and particles through kinetic expression using a population balance. Both of these two models divide a dissolved air flotation (DAF) unit into two zones: contact (reaction) and separation, as shown in Figure 2.7. The contact zone encourages further attachment between bubbles and particles or flocs, while the separation zone promotes clarification as bubble/floc agglomerate float to the surface. Table 2.4 provides a summary of a selection of contributions proposing or using these models, based on the review by Edzwald (2010).

Single collector collision theory (SCC model)

The SCC theory modelling approach was first used in air filtration models (Edzwald and Van Benschoten, 1990; Edzwald, 1995), and later adapted to model granular water filtration (Haarhoff and Edzwald, 2004). The model describes collection of particles by bubbles in froth flotation and in dispersed air flotation (Edzwald, 2010). The SCC approach considers within the contact zone, bubbles in the "white water" blanket act as collectors of particles which accounts for particle transport to the bubble interface.

Table 2.4: DAF contact and separation zone models. Adapted with permissions from Edzwald (2010).

Primary Equation	Model Basis	Comment	Author(s)
Single collector collision model			
$\eta_D = 6.18\left[\frac{k_bT}{g(\rho_w-\rho_b)}\right]^{2/3}[1/d_p]^2$ **(i)** $\eta_I = [(d_p/d_b)+1]^2 - (3/2)[(d_p/d_b)+1]$ $+(1/2)[(d_p/d_b)+1]^{-1}$ **(ii)** $\eta_S = [(\rho_p-\rho_w)/(\rho_w-\rho_b)][d_p/d_b]^2$ **(iii)** $\eta_T = \eta_D + \eta_I + \eta_S$ *(iv)* $\frac{n_{p,e}}{n_{p,i}} = \left[exp\left(-\frac{\left(\frac{3}{2}\alpha pb\eta_T\phi_b\nu_b t_{cz}\right)}{d_b}\right)\right]$ **(v)**	1. At dynamic steady state, blanket of bubbles (white water blanket) modeled in the contact zone with a high bubble number concentration. 2. Bubble acts as collectors. 3. Particle transport terms expressed with respect to the single collector efficiencies. Expressions for interception (n_I), settling (n_s) and inertia (not shown since not important for DAF) developed from particle trajectory analysis. Brownian diffusion (n_B) expression is obtained from Stokes-Einstein relationship.	1. Assuming plug flow hydraulics, performance equation (Equation (v)) is for continuous steady flow through the contact zone. 2. Particle trajectory analysis does not incorporate interparticle forces, which can be attributed to London-van der Waals and electrostatic force.. Short range hydrodynamic effect of water layer model. All of these effects are accounted for between bubble and particle not considered in in the empirical attachment efficiency term a_{pb}.	(Edzwald and Van Benschoten, 1990; Edzwald, 1995; Haarhoff and Edzwald, 2004)
Rise velocity equation for Floc-bubbles aggregates			
$v_{fb} = 4g(\rho_w-\rho_b){d_f b}^2/3k\mu_w$ **(vi)** where $d_{fb} = (d_f^3 + N_b d_b^3)^{1/3}$ **(vii)** $\rho_{fb} = \rho_f d_f^3 + N_b\rho_b d_b^3/d_b^3 + N_b d_b^3$ **(viii)** $v_{fb} = (4/3K)^{0.8}[g^{0.8}(\rho_w-\rho_f b)^{0.8}{d_f b}^{1.4}$ $/(\rho_w)^{0.2}(\mu_w)^{0.6}]$ **(ix)** $v_{fb} = N_b g\rho_w d_b^3\varphi^{0.5}/18\mu_w d_{fb}$ **(x)** $v_{fb} = g\rho_w d_b^3\varphi^{0.5}/18\mu_w(d_b^3 + jd_f^3)^{1/3}$ **(xi)**	1. Equation (vi) for Re $\leq$ 1, holds at 20°C for d_{fb} $\leq$160 µm with 4 attached 100 µm bubbles. K accounts for the shape of the aggregate and its effect on increased resistance to drag. 2. Equation (ix) for transition zone Re 1 – 50. 3. For Equation (x) Re $\leq$ 1 and applies to case of large number bubbles attached to each floc. 4. For Equation (xi) Re $\leq$ 1 and applies to case of floc size smaller than bubble size and multiple flocs (j) can be attached to each bubble.		(Haarhoff and Edzwald, 2004) (Matsui et al., 1998)

Also, in this approach, the effect of streamlines of flow diverting around the bubble is considered and an expression for interception and settling is derived from particle trajectory analysis. The inter-particle forces are not considered in SCC efficiency (η_T), so whether potential collisions are successful resulting in attachment is accounted for by an empirical coefficient α_{pb}.

Separation zone modelling

The bubbles in the contact zone are smaller than the bubbles in the separation zone. This is due to coalescence or even due to reduction of water pressure as the bubbles move from the bottom of the contact zone toward to the surface and into the separation zone (as shown in Figure 2.7). The main focus in the separation zone is the rise velocity for floc-bubble aggregates, and these factors can be modelled based on the Hazen theory which is similar to the sedimentation tank theory (Edzwald, 2010). The earlier models of separation zone for DAF systems assumed a vertical plug flow from the surface to the underdrain system. Stratified flow was explained as water travelling in a horizontal flow layer along the top of the tank to the far end, and then travelling back towards the front in a second horizontal layer below the first layer. Models predicting stratified flow often employ CFD techniques, but are limited as they do not identify the desired stratified flow conditions and do not predict the quantitative impact of the stratification on bubble removal (Lakghomi et al., 2012). Hedberg et al. (1998) and Amato et al. (2001) conducted empirical studies that suggest improvements in the removal of single bubbles in the separation zone can be achieved by producing larger bubble aggregates that have a higher rise velocity. This finding is in agreement with those of Edzwald (2010) and Leppinen and Dalziel (2004) who also found that removal efficiency was improved with large bubble aggregates in the separation zone.

Two dimensional (2-D) DAF modelling

As for models of other clarifiers, the prediction capabilities of DAF models can be improved by using CFD techniques to show how the velocity of the water flow changes as a function of flow rate, water temperature, aspect ratio, size of the tank, and baffle height . Several authors have stated how CFD can be used as a design tool (a list can be found in Edzwald (2010)). Amato and Wicks (2009) report by considering the effects of the baffle height on water velocities and bubble concentration in the separation zone,

CFD can be used to evaluate a plant expansion by increasing the flow of an existing DAF tank.

Previous CFD models of DAF units, such as those reported by Kwon et al. (2006), Amato and Wicks (2009) and Edzwald (2010), neglected bubble aggregation and were based on the assumption of a uniform bubble size. Looking at other application of CFD studies, such as mining, have used population balance algorithms to describe bubble coalescence and break-up (Edzwald, 2010; Chen et al., 2004) and it is predicted that the inclusion of bubble aggregation in a CFD model would make the model more accurate.

While CFD is a useful design tool, few verified models exist. There are assumptions about the bubbles that have to be made about; for example, as the bubble size significantly affects the predictions. Also, due to the difficulty of including the solid phase, this phase is usually neglected; although in practice, the solid phase particles affect the velocity predictions and air bubble concentrations. Currently, there is more research being conducted in order to develop a robust CFD model (Lakghomi et al., 2015; De Souza Vasconcelos et al., 2015; Samstag et al., 2016).

Summary and outlook

Flocculation clarifier and dissolved air flotation are the main clarification processes utilised for clean water treatment. There have been numerous advances in the development of mathematical models that capture the phenomena occurring. Kynch's model of sedimentation (Concha and Bustos, 1991) has been used as a starting point for many sedimentation models throughout the years. Extensions have been made to the model to simulate batch and continuous sedimentation within cylindrical columns, many of the models utilise macroscopic balances. The sedimentation process in the secondary settling tank is commonly approached from one-dimensional modelling. Several authors have attempted to extend the models to incorporate more detailed physical phenomena in order to enable a more robust and accurate model (Concha and Bustos, 1991; Burger and Concha, 1998; Burger et al., 1999). The flotation models consider a number of phenomena which are of great importance in plant operation, and however, are therefore very complex and require a number of parameter values which can only be obtained from experimental data or fitted from plant data. Therefore unfortunately limiting their current applicability. As pointed out by Edzwald (2010), more research is needed on the magnitude of bubble coalescence, collisions and attachment, and floc detachment that

may occur in DAF units and how these effects should be incorporated into mathematical models.

There has been a substantial amount of mathematical modelling research in the wastewater industry focusing on the development of a robust secondary settler tank, which has be applied to a sludge clarification unit in the clean water industry (Clarke et al., 1978; Wilson et al., 1979; Head et al., 1997). This brings encouragement in the application of this mathematical modelling approach to the clean water industry as it becomes an emerging research area. One-dimensional models of flocculation clarifiers (sedimentation tanks) are promising as they are able to be developed to accurately represent areas of interest at a reduced computational time than a two-dimensional model.

2.3.4 Filtration

The purpose of filtration in water treatment is the removal of solid particles from the water by passing the solid/water mixture through a porous medium or other suitable material to capture the solid particles whilst allowing the water to pass, thus achieving the required quality of filtered water. This unit is usually the third physical unit in the water treatment process and is often the last line of defense to remove floc and colloidal particles from entering the distribution by retention in the porous medium. A porous medium is a solid matrix containing voids which interconnect to enable the fluid flow through the medium at a low speed (Jegatheesan and Vigneswaran, 1987). Upon filtration, the media thereby retains most of the solid matter within the pore structure.

There are three basic types of filtration methods used in water treatment: slow sand filters (Huisman and Wood, 1974), rapid gravity filters (Han et al., 2008) and pressure filters (Landman et al., 1995), with rapid gravity filters being the most common. Slow sand filters are the oldest and original type of sand filter. These filters operate at low-loading rates and thus they are deemed as 'slow'. In this type of filter, two processes are used to treat the water: physical straining and biological action using fine sand as a medium, where at the top of the sand and the uppermost part of the sand bed there is a layer of biological growth (also known as schmutzdecke), which is vital for effective operation.

Rapid gravity filters differ from slow sand filtration as they operate at high loading rates using a coarser media with a high permeability rate. In this type of filtration, water

is treated by physical treatment alone and the media used can be granular activated carbon. Pressure filters share many of the same characteristics as rapid gravity filters except that they operate under pressure in a large closed vessel. They can be situated either vertically or horizontally with a set of frontal pipe work and valves. Slow sand filters and rapid sand filters are widely used for the removal of suspended solids present in water, but sand filters have a number of limitations and drawbacks such as high energy requirements for back-washing. One of the most serious problems involved with sand filters include maintaining bed homogeneity during operation. Inhomogeneities in the bed leads to formation of channels in the bed, poor distribution of the liquid flow through the bed, and thus very low particulate removal (Brika, 2010). The advantages and disadvantages of the various filter types can be found in Table 2.5.

A comprehensive review of granular media filtration processes is provided by Cleasby and Logsdon (1999). The various types of filters used for particle removal in potable water filtration can be classified based on several factors, including (Tobiason et al., 2010):

1. **Dominant overall mechanism for particle removal:** Particle removal mechanisms can be divided into three main classifications: *deep bed filtration, straining filtration,* and *cake filtration.* Deep bed filtration occurs when the pore spaces of a filter receive particle deposits which transport to, and attach themselves on, the surface of the granular media. Straining filtration occurs when the particle is too large to pass through the pore opening; and this type of filtration is predominantly used in low pressure membrane filtration. Cake filtration is when water to be filtered passes through a cake comprised of previously deposited particles.

2. **Filtration media used:** The filtration media used are comprised of specific depths of one or more types and sizes of granular media, such as rapid sand, dual-media and slow sand filters.

3. **Hydraulic loading rate:** The hydraulic loading rate is the flow rate of water applied per unit area of the filter. It is the velocity of the water approaching the face of the filter. It has a significant impact on the capital cost of treatment because the required filtration surface area to produce a desired flow decreases as the hydraulic loading rate increases.

In water and wastewater treatment, particles of various sizes present in water can be removed by deep bed filtration, which involves complex mechanisms. In order for

Table 2.5: Advantages and disadvantages of various filter types used in clean water treatment.

	Advantages	**Disadvantages**	**Author(s)**
Slow sand filtration	Works without coagulants. Produces excellent water quality. Low cost and ease of construction/operation.	Large area required. Labour intensive to operate. Not effective with highly turbid waters. Algal growths cause operational difficulties.	(Huisman and Wood, 1974)
Rapid gravity filtration	Low construction costs. Produces excellent water quality (quality is still less than slow sand filtration). Operation and backwash can be observed.	Increased operation costs. Increased maintenance.	(Han et al., 2008)
Pressure filtration	Placed directly in pumping line with little head loss. Produces good water quality. Low initial costs.	Unable to observe the filter media. Unable to determine the operating condition of the media as it changes.	(Landman et al., 1995)
Membrane filtration	Good degree of treatment. Produces good water quality. Operation and maintenance is simple.	Regular maintenance.	Crittenden et al. (2012)

removal to be effective, there are various factors to be considered such as physical and chemical characteristics of the water, the particles and the filter medium (Vigneswaran et al., 2009).

Stages of deep bed filtration

The filtration process can be categorised into two stages: the *initial stage* and the *transient stage*. The initial stage is when the filter bed is clean and particle deposition occurs onto the clean filter, which has a negligible effect on the properties of the filter during the initial stage. The transient stage describes the rest of the filtration process. Where deposition occurs on filter grains which are already partly covered by deposited particles. Depending on the chemical conditions of the suspension and filter medium, the removal of particles can either improve or degenerate during this stage.

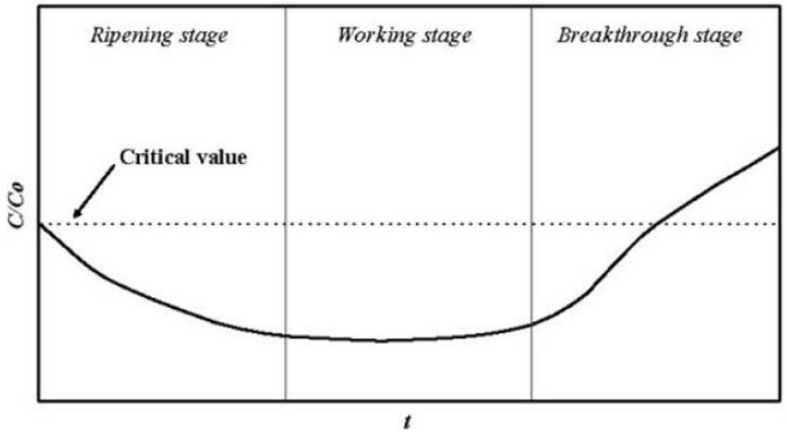


Figure 2.8: Typical curve showing filter performance over different stages of transient filtration. The relative suspended solid particle concentration, c/c_0 is shown over time, t (Vigneswaran et al., 2009).

Figure 2.8 shows the three sub-stages that occur in the transient stage during a filter run, which are the *ripening stage*, *working stage* and *breakthrough stage*. The improvement of the filter quality (c/c_0) with time is shown in the ripening stage, followed by the working stage in which the particle removal remains essentially constant. Finally, in the latter part of filtration, the breakthrough stage occurs where the particle removal starts to deteriorate and the filter efficiency decreases with time, at this time a back-washing occurs and resets the unit to the ripening stage.

For water filtration, there are a wide range of options that are available and have been presented in literature. Deep bed filtration dominates the main research area in which both macroscopic (deal with the accumulative collection of deposits) and microscopic (considers the size of the individual particle as well as the number of particles) approaches have been considered. Equations used to describe phenomena based on a macroscopic and microscopic approaches are discussed in this section. Very few filtration models have been formulated where filtration back-washing to clean the filter medium occurs in order to restore the efficiency of the filtration unit. However, optimum conditions and the effects of surface properties are also discussed in this section.

2.3.4.1 One-dimensional modelling

There have been various mathematical models that have been developed to describe particle capture in a filter (Rajagopalan and Tien, 1976; O'Melia and Ali, 1978; Johnson

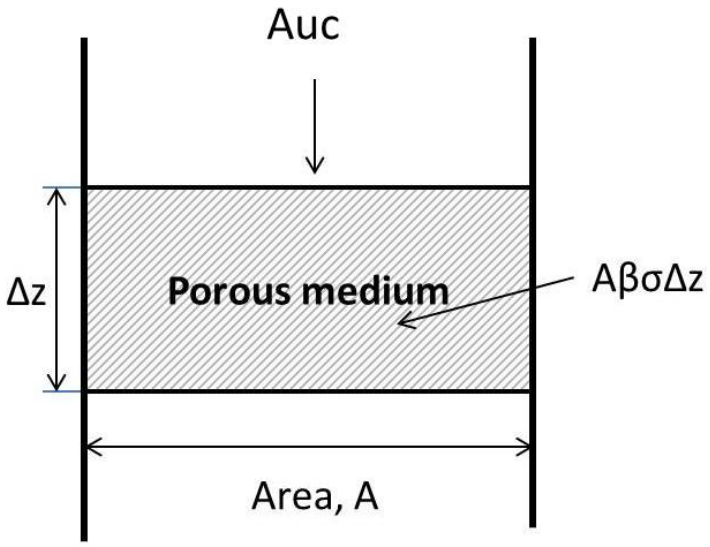


Figure 2.9: Filtration: Porous medium element.

and Elimelech, 1995). Studies have been done to understand dynamic change in the transient stage of filtration.

Macroscopic approach

A macroscopic modelling approach does not explicitly account for the flow field of the granular bed or the physical and chemical characteristics of the suspension (Ison and Ives, 1969). In 1937, Iwaski was the first to attempt a mathematical description of granular media filtration. The author proposed a first order kinetic equation, which was later verified experimentally by Ison and Ives (1969):

$$-\frac{\partial c(t,z)}{\partial z} = \lambda c(t,z) \tag{2.3.18}$$

where *c(t,z)* is the concentration (mg/L) of a particle at a given time t (s), and depth z (m), measured from the inlet of the filter, λ is the filter coefficient. The macroscopic conservation equation can be obtained in view of the phenomena affecting the flow and deposition of a suspension of solid particles passing through a downflow or upflow granular depth filter with initial porosity, ε_0, under constant flow rate or pressure drop conditions. Consider a porous medium element of depth, Δz, and area, A (m^2) (Figure 2.9), which contains:

- a volume $A\sigma\Delta z$ of retained particles

- a volume $A\varepsilon c\Delta z$ of moving particles entrained by the liquid
- a deposit of real volume $A\beta\sigma\Delta z$ imprisoned by the retained particles

where σ is the specific deposit of particles (mg/L) onto the filter medium expressed in terms of the ratio of the volume of deposited material over the differential volume under consideration (-), c is the volumetric concentration of particles within the zone (mg/L), ε is the porosity (-). With varying assumptions, the rate of particle deposition can be written in terms of the specific deposit, σ, or the particle concentration, c:

$$\frac{\partial\sigma}{\partial t} = \lambda uc \tag{2.3.19}$$

The governing parameters of the macroscopic model, the filter coefficient, λ, and the specific deposit, σ, are implicit functions of the physical and chemical characteristics, such as attachment and transport efficiency between particles and to the filter, of the suspension and filter medium, as well as of filtration velocity, u. The parameters vary with time and filter depth during the filtration process (as shown in Figure 2.8). In order to predict the concentration profile, the value of the filter coefficient λ must first be estimated. Yao et al. (1971) used the theory of floc formation of Smoluchowski (as outlined in subsection 2.3.2) as a basis to determine the clean bed filtration rate λ_0. Prior to this work, several authors tried to determine the clean bed filtration rate λ_0 in an empirical way for different circumstances. The main limitation of the macroscopic approach is that the physical and chemical characteristics of the filter medium, the suspension and the flocculants used are not explicitly described. This is where microscopic modelling will be beneficial to provide some solutions to the current limitations in macroscopic modelling.

Microscopic approach

In a microscopic modelling approach, the filter bed is modelled as a gathering of single or unit collectors, which fluid flows around or through the filter bed. In porous media, as a particle approaches a media grain, the motion deviates from the streamline due to different forces and torques acting on the particles, mainly related to transport and attachment. The main transport mechanisms are sedimentation, interception, Brownian diffusion and hydrodynamic action (Keir et al., 2009), as illustrated in Figure 2.10.

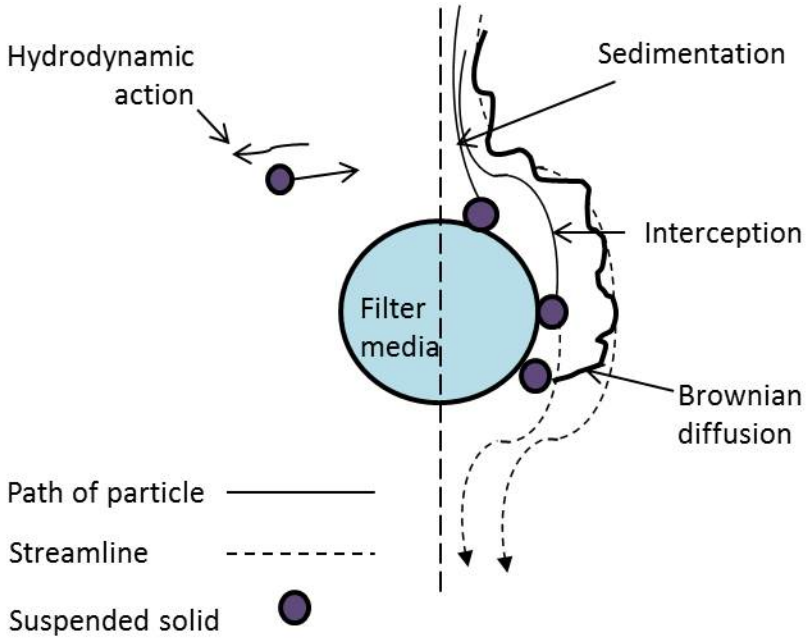


Figure 2.10: Basic transport mechanisms in a granular filter (Binnie and Kimber, 2009; Tobiason et al., 2010).

- Sedimentation takes into account the gravitational forces on the particles to be removed. If the density of the particle is greater than that of water, the dense particles will be removed more effectively by settling to the bottom of the unit.

- Interception occurs when particles moving uniformly collides with a grain of filter media. This enables the particle to be captured, thus being removed from the liquid flow.

- Brownian diffusion is a random movement observed due to the thermal agitations of the fluid molecules, which affects very small particles suspended in the medium.

- Hydrodynamic action arises from a random drifting across the flow streamlines which may lead to contact with the filter grain surface. Flow through the filter bed is typically laminar with some velocity profile, and hence a shear field. For a uniform shear field and a spherical particle, rotation of the particle causes a curving path across the shear field. For non-uniform shear field and non-spherical particles (which is most common in practice), the particle is deflected in a similar, but unpredictable manner. This is due to the velocity gradient in each pore surrounding the grains of filter media. A small particle passing through a grain of filter media will tend to be rotated by the velocity gradient. This will cause pressure differences across the particle, which will move it towards the filter media.

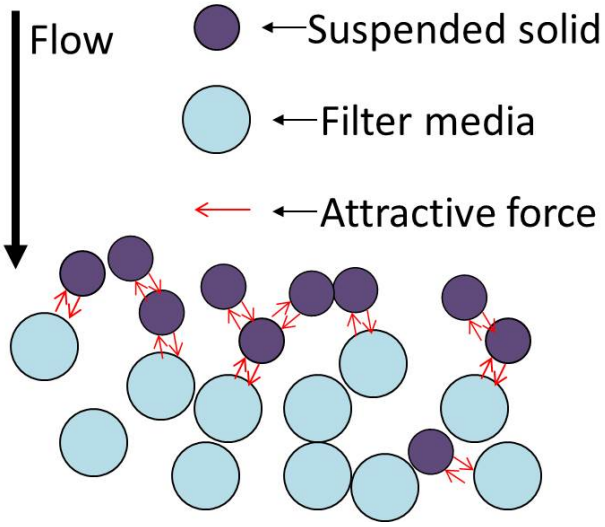


Figure 2.11: Particle attachment to filter media and to other particles.

A detailed discussion of these mechanisms can be found in Jegatheesan and Vigneswaran (2003). The authors state that these mechanisms are likely to occur simultaneously as particles in a flowing suspension will be subject to some or all of the mechanisms at varying degrees, and the level of impact will depend on fluid flow conditions, the geometry of the filter pores and the nature of the particles.

Figure 2.11 shows that once a suspended solid particle has made contact with the filtering media, it needs to be retained by an attachment mechanism to stick to the media. In the literature, the attachment mechanisms are considered to be gravity, London-van der Waals attraction, and double-layer forces (Keir et al., 2009). Adin and Rebhun (1974) state that the efficiency of a filtration process for a specific set of hydraulic conditions depends on the attachment forces and can be described by a relationship between attachment and shear forces. As the hydrodynamic shear forces become greater than the attachment forces, breakthrough of suspended solid particles occurs.

Transport efficiency, η, is defined as the fraction of contacting for a given collector relative to the particles approaching (Elimelech and O'Melia, 1990). Elimelech and O'Melia (1990) list the common equations for collection efficiency, with the most common correlation being the one developed by Rajagopalan and Tien (1976). Their studies were developed further to incorporate back-washing, and can be used to estimate when the best back-washing time would be (Fitzpatrick, 1998; Brouckaert et al., 2006). Back-washing involves reversing the flow of water through the filter in order to fluidise the bed and lift the particle building up on the filter medium and sending them to

drain. This is important not only for the maintenance of the filter but also for the filter efficiency by restoring the ripening stage of the filter cycle. Brouckaert et al. (2006) show that the particle/filter grain transport efficiency in the clean filter, η_0, can be calculated from:

$$\eta_0 = 4A_s^{1/3}Pe^{-2/3} + A_s N_{LO}^{1/8} N_R^{15/8} + 3.38\,x\,10^{-3} A_s N_G^{1.2} N_R^{-0.4} \tag{2.3.20}$$

where

$$A_s = \frac{1\,(1-p^5)}{w} \tag{2.3.21}$$

$$w = 2 - 3p + 3p^5 - 2p^6 \tag{2.3.22}$$

$$p = (1-\varepsilon)^{1/3} \tag{2.3.23}$$

The first term on the right hand side in Equation 2.3.20 represents filtration due to Brownian diffusion. A_s is a parameter defined by the Equation 2.3.21; and Pe is dimensionless Peclet number given by $^{D_\infty}/_{ud_c}$, where D_∞ is the bulk particle diffusion coefficient (m^2/s), u is the superficial velocity (m/s) and d_c is the clean filter grain diameter (m). The second and third terms represent the combined effects of interception and gravity when the retardation and London-van der Waals attraction are included. w and p are parameters defined by the Equations 2.3.22 and 2.3.23, respectively; N_{LO} is dimensionless van der Waals number given by $^{4A}/_{9\pi\mu d_p^2 u}$, where A is the Hamaker constant (1 x 10^{-20}J), μ is the viscosity of water (Pa. s) and d_p is the suspended solid particle diameter (m); N_R is the dimensionless ratio of particle to collector size given by $^{d_p}/_{d_c}$; and N_G is the gravitational force number given by $^{(\rho_p-\rho)gd_p^2}/_{18\mu u}$, where ρ_p is the particle density (kg/m^3) and g is gravity (m/s^2).

Model for transient stage of filtration

Within the microscopic approach, There are a variety of models that have been developed to calculate particle capture in a filter. Table 2.6 presents a summary of the most cited models in the literature which predict the removal efficiency during transient condition of a filter, and lists their strengths and weaknesses.

Although filtration models can be used very effectively to assess the influence of each variable, such as filter velocity, on filter performance, they all have several similar weaknesses:

- Existing models are based on the attachment of spherical particles on a single size

Table 2.6: Summary of recent filtration models and their strengths and weaknesses.

Models	Strengths	Weaknesses	Author(s)
Detachment mechanisms	Can simulate filter performance satisfactorily and easily at all filtration velocities.	Inclusion of factors relating to the attraction in the transient state modelling in an explicit manner is required.	(Jegatheesan, 1999; Han et al., 2008)
Filtration and adsorption	Can simulate filter performance satisfactorily.	Only at low filtration velocity.	(Jegatheesan, 1999)
Retained particles blocking other particle collection	Based on random sequential adsorption mechanism, which can be used to predict the transient stage and deposition of colloids.	Cannot be applied for unfavourable surface condition.	(Johnson and Elimelech, 1995)
Effects of change in the surface charge of filter grains	Useful in predicting the accumulation on the filter grain surface due to the deposition of particles.	Model is valid in predicting the changes in the filter media structure only at low inception numbers.	(Jegatheesan and Vigneswaran, 2003)

spherical media grain. Media characteristics such as angularity or media range based on the effective size has not been considered but is clearly of importance as neglecting this means hydrodynamic forces are not being represented.

- The studies mentioned in the table consider only deep bed filtration which, for applications in the developed world, is the main option However, in emergency scenarios where pre-filtration treatment is not a likely option, minimising the effect of surface straining in order to keep the filtration system efficient can be of equal importance to optimising depth filtration (Rajagopalan and Tien, 1976).

Model for filtration back-wash

Filtration operation involves back-washing to clean the filter medium. As stated earlier, backwashing involves reversing the flow of water through the filter in order to fluidise the bed to lift the particles building up on the filter medium and send them out to the drain. This is important not only for the maintenance of the filter but also for the filter efficiency by restoring the ripening stage of the filter cycle. Numerous research efforts have been made in studying the behaviour of fluidised beds (which is the phenomena

occurring during back-wash) because of their use in the chemical and mineral processing industry (Amirtharajah, 1971; Kawamura, 1975; Huang and Basagoiti, 1989; Ahmad, 1996; Brouckaert, 2004). There have been several modelling attempts to predict the process of filtration back-wash, including predicting the conditions for optimum backwash (Amirtharajah, 1971; Kawamura, 1975) and determining the effect of surface properties for floc, clay and bacteria on the efficiency of backwash (Huang and Basagoiti, 1989; Ahmad, 1996). However, Brouckaert (2004) states that the main limitations of existing back-wash models is that they do not sufficiently account for the intense mixing that occurs at the beginning of backwash as the most clogged regions of the filter bed collapse and disintegrate. This is due to the difficulty in capturing the initial stage because the mixing conditions change very rapidly with time.

Headloss development

Headloss in a filter bed is an important factor for the filter bed conditions, and can be used as an indicator to start filter washing. Headloss through the filter media is usually monitored by different pressure-cell devices that measure the water pressure above and below the filter media. When terminal headloss is reached, the filter should be washed, otherwise turbidity breakthrough may occur. One of the most practical headloss monitoring methods is to measure the headloss at different depths within the filter bed with several pressure taps (Crittenden et al., 2012).

For a clean bed, the pressure drop across the filter bed is given by the Carmen-Kozeny equation. This equation was derived assuming that the flow is laminar, the filter media are uniform spheres, and the pressure drop results entirely from the form-drag loss as fluid moves around the media. The Carmen-Kozeny equation can be expressed as a change in headloss over a length of clean filter bed:

$$-\frac{\Delta P}{L} = \frac{150\mu u\left(1-\varepsilon_0\right)^2}{d_c^2\varepsilon_o^3} \tag{2.3.24}$$

The pressure drop after a backwash can be expressed as:

$$\Delta P = h\rho g = L\left(\rho_s - \rho\right)g\left(1-\varepsilon\right) \tag{2.3.25}$$

where $\triangle P$ is pressure drop, h is the headloss (m), L is the filter bed depth (m), u is the superficial velocity (m/s) and μ is the viscosity of water (Pa. s). Equation 2.3.24

predicts that the headloss should increase as a function of decreasing grain diameter, increasing superficial velocity, increasing viscosity and decreasing density of the influent. It is beneficial to factor in headloss when looking to model filtration performance.

Summary and outlook

Filtration is generally the final physical removal process in clean water treatment. This is achieved by passing a mixture of suspended solid particles and water through a porous medium to capture the solid particles whilst allowing the water to pass. Tobiason et al. (2010) provide a list of the various filters that can be used and classified by several factors with the dominant overall mechanism for particle removal being highlighted. For water treatment, the preferred mechanism is deep bed filtration. Numerous models have been proposed to predict the removal efficiency in deep bed filtration at initial and transient stages and at both macroscopic and microscopic levels. In general, filtration models based on the concept of adsorption can simulate the filtration performance at low filtration velocity (Ali and Gupta, 2006) whereas models based on the detachment mechanism (Jegatheesan, 1999; Han et al., 2008) can simulate the filter performance acceptably and easily at all filtration velocities. The detachment mechanisms can also be used to show the three stages that usually occur during a filtration run: ripening, working and breakthough stages, which enables effective timing for back-washing.

In order to develop a more detailed predictive model of back-wash efficiency, the model should be based on easily measured parameters such as rate of headloss development, which is an important indicator for all the filter bed conditions. Headloss can be used as an indicator to start filter washing, initiating turbidity decrease through removal of total suspended solids (flocs) and filter run time. Such a model can be easily integrated with existing models of the filtration phase of the filter cycle, including models of filter ripening.

2.3.5 Disinfection

Disinfection is the final main unit operation in clean water treatment before the water enters the distribution system. In this process, most of the remaining pathogenic organisms are killed or controlled. The most commonly used disinfection treatment systems are ozonation, ultraviolet irradiation (UV) and chlorination using chemicals such as chlorine dioxide and chlorine based compounds. UV water treatment is an effective

Table 2.7: Advantages and disadvantages of various disinfection treatment used in clean water treatment.

	Advantages	**Disadvantages**	**Author(s)**
Ozonation	Utilises a short contact time. Ozone decomposes rapidly so no harmful residuals. Ozone is generated on site, thus, fewer safety problems with shipping and handling. Increases dissolved oxygen concentration of the effluent.	Low dosages may not effectively inactivate some viruses, spores and cysts. Requires complicated equipment and efficient contacting systems. Corrosion resistant material is required. Off gases must be destroyed to prevent exposure.	(Weiss, 1935; Am Water Works Res et al., 1991; Reynolds and Richards, 1996)
Ultraviolet irradiation (UV)	Physical process, which eliminates the need to generate, handle, transport or store toxic chemicals. User friendly for operators. Utilises short contact time. Equipment requires less space than other methods.	Low dosage may not effectively inactivate some viruses, spores and cysts. Potential for bacterial reactivation. Cleaning method to prevent fouling. Not cost-effective.	(Linden and Rosenfeldt, 1990; Reynolds and Richards, 1996)
Chlorine	Cost effective. Well established technology. Effective against wide spectrum of pathogenic organisms. Flexible dosing control. Eliminates odours.	Toxic to aquatic life. Highly corrosive. Chlorine reacts with some organic compounds that create more hazardous compounds. Low doses of chlorine will not be able to inactive all parasitic species, due to resistance.	(Reynolds and Richards, 1996; Clark et al., 2001)

way to disinfect drinking water supplies, and this process is becoming increasingly popular as an alternative to chlorine disinfection systems as no chemicals are added to the water. Details of the advantages and disadvantages of ozonation, ultraviolet irradiation and forms of chlorine can be found in Table 2.7.

For water disinfection, there are a wide range of options that are available and have been presented in literature. Due to the complex phenomena occurring most modelling within this area are empirical models and the development of these are discussed in this section.

2.3.5.1 Kinetic model

Several authors have proposed mathematical models of disinfection based on empirical observations (Lawrence and Cappelli, 1977; Hijnen et al., 2006). More detailed

modelling approaches have also been considered, in particular, kinetic modelling which simplifies and idealises complex phenomena occurring within a system. Based on the following assumptions being satisfied, kinetic inactivation models are derived (Lawrence and Cappelli, 1977; Gyurek and Finch, 1998; Hijnen et al., 2006):

1. No back mixing.
2. Uniform dispersion of disinfectant molecules and organisms.
3. Sufficient mixing to ensure liquid diffusion is not rate limiting.
4. Fixed temperature and pH.
5. Constant disinfectant concentration during the contact time.

These assumptions have been applied to the various disinfection methods available. Several kinetic models have been derived from the following differential rate law:

$$\frac{dN}{dt} = -kmN^x c^n t^{m-1} \tag{2.3.26}$$

where dN/dt is the rate of inactivation of microorganisms, k is reaction rate constant found experimentally, N is the number of microorganisms that did not inactivate at contact time t, c is the concentration of disinfectant and m, n, and x are empirical constants. Table 2.8 presents a summary of kinetic models that are currently available. The equations presented in this table are used to describe the inactivation of microorganisms within disinfection techniques and all equations are applicable to chlorination, ozonation and ultraviolet irradiation.

Chlorination

A representation of second-order kinetics for chlorine consumption in disinfection was developed by Zhang et al. (2000), who incorporated chlorine consumption into a numerical model to predict the formation of disinfection by-products (DBP) for clean water applications. The model was refined to predict the required chlorine demand in the disinfection process. The main concern was the distribution of the major DBPs in the contact tanks, this includes primarily total trihalomethanes (TTHMs), dichloroacetic acid (DCAA) and trichloroacetic acid (TCAA).

Table 2.8: Summary of all kinetic inactivation models for disinfection. Reproduced with permissions from Gyurek and Finch (1998).

Primary Equation	Model Basis	Comment	Author(s)
Chick-Watson			
$-kC^nT$	1. Disinfectant is present in excess. 2. Reaction is irreversible. 3. The microorganisms are genetically similar.	1. The simplicity of the Chick-Watson model makes it attractive for design and regulatory practice. 2. Can adequately describe ultraviolet radiation.	(Chick, 1908; Watson, 1908)
Hom rational			
$-kC^nT^m$ $-\frac{log[1+N_0^{x-1}(x-1)kC^nT]}{(x-1)}$	Can describe the shoulder and tailing off phenomena (which are part of the three-stage inactivation curve: shoulder, linear and tailing) for x $<$ 1 and x $>$ 1.	Model created by observing that plots of log survival on contact time for chlorine disinfection of natural algal-bacterial systems were curvilinear rather than linear.	(Hom, 1972; Majumdar et al., 1973; Roy et al., 1981)
Hom-Power law			
$-\frac{log[1+N_0^{x-1}(x-1)kC^nT^m]}{(x-1)}$	Model may provide better fit than either the Hom or Rational model for survival curves in which the inactivation rate initially increases and then decreases during the contact time.	A kinetic model with as many as four parameters can lead to over-parametrisation resulting in highly correlated parameter estimates.	(Anotai, 1996)
Selleck			
$-nlog[1+\frac{CT}{k}]$	Proposed when a decrease in inactivation rate during contact time occurred even when the disinfectant concentration remained constant.	Model has been used to describe survival curves having an initial shoulder and a declining inactivation rate, which are often observed in chlorination of wastewater.	(Gard, 2008; Selleck et al., 1978; Haas, 1979)

Table 2.8 continued: Summary of all kinetic inactivation models for disinfection. Reproduced with permissions from Gyurek and Finch (1998).

Primary Equation	Model Basis	Comment	Author(s)
Multiple target			
$log[1-(1-e^{-kCT}))^{n_c}]$	Mixed second-order kinetics describe the rate of inactivation of a critical target.	The multiple-target model is not suitable for describing microbial inactivation kinetics because it is unlikely clumps will be of equal size and cell damage will be randomly distributed among targets.	(Kimball, 1953; Wei and Chang, 1975)
Series event			
$\frac{-kCT + ln\left[\sum_{k-0}^{l-1} \frac{(kCT)^k}{k!}\right]}{ln(10)}$	1. Series-event model assumes that a number of first-order reactions with respect to concentration are needed to inactivate the organism. 2. Series-event model describes shoulder behaviour when $l > 1$.	Inappropriate because the series-event model assumes that the occurrence of an event in a viable organism is independent of the occurrence of previous events.	(Wei and Chang, 1975; Severin et al., 1984)
Multiple series event			
$log\left[1-\left(1-e^{-kCT}\sum_{k=0}^{l-1}\frac{(kCT)^k}{k!}\right)\right]$	Multiple series-event model simplifies to the multiple-target model when uniform clumps are assumed to be made of single-hit organisms.	Possible to describe tailing-off behaviour (seen in graphs) using a number of multiple series-event models, each corresponding to a different clump size L, the complexity in doing so limits the applicability of the series-event model.	(Wei and Chang, 1975; Severin et al., 1984)

Clark et al. (2001) presented a mathematical model based on the use of two second-order terms for predicting chlorine consumption loss or decay. It was found that the water quality variables needed to predict the model parameters, in order of importance, where: initial chlorine concentration, UV absorbance, total organic carbon (TOC) concentration, pH, bromide concentration, and alkalinity. More recent research conducted by Muslim et al. (2009), provided a dynamic single-input single-output model based on CFD to describe chlorine dosing and the decay process in chlorine contact tanks. The model provided a new direction in evaluating a control scheme particularly pertinent to fluid mixing problems.

Ozonation

Weiss (1935) presented two analytical kinetic ozone decomposition models for ozone decomposition in water. The first model was called Staehelin, Hoigne and Buhler (SHB), and was experimentally developed for acidic to neutral pH conditions. With an empirical approach, Lovato et al. (2009) developed the SHB model by relating the pH solution to one of the 18 kinetic constants. The Tomiyasu, Fukutomi and Gordon (TFG) model, on the other hand, considered high pH values (Audenaert et al., 2010). Westerhoff et al. (1997) compared both models and found that they predicted different kinetics for molecular ozone, HO radicals, and other intermediate species; however, both models were able to predict similar O_3/HO ratios.

Ultraviolet irradiation

Different approaches to modelling ultraviolet irradiation (UV) in water treatment have been considered in the literature: 1) the disinfection field is considered as a continuum and solved in an Eulerian framework, and 2) the microorganism particles and their inactivation are tracked using a Lagrangian frame of reference. There have been several studies that suggest the efficacy of UV inactivation can occur due to photoreactivation of the damaged microorganism (Eker et al., 1991; Whitby and Palmateer, 1993; Lindenauer and Darby, 1994; Chan and Killick, 1995).

Photoreactivation is the phenomenon by which UV-inactivated microorganisms recover activity through the repair of dimers in the DNA under near-UV light (Oguma et al., 2001). Few papers have focused on modelling the reactivation processes, which focus on describing qualitative studies of the process (Harris et al., 1987; Lindenauer and Darby,

1994; Hassen et al., 2000; Oguma et al., 2004). There are other authors who have tried to model both the reactivation and inactivation phases by comparing experiments that did and did not include reactivation (Tosa and Hirata, 1999; Beggs, 2002). Kashimada et al. (1996) offered a model to predict the reactivation phase independently, but the experiments carried out were insufficient to be generalised, and a better understanding of the factors affecting the kinetics of activation is therefore required. There have also been studies suggesting numerical simulations based on exploiting techniques from CFD can be utilised in the modelling efforts for UV disinfection (Lyn et al., 1992). Lyn et al. (1992) used a steady state two-dimensional depth averaged model to predict the turbulent flow in a vertical-type open channel UV reactor. The model was extended by Lyn (1999) compared numerical predictions with experimental measurements and examined in more detail the simulation of not only flow, but also disinfection in open-channel UV disinfection systems.

Summary and outlook

The disinfection of water treatment plants is mainly a chemical process, nevertheless a process model would have to take into consideration other phenomena, such as turbulent flows for mixing which can be assumed to be created by equipment, such as baffles. Presented in this section are the key kinetic models, which mostly dominate disinfection modelling and incorporate factors to account for the complexity of the fundamental phenomena occurring. These models can be used to model the varying forms of disinfection, such as ozonation, ultraviolet irradiation and chlorine treatment as they focus on the inactivation of microorganisms. There is a need to develop and optimise analytical methods to determine the amount of by-product to gain the advantage of using lower amounts of reagents.

2.4 Challenges and opportunities

Although continuous progress has been made in recent years in improving the accuracy of mathematical models to predict clean water treatment processes, much research work still need to be carried out. In order for first principle modelling approach to be applied in this industry, there needs to be more research into the fundamental understanding of the behaviour of the process and the hydrodynamic relationships. A few examples of

these current limitations can be found in Table 2.9, along with suggestions for possible improvements that could be able to address these challenges.

Water supply companies are gradually shifting to centralised, fully-automated operations (Worm et al., 2010). The motivation for this change is the need for increased efficiency and a better and more stable water quality. More sophisticated operation would be required for a fully automated treatment plant, so operators would need to periodically train in the use of a clean water treatment plant simulator which can be developed by using first principles to create a mathematical model that enables an understanding the system behaviour to be achieved. Worm et al. (2010) discusses the successes in setting up this type of simulator for the first time. The simulation in the study incorporates four simultaneous models: a water quality model, a hydraulic model, a process control model and a field object model. In general, there is a need to develop plant-wide dynamic models able to describe start-up, shut-down, how to deal with various problems, and changing concentrations in a multipurpose plant. These models should be validated with real industrial data so that the applicability and validation of the models can be tested. With such a comparison, the weakness of the mathematical model can be identified and improved.

2.5 Overall concluding remarks

In order for first principles modelling approaches to be applied to the design and development of processing steps for clean water treatment processes in industry, a large body of evidence and best practices must be developed and validated in the literature. This literature review considered mathematical models available for the four key processing steps, coagulation and flocculation, clarification, filtration and disinfection. The key findings are summarised in this section:

Coagulation and flocculation are important processes in clean water treatment as flocs are formed through aggregation with the aid of chemical coagulants and mixing. From researching several authors in literature, there are two main conclusions. Firstly, the experimental results established by idealised particle suspensions are not likely to provide accurate representation of the behaviour for real systems. Secondly, focusing on the microscopic behaviour of particles in an attempt to find correlations between process parameters (e.g. mixing intensity, coagulant dosage) and flocculation kinetics (e.g. collision efficiencies) would be extremely difficult. A mathematical model that

Table 2.9: Current limitations of modelling the various clean water treatment processes.

Current limitations	**PSE methods currently being applied**	**Improvements that can be made**	**Author(s)**
Jar testing models focus on chemistry within units and not on process interactions.	1. Artificial Neutral networks to model dosage. 2. Adaptive Neuro-Fuzzy Inference system.	Inclusion of flow and concentration of water using fundamental modelling.	(Valentin et al., 1999; Wu and Lo, 2008; Heddam et al., 2012)
1. Within Flocculation nearly all models are based upon Smoluchowski's coagulation equation. 2. Smoluchowski's theory has been found to only be valid in particular cases of coalescences of small particles with large ones.	One and two dimensional modelling.	Utilising process focussed modelling to investigate how the concentration increase with the floc size distribution.	(Gregory, 1981; Wiesner, 1992; Spicer and Pratsinis, 1996; Veshchunov, 2011)
Mixed flocculators are more complex to model.	1. Monte Carlo stochastic simulations. 2. Bulk flow patterns, primarily at lab scale.	1. Multiphase modelling. 2. Population balances. 3. CFD.	(Parker et al., 1972; Haarhoff et al., 1997; Bridgeman et al., 2009)
There are various factors, such as particle velocity and size, that can influence the settling process in clarification, finding an efficient way to combine all factors is a difficult task.	1. Shear forces in water flow. Hydrodynamic processes. 2. Removal efficiency models.	Fundamental understanding of the behaviour of particle suspension suspensions (as particle suspension dynamics play a major role in the migration and removal of particles in a fluid flow).	(Kim and Kramer, 2006; Al-Sammarraee et al., 2009)
Formation of sludge blankets in the clarification. Existing models developed to portray real works are time consuming to solve and the simulation outcomes do not provide accurate results.	Partial differential equations representing kinematic model.	1. Fundamental understanding of the various aspects of the floc blanket theory by drawing upon models derived in the wastewater industry. 2. Dynamic effects of moving flows and suspended particles.	(Wilson et al., 1979; Concha and Bustos, 1991; Burger and Concha, 1998; Burger et al., 1999)
In filtration, models developed have limited inclusion of media characteristics, such as angularity or media range.	Optimisation of filtration depth.	Minimising the effect of surface straining in the models.	(Jegatheesan, 1999; Jegatheesan and Vigneswaran, 2003; Han et al., 2008)

can draw upon the key aspects of the microscopic behaviour whilst integrating the hydrodynamic forces would be extremely beneficial in the development of a process model that is able to predict real system behaviour.

Clarification is a solid-liquid separation processing step, where flocculation clarifier and dissolved air flotation are the main clarification processes utilised for clean water treatment. There have been numerous advances in the development of mathematical models that capture the phenomena occurring in these clarification systems. There has been a substantial amount of mathematical modelling research in the wastewater industry focusing on the development of a robust secondary settler tank, which has be applied to a sludge clarification unit in the clean water industry. The sedimentation process in the secondary settling tank is commonly approached from one-dimensional modelling.

Filtration is the last physical removal processing step in the clean water treatment process, and the preferred mechanism is deep bed filtration. Numerous models have been proposed to predict the removal efficiency in deep bed filtration at initial and transient stages, and at both macroscopic and microscopic levels. These models combined currently provide a good prediction of filter behaviour; however, they can be strengthened with the incorporation of a predictive filter back-wash model.

Disinfection is mainly a chemical process to enable inactivation of microorganism present in the treated water. There are various established kinetic models that have been utilised to represent the usage of ozonation, ultraviolet irradiation and chlorine. Based on the review of the current literature, it is found that in order to move towards a more mechanistic model, a better understanding of the factors affecting the kinetics of activation is required, as it will enable accurate prediction of the efficiency of the various disinfection techniques.

2.6 Conclusions

In summary, this chapter describes the current state-of-the-art of modelling and optimisation related to the clean water industry. It is clear that process systems engineering can play a major role not only in the modelling of water treatment processes, but also in increasing the fundamental understanding of the physical and chemical phenomena occurring within each processing step. Thus, development of novel computational

models and optimisation algorithms that can be integrated into the water industry through advanced computing tools can be achieved by drawing upon PSE expertise. The modelling of water treatment plants is a current topic of interest and can be achieved by possible research into the integration of individual models of the water treatment units into bigger systems of models. More effort needs to be directed towards the development of dynamic process control models to provide savings on costs and emissions by reducing the use of chemicals and energy in order to meet regulation standards.

An integrated approach to modelling has been shown in literature to provide a competitive advantage to different sectors. An integrated approach can also be a driving force for operational-level optimisation based on explicit objectives in the development of novel designs and prediction of changes in the traditional concept of drinking water treatment. The developed models can incorporate water quality data to predict the changes in process parameters by preceding processing steps or how this change influences subsequent processing steps. As can be seen in literature, current work shows that an understanding of the phenomena will develop understanding for better process design.

In this work, the focus is to develop a conceptual understanding of clean water treatment processes utilising first principles modelling techniques. The main objective is the consideration of a complete mathematical model of an entire water treatment plant which enables a wider view on how changes in one processing unit will affect the treatment process as a whole.

Chapter 3

Modelling of clean water treatment units

The main objective of this chapter is to draw upon knowledge from the literature in order to establish mathematical models of the main clean water treatment processing steps. The knowledge gained from the previous chapter is considered and the selected mathematical model for each of the various units are described, followed by details of the numerical integration technique used for the dynamic simulations of the unit processes. The models are simulated using gPROMS (Process Systems Enterprise, 2014), then verified against previous studies in the literature, and finally the sensitivity of each model is tested.

3.1 Introduction

As outlined in Chapter 2, there are a variety of models developed in the literature to describe the behaviour of the different processing units of a clean water treatment work and it highlights that a better knowledge and understanding of the individual clean water processing units is advantageous. The main objective of this chapter is to describe the approaches taken in modelling of the three main physical processing units: coagulation and flocculation, clarification and filtration. The next section outlines the

development of mathematical models for these processing units based on first principles which are validated with data from literature. The models are predominately taken from literature, but are presented and compared here in a unified approach. The validity of the models will initially be considered at steady state to allow for proper comparison with previous work in the literature. The derivation of the models will be based on the previous work outlined in Chapter 2 and will be used in Chapter 4 in the development of a detailed mathematical model for a complete water treatment work.

Disinfection is a very complex process and the exact mechanisms are still not properly understood, hence a simplified approach will be considered for this step and detailed in Chapter 5.

3.2 Modelling of coagulation and flocculation

In this section, coagulation and flocculation are being modelled together as one process, as these mechanisms are closely integrated. Two alternative mathematical models are described to simulate the formation of flocs following the addition of chemicals to promote the aggregation of colloidal particles.

3.2.1 Unit principle

Colloidal particulates in the raw water are grown in the coagulation/flocculation step by neutralisation of negative charges due to the addition of chemicals. This can be done by a number of mechanisms, but the addition of a chemical coagulant under rapidly mixed conditions is the most traditional method in clean water treatment (Crittenden et al., 2012). Once the coagulant has been added, the particles become destabilised, which encourages the rapid formation of small agglomerates.

Following this initial coagulation, flocculation follows, which is a gentle mixing stage taking place either in a slow mixing unit or using movement through baffled chambers, thus increasing the particle size from small colloidal particles to visible suspended solid particles. Through the a process of slow mixing, colloidal particles are brought into contact with one another. Collisions of the colloidal particles cause them to agglomerate to produce larger, more visible flocs. The floc size continues to grow through additional collisions and interaction with the inorganic polymers formed by the coagulant or

with organic polymers added. A traditional coagulation/flocculation unit is shown schematically in Figure 3.1a, which has the rapid mixing of chemicals before the slow mixing occurs (Haarhoff et al., 1997). This unit is typically utilised when the location of the plant is not able to accommodate flocculation chambers that can promote the slow particle growth. Figure 3.1b shows an alternative unit operations as there is no initial rapid mixing of the chemicals, and instead the slow mixing process begins as soon as the chemical coagulants as added (Argaman, 1971). This unit of operations are often found in series as shown in Figure 3.2. Factors that can promote coagulation and flocculation are velocity gradient (which is the degree of mixing based on the power provided), pH and time. pH is a key factor in removal of colloids because it affects the choice of chemical coagulant for particle aggregation, while time and velocity gradient are also important factors to increase the probability of particle aggregation (Pillai, 1997).

3.2.2 Model development

The main purpose of the mathematical models for the coagulation and flocculation unit is to describe the growth of flocs, also known as secondary particles, from the colloidal/primary particles entering the system and develop an understanding of the relationship between the break up of flocs back into primary particles.

This section is divided into two subsections, which focus on the alternative coagulation/flocculation units being considered. A model developed by Argaman and Kaufman (1970) form the starting point for this work. The development of the models and the corresponding assumptions are explained in the following section.

Floc formation through rapid mixing

Flocculation via rapid mixing is mainly designed as a pre-treatment step for the removal of suspended solids, which results in the reduction in turbidity. During the floc formation process, heavy metals, pathogenic microorganisms and organic matter are incorporated in the resulting flocs particles. As discussed in Chapter 2, the basis of most of the current theories used to model flocculation dates back to work by Smoluchowski from 1917 (Gon Lee et al., 2000).

In the literature, number concentration is often used to describe the concentration of suspended solid particles, as the number concentration is often based on empirical

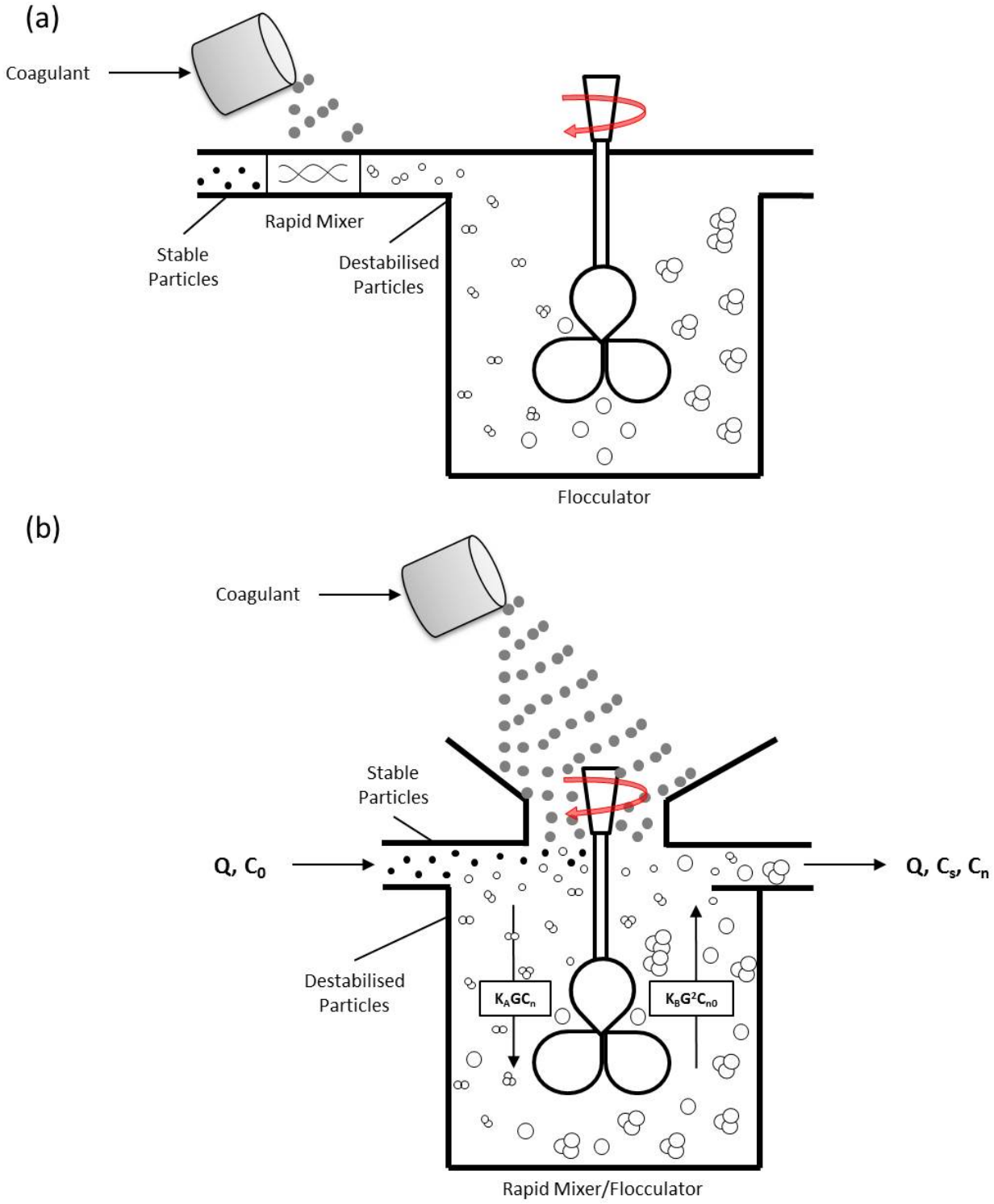


Figure 3.1: Schematic impressions of a) coagulation and flocculation flowsheet, b) floc formation chamber.

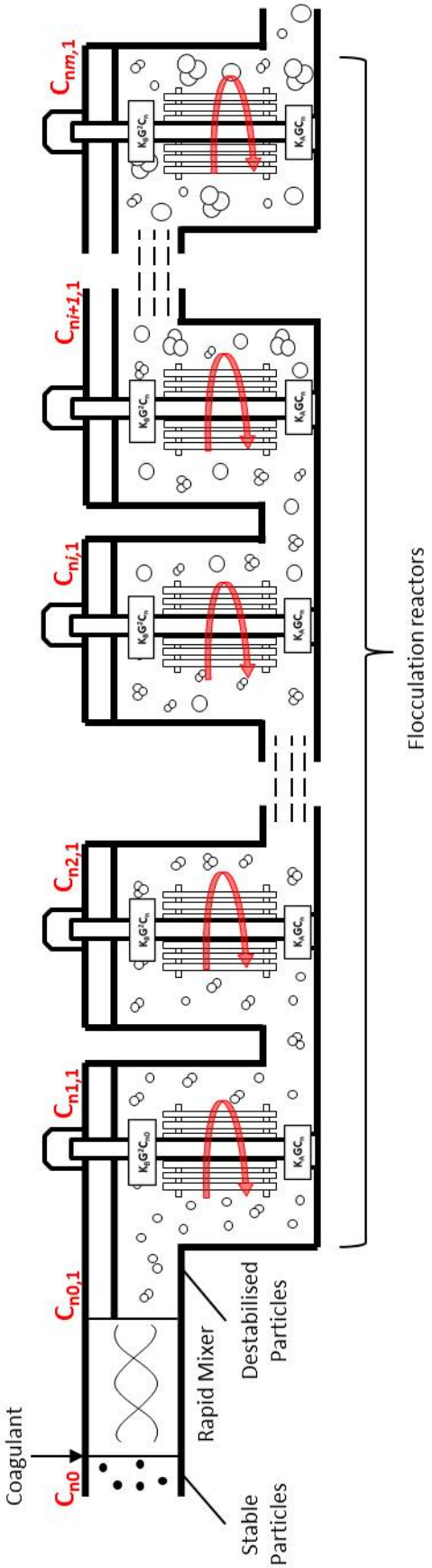


Figure 3.2: Schematic diagram of multi-compartment flocculator.

relations where it is easier to determine the approximated number of particles per millilitre of water. In the absence of satisfactory means for determining the number concentration, particle mass concentration may be substituted for number concentration (Rietveld et al., 2009).

During the coagulation/flocculation processing step, destabilisation and aggregation of colloidal/primary particles occurs. During the flocculation stage, mixing is used to promote the aggregation of colloidal/primary particles to flocs; however this mixing can also cause the flocs to break up into the colloidal/primary particles as these mechanisms occur simultaneously. With a number of simplifying assumptions, Argaman and Kaufman (1970) developed an equation for floc formation in a single CSTR. By assuming that the model constants remained constant in consecutive tanks, the model was extended to, and verified for, a number of floc formation tanks in series.

James (1993) shows the derivation for a one-dimensional equation of a dissolved or suspended compound in water using an advection-dispersion model, which has been subsequently utilised by Rietveld (2005). In the advection-dispersion model, there are three basic mechanisms distinguished that are responsible for the transport of dissolved and suspended solids in natural waters:

- Advection refers to transport due to the bulk movement of the water.
- Diffusion is the transport due to migration of a solute in response to a concentration gradient as a result of Brownian motion.
- Dispersion is the transport due to turbulence of the fluid and velocity shear.

The general material balance of particles can be written as:

$$accumulation\,rate\; = (flow\,in)\; -\; (flow\,out)$$

The equation for one-dimensional flow of a dissolved or suspended compound in water assuming that the turbulent dispersion can be described with Fick's law for molecular diffusion, and that the uniform flow in x-direction, with a constant dispersion coefficient D_x (m^2/s) can be written as:

$$\frac{\partial c}{\partial t} + \frac{\partial \left(uc - D_x \frac{\partial c}{\partial x}\right)}{\partial x} = 0 \tag{3.2.1}$$

where

u velocity of primary particles in water through CSTR (m/s)
c concentration of suspended solids as primary particles (mg/L)
D_x dispersion coefficient in water (m^2/s)

The rate at which molecules are transferred into new compounds can be described by reaction kinetics. The rate of transformation of any i^{th} reactant or product is defined as the quantity of material changing per unit time per unit volume, given as:

$$\frac{\partial c}{\partial t} = -f_i(c) \tag{3.2.2}$$

where f_i is the decay function of i^{th} reactant in water (mg/L.s). Simple reactions can be described by an expression for f_i. Complex reactions consist of numerous reaction paths and require multiple reaction rate expressions to describe the overall reaction rate. Finally, reactions that proceed in one direction are designated irreversible. Reactions occurring in both forward and reverse directions are known as reversible. Often, irreversible homogeneous reactions with unknown mechanisms can be modelled with an Υ-order rate expression (Montgomery, 1985):

$$\frac{\partial c_i}{\partial t} = -f_{1,i}(c) = -k_1 c_1^{\Upsilon}$$

where k_1 is the reaction rate ($(\mathrm{mg/L})^{1-\gamma} s^{-1}$), and Υ is the order of reaction (-). The overall equation for one-dimensional flow of a dissolved or suspended compound in water is subject to transport, transfer and degradation in the water and solid phase (Rietveld, 2005) is written as:

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2\left(c, c_s\right) = 0 \tag{3.2.3}$$

where:

f_1 decay function of suspended solids in water (mg/L.s)
f_2 transfer function of suspended solids from water (mg/L.s)
s subscript for variables related to suspended solids in the solid (floc) phase

The first term is the change of concentration with time. The second term is the turbulent dispersion of the gradient type (following Fick's law). The third term indicates the transport of the concentration through the CSTR by advection. The fourth term represents a function for the decay of the suspended solids. The last term represents a function for the transfer of the suspended solids from the water to the suspended

solid phase. As mentioned in Chapter 2, in some of the available literature (Hannouche et al., 2011; Kemker, 2014), a linear relation between suspended solids concentration and turbidity is assumed to allow a qualitative relationship to be formulated. Based on a detailed theoretical analysis, Argaman and Kaufman (1970) developed a differential equation describing the overall kinetics of flocculation in turbulent mixing occurring in a batch reactor. In the Argaman-Kaufman equation it is assumed that the primary particles collide into flocs and that these flocs are removed by the subsequent particle removal device:

$$\frac{dc_n}{dt} = -K_A G c_n + \left(K_B c_{n0}\right) G^{\phi} \tag{3.2.4}$$

where:

c_n	number concentration of primary particles (m^{-3})
c_{n0}	initial number concentration of primary particles (m^{-3})
K_A	collision constant (-)
K_B	break-up constant (s)
G	velocity gradient (s^{-1})

For the transport of suspended solids in water and in flocs, the overall equations for transport of particles in the water and solid phase are written in Equation 3.2.5 and Equation 3.2.6, respectively:

$$\frac{\partial c}{\partial t} - D_x \frac{\partial^2 c}{\partial x^2} + u \frac{\partial c}{\partial x} + f_1(c) + f_2\left(c, c_s\right) = 0 \tag{3.2.5}$$

$$\frac{\partial c_s}{\partial t} - D_{x,s} \frac{\partial^2 c_s}{\partial x^2} + u \frac{\partial c_s}{\partial x} + f_{1,s}(c_s) + f_{2,s}\left(c, c_s\right) = 0 \tag{3.2.6}$$

Neglecting dispersion and decay as both are normally only present in the solid phase (Rietveld, 2005), Equations 3.2.5 and 3.2.6 are reduced to:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + f_2\left(c, c_s\right) = 0 \tag{3.2.7}$$

$$\frac{\partial c_s}{\partial t} + u_s \frac{\partial c_s}{\partial x} + f_{2,s}\left(c, c_s\right) = 0 \tag{3.2.8}$$

The transfer function of suspended solids from water f_2 occurs as the flocs break up as a result of the degradation of primary particles from floc surfaces due to eddies in the viscous dissipation range. Edzwald and Laminski (2007) state that based on an analysis by Parker et al. (1972), the parameter ϕ in Equation 3.2.4 is equal to 2. Incorporating

the parameter value into Equation 3.2.4 gives:

$$f_2(c, c_s) = -f_{2,s}(c, c_s) = K_A G c_n + (K_B c_{n0}) G^2 \tag{3.2.9}$$

By combining Equations 3.2.7, 3.2.8 and 3.2.9, the following equations are formed:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - K_A G c + (K_B c_{n0} G^2) = -u\frac{\partial c}{\partial x} - K_A G\left(c - \frac{K_B}{K_A} G c_{n0}\right) = -u\frac{\partial c}{\partial x} - k_2(c - c_e) \tag{3.2.10}$$

$$\frac{\partial c_s}{\partial t} = -u\frac{\partial c_s}{\partial x} + K_A G(c - \frac{K_B}{K_A} G c_{n0}) = -u\frac{\partial c_s}{\partial x} + k_2(c - c_e) \tag{3.2.11}$$

where c_e is the equilibrium concentration of suspended solids captured into flocs (mg/L). From the above equations, it can be seen that no floc formation will occur when G or K_A are zero, which agrees with the theory that collision is needed for floc formation, and mixing of the system promotes aggregation of the primary particles. It can also be concluded that when K_B is equal to zero, all primary particles will agglomerate into flocs and there will be no break up.

Floc formation in a flocculation chamber/compartments

Floc formation through rapid mixing occurs in a CSTR, where the velocity gradient plays an important role on the amount of flocs formed. This alternative unit operation is flocculation occurring in chambers (as opposed to a reactor) that are arranged in a series (creating a compartment). In the continuous-flow system shown in Figure 3.2, raw water containing suspended solids at concentration c_{n0} is entering a rapid mixing chamber to which chemical coagulants are added. After the destabilisation of these primary particles, the exit suspended solid concentration from the rapid mixing unit is denoted $c_{n0,1}$.

Gentle mixing, which occurs through turbulent waters, promotes the aggregation of primary particles into flocs. Neglecting the assumption that the velocity gradient, G, is the same in all flocculation reactors (Argaman and Kaufman, 1970), the mass balance of primary particles for a CSTR in series yields at steady state the following equation :

$$QC_{ni,1} - Qc_{ni+1,1} - K_{A,i+1} c_{ni+1,1} G_{i+1} V + K_{B,i+1} c_{n0,1} G_{i+1}^2 V = 0 \tag{3.2.12}$$

where:

Q	flow of water (L/s)
V	volume of reactor (L)
$c_{n0,1}$	concentration of primary particles at time t=0 (mg/L)
$c_{ni,1}$	concentration of primary particles in the output of the ith a flocculation compartment (mg/L)
Cc_1^{ni+1}	concentration of primary particles in the output of the $(i+1)$th flocculation compartment (mg/L)

Assuming ideal hydrodynamic behaviour, the average hydraulic retention (residence) time (T) can be obtained through V/Q. Thus, dividing Equation 3.2.12 by V and re-arranging for T:

$$c_{ni,1} - c_{ni+1,1} - K_{A,i+1}c_{ni+1,1}G_{i+1}T + K_{B,i+1}c_{n0,1}G_{i+1}^2T = 0$$

Then, dividing by $c_{ni+1,1}$:

$$\frac{c_{ni,1}}{c_{ni+1,1}} - 1 - K_{A,i+1}G_{i+1}T + K_{B,i+1}\frac{c_{n0,1}}{c_{ni+1,1}}G_{i+1}^2T = 0$$

and expanding by $\frac{C_{ni,1}}{C_{ni+1,1}}$:

$$\frac{c_{ni,1}}{c_{ni+1,1}} - 1 - K_{A,i+1}G_{i+1}T + K_{B,i+1}\frac{c_{n0,1}}{c_{ni+1,1}}\frac{c_{ni,1}}{c_{ni,1}}G_{i+1}^2T = 0$$

Finally, rearranging the equation:

$$\left(1 + \frac{c_{n0,1}}{c_{ni,1}}K_{B,i+1}G_{i+1}^2T\right)\frac{c_{ni,1}}{c_{ni+1,1}} = 1 + K_{A,i+1}G_{i+1}T$$

Therefore, for varying values of G in m compartments in series, the ratio of inlet-to-exit concentration is given by:

$$\frac{c_{ni,1}}{c_{ni+1,1}} = \frac{(1 + K_{A,i+1}G_{i+1}T)}{\left(1 + \frac{C_{n0,1}}{C_{ni,1}}K_{B,i+1}G_{i+1}^2T\right)} \tag{3.2.13}$$

and the overall change in concentration in the whole series of m compartments with equal average velocity gradients, G, incorporating the relation average hydraulic retention (residence) time multiplied by the number of flocculation chambers, $(\mathrm{T} \cdot m)$, which expresses the value responding to the total hydraulic retention (residence) time[1] (τ) can be written as (Argaman and Kaufman, 1970):

$$\frac{c_{n0,1}}{c_{nm,1}} = \frac{\left(1 + K_A G \frac{\tau}{m}\right)^m}{1 + K_B G^2 \frac{\tau}{m} \sum_{i=0}^{m-1} \left(1 + K_A G \frac{\tau}{m}\right)^i} \tag{3.2.14}$$

The main limitation with using these models is that the derived expression assumes that the floc suspension is of constant size distribution so using a plug flow reactor is not applicable as the floc size distribution will not be constant with time.

3.2.3 Numerical simulation and validation

In this section, the two flocculation models derived above will be simulated in gPROMS. First, the models will be validated against the literature and then the limitations of the models will be tested through a sensitivity analysis.

Model Parameters

Argaman (1971) conducted pilot-plant experiments in a flocculator to determine the parameters which will be used in this work for model validation. The experiments were conducted on an operating water treatment plant. Argaman (1971) interprets the experimental results by using theoretical results of flocculation kinetics in turbulent fluid. The experimental results (which can be found in Appendix B) are determined from the values for K_A and K_B. All the parameter values can be found in Table 3.1.

Model validation and sensitivity analysis

The experimental and theoretical values determined by Argaman (1971) are compared (in Table 3.2) with the predicted values calculated using the floc formation in rapid

[1] Total hydraulic retention (residence) time is a measure of the average length of time that a compound (water) remains in a unit (flocculation chamber).

Table 3.1: Model parameters for coagulation and flocculation model verification (Argaman, 1971).

Description	**Parameters**	**Value**
Collision constant (-)	K_A	1.8 x 10^{-5}
Break-up constant (s)	K_B	0.8 x 10^{-7}
Total hydraulic retention (residence) time (s)	τ	1800
Number of flocculation reactors (-)	m	4
Velocity Gradient (s^{-1})	G	20
Initial primary particle concentration (mg/L)	c_{n0}	10
Volumetric flowrate (L/s)*	Q	0.44

*Based on a symmetrical basin with volume 52,000 gal, the area is approximately $36m^2$. This can be used to estimate the velocity.

Table 3.2: Actual and predicted performance of a multi-compartment flocculator (Argaman, 1971).

	Values of $\frac{c_1^{n0}}{c_1^{nm}}$			
Number of compartments, i	Floc formation in rapid mixing (This work)	Floc formation in a flocculation chamber (This work)	Simulated in literature (Argaman, 1971)	Prototype actual performance (Argaman, 1971)
1	-	1.15	1.15	1.08
2	-	1.33	1.32	1.18
3	-	1.55	1.48	1.45
4	1.78	1.80	1.73	1.75

mixing (Equations 3.2.10 and 3.2.11) and floc formation in a flocculation chamber model (Equations 3.2.13 to 3.2.14).

From the results, it can be seen that there is consistently good agreement between the models developed in this work and literature. This suggests that these two models can be used to represent the phenomena occurring in the coagulation and flocculation units. To test the limitations of the models, sensitivity analysis will be conducted to:

1. Test the relationship between the velocity gradient and hydraulic residence time in the floc formation in flocculation chambers
2. Test how the floc formation by rapid mixing reacts to a set of illustrative case studies

These two sensitivity analyses are relevant to actual water treatment plants because the amount of time a colloidal/primary particle spends in a flocculation chamber or is

rapidly mixed will have an affect on the suspended solids concentration. Floc formation can be hindered if the velocity gradient is too high promoting floc break up in the effluent stream.

Sensitivity study 1: Floc formation in a flocculation chamber

Figure 3.3 shows the relationship between the velocity gradient, G, and the total hydraulic retention (residence) time, τ, for the two examined case studies (flocculation chamber with one and four compartments, respectively) for two different values of collision constant, K_A and break-up constant, K_B. It can be seen that for any desired flocculation performance, there is a minimum retention (residence) time, below which the performance can not be determined regardless of the velocity gradient. This observation agrees well with those found in the literature where it is stated that the product $G \cdot \tau$ in itself is not an adequate parameter for describing the effects of stirring energy and residence time on flocculation performance (Argaman, 1971; Crittenden et al., 2012).

Both figures illustrate the effect of compartmentalisation, particularly when the high performance is desired. Figure 3.3a shows that for 75% removal of primary particles ($c_1^{n0}/c_1^{nm} = 4$), the total hydraulic retention (residence) time (*ca.* 700 s) required in a four-compartment reactor is approximately half of the required time (*ca.* 2000 s) for a single-compartment reactor. This is in contrast to what is observed in Figure 3.3b, where the graph shows that for 75% removal ($c_1^{n0}/c_1^{nm} = 4$), the single-compartment reactor has a smaller retention (residence) time (*ca.* 13000 s) than a four-compartment reactor (*ca.* 48000 s). This observation can be attributed to the smaller break-up constant, K_B, as for low velocity gradients, G, or for strong flocs (with a small breakup constant), the denominator of the equation 3.2.14 approaches unity; therefore increase in the number of compartments would have no added effect on efficiency but would be detrimental to the process, as if $K_B < K_A$, the process will be dominated by kinetics and this will promote floc break up.

Sensitivity study 2: Floc formation in a rapid mixing unit

Figure 3.4 shows the relationship between primary particles forming suspended solid particles (flocs) and how the system would react to changes. The two case studies implemented here are: (1) an initial 10% increase in the primary particle concentration (in reality, this could be due to an increase in flowrate from an additional water source) and (2) a 20% decrease in the impeller speed or velocity gradient (which could occur when there is a need to promote aggregation in the system).

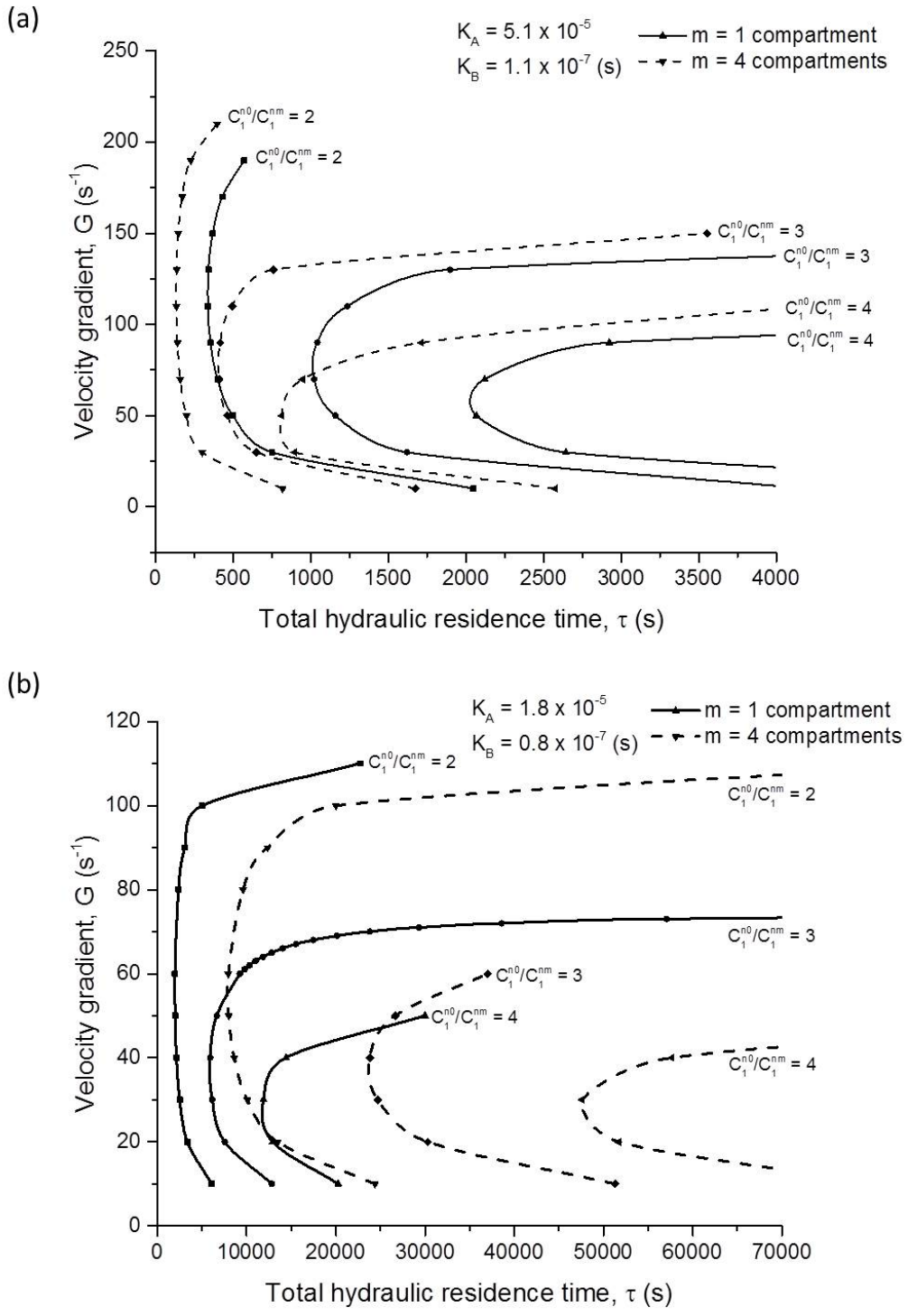


Figure 3.3: Sensitivity analysis: Relationship between the velocity gradient, G, and the total hydraulic retention (residence) time, τ, for two different case studies (flocculation chamber with one and four compartments, respectively) for two different values of collision constant, K_A and break-up constant, K_B.
a) Collision constant $K_A = 5.1 \times 10^{-5}$ and break-up constant $K_B = 1.1 \times 10^{-7}$
b) Smaller collision constant $K_A = 1.8 \times 10^{-5}$ and break-up constant $K_B = 0.8 \times 10^{-7}$.

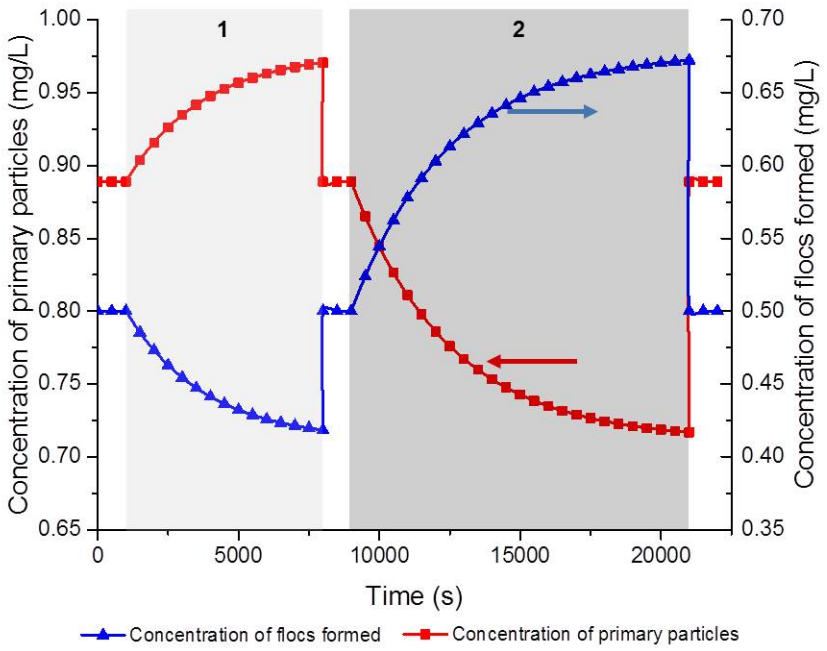


Figure 3.4: Sensitivity analysis: Relationship between primary particles forming suspended particles (flocs) in a rapid mixing unit and how the system would react to specific changes. Two disturbances are implemented (black dotted line): 1) 10% increase in the primary particle concentration, and 2) 20% decrease in the impeller speed or velocity gradient.

From Figure 3.4, it can be seen that following the first disturbance, with an increase of primary particles to 0.97 mg/L, the system responds by finding a new suspended solids steady state at a lower concentration (0.43 mg/L). This is because collision and break up parameters, K_A and K_B respectively, have not changed as they are considered to be in equilibrium and the unit is now operating under its initial removal efficiency. The system is then restored to its original steady state, before another disturbance of 20% decrease in the velocity gradient is introduced.

Figure 3.4 shows a steep increase in the formation and concentration of flocs (suspended solids) with the step decrease in velocity gradient. This is expected as slow mixing promotes the aggregation of particles. As discussed in the previous sensitivity analysis, a higher number of suspended solids would be formed from the collision of primary particles with a low velocity gradient and small break up constant, which is in good agreement with the literature (Argaman, 1971; Rietveld et al., 2009) and shows the model is responding to system changes appropriately.

3.2.4 Concluding remarks

The primary objective of the current study was to investigate the formation of flocs from primary particles and the relationship between the break up of flocs back into primary particles. Numerous flocculation models have been developed in the literature originating from Smoluchowski's equation.

The mathematical model derived in Section 3.2.2 was used to simulate the Argaman - Kaufman flocculation model; although data available for model validation is limited, it can be said that the findings revealed that the model was in good agreement with the existing data; however, relies heavily on an empirical relationship to estimate the parameters needed. When comparing the simulated result with the data provided in literature, it is clear that the trends are similar. In order to accurately predict the performance of a full-scale water treatment plant, an experimental study should be carried out to determine the actual values of the collision and break up constant K_A and K_B to reflect the same suspension and chemical expected in the treatment process.

3.3 Modelling of clarification process

In this section, a mathematical model based on sedimentation clarification is proposed to represent the clean water clarification process. In addition, there is a discussion as to why dissolved air flotation will not be modelled in this work. The mathematical model proposes to simulate floc (suspended solids) concentration and height of sludge blanket within the sedimentation tank in time and space.

Dissolved air flotation

Dissolved air flotation is a commonly used clarification process; most models created to represent the phenomena are developed through Computational Fluid Dynamic (CFD) modelling, as obtaining an accurate predictive one-dimensional model of the process unit is quite complex due to the presence of a large number of empirical parameters such as particle-bubble attachment efficiency, air-to-solids volume ratio, bubble volume concentration etc. One-dimensional models that currently exist in the literature are able to successfully show the bubble-filter efficiency in the contact zone and the removal efficiency in the separation zone both as products of residence time with empirical

parameter inputs (more details can be found in the work of Bloom and Heindel (2003)). The empirical parameters rely heavily on experimental data for predictions meaning the models developed work on a case-by-case basis. As the aim of this work is to produce predictive mathematical models, currently detailed modelling of dissolved air flotation would be out of the scope.

3.3.1 Unit principle

The clarification unit is important as it ensures the filters can be operated more easily and cost-effectively to produce quality water. Sedimentation is a solid-liquid separation process in which particles settle under the force of gravity and the clear water rises to the top of the tank to be removed with the effluent flow. This process has been widely used in water treatment to remove flocs, inorganic and turbidity-causing particles.

3.3.2 Model development

The model developed represents the increase in suspended solids concentration within the clarification unit. For simplicity purposes, the two main variables being considered are the time and the convective settling function.

Model development of sedimentation clarification unit

As mentioned in Chapter 2, the mathematical modelling of conventional clean water treatment units can also benefit from various models developed to simulate wastewater treatment process units as the wastewater industry is more advanced in mathematical modelling of their processes. Due to the similarities in the phenomena occurring in a secondary settling tank (SST) utilised in the activated sludge process[2], this will be used to describe the sedimentation clarification unit in clean water treatment. This section will present a one-dimensional model to predict effluent solids concentration in addition to the sludge blanket height in the secondary settling tank (SST).

Figure 3.5 shows the schematic impression of an ideal SST. Generally, this unit can be divided into three distinct zones according to their key functions: *Clarification*

[2]Activated sludge process is utilised in the wastewater treatment that has a post treatment clarification unit.

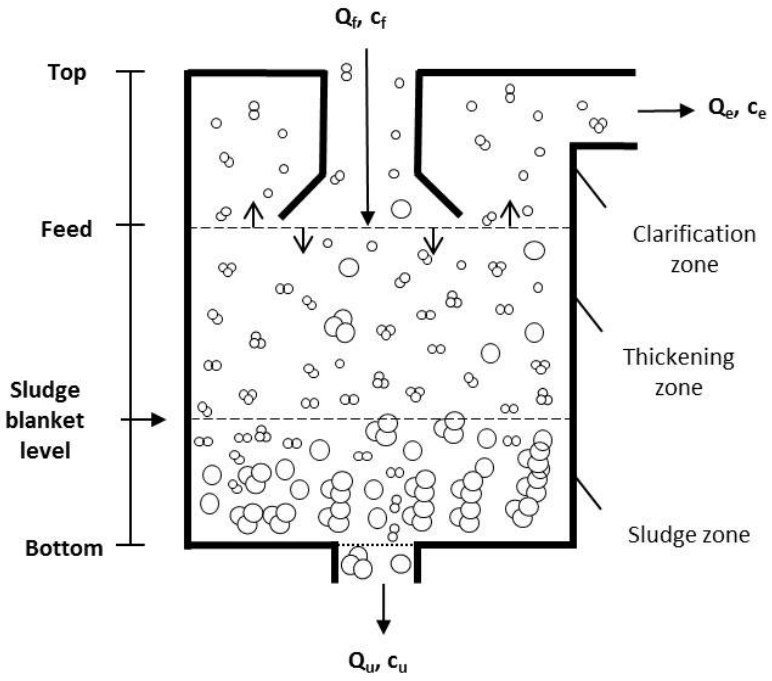


Figure 3.5: Schematic impression of an ideal secondary settling tank (SST) unit.

zone, Thickening zone, and *Sludge zone*, where the feed inlet layer is assumed to lay between these the clarification and thickening zones. The clarification zone is where the influent flow is clarified to produce a low amount of suspended solids concentration in the effluent. The thickening and sludge zone is where the suspended solids are concentrated for removal. From the feed inlet layer, the hydraulic flow divides to an upwards flow (Q_e) towards the effluent weir and the downwards flow (Q_u) towards the SST bottom.

The conservation of mass and continuity equation can be used to express the SST in the form of a partial differential equation (Jeppsson and Diehl, 1996; Burger and Concha, 1998; Burger et al., 2011):

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial z} F\left(c,\, z,\, t\right) = \frac{\partial}{\partial z}\left(d_{disp}(z)\right) + \frac{Q_f(t) c_f(t)}{A} \delta(z) \tag{3.3.1}$$

where

c	concentration (mg/L)
F	(convective) flux function (mg/m^{2}s)
d_{disp}	dispersion function (m^2/s)
Q	volumetric flow rate (L/s)
A	cross-sectional area of SST (m^2)
z	depth (m)
f	subscript for inlet feed

The first term on the left hand side is the change of concentration with time. The second term on the left-hand side models hindered settling[3] combined with bulk flows that separate due to feed, underflow and overflow operations. The third term models dispersion, and the final term is a singular source term which models the feed mechanism. The model presented here is a convection-dispersion model where the effects of compression are not incorporated into the model as it is an added complexity which provides little reward once the surrogate models are developed (Burger et al., 2012). There are a variety of other assumptions made in the model development:

1. The particles concentration is uniform in the horizontal direction. It is therefore a one-dimensional model (in the vertical z-direction).

2. The liquid and solid phases are incompressible, meaning there is no mass transfer between them as the water is being clarified by removal of fully formed suspended solid particles.

3. The particles are of similar sizes and shapes. This assumption is to simplify the model as there is much discussion on the actual fractal shape of suspended solid particles (Jarvis et al., 2005).

4. The velocity of sedimentation depends only on the local particle concentration (this is a restrictive assumption as it does not account for the population of suspended solid particles).

5. The velocity tends to zero as suspended solids concentration, c, tends to a maximum value c_{max} as the solids have reached the top of the sludge blanket indicating the end of settling.

[3]Within hindered settling, the mass of particles will settle as a unit with individual particles remaining in fixed positions with respect to each other. Zones of different concentrations may develop from segregation of particles with different settling velocities.

With the unit area being constant, and taking into account the the two volumetric upward and downward flows and hindered settling velocity within the SST:

$$F(c,\, z,\, t) = \begin{cases} & -Q_e(z)c/A \; for \; z < Top \\ f_{bk}(c) & -Q_e(z)c/A \; for \; Top < z < 0 \\ f_{bk}(c) & -Q_e(z)c/A + Q_u(z)c/A \; for \; z = 0 \\ f_{bk}(c) & +Q_u(z)c/A \; for \; 0 < z < Bottom \\ & +Q_u(z)c/A \; for \; z > Bottom \end{cases} \tag{3.3.2}$$

where the convective flux function involves the Kynch batch density function (Kynch, 1952), f_{bk}:

$$f_{bk} = c.v_{hs} \tag{3.3.3}$$

The hindered settling velocity $v_{hs}(c)$ is a function of concentration only (Kynch, 1952):

$$v_{hs}(c) = v_0 e^{-rc} \tag{3.3.4}$$

$$f_{bk}(c) = v_0 c e^{-rc} \tag{3.3.5}$$

where

Top	height of clarification zone (m)
Bottom	depth of thickening zone (m)
f_{bk}	Kynch batch flux density function (mg/(m^{2}s))
v_{hs}	hindered settling velocity (m/s)
v_0	settling velocity of a single particle in unbounded fluid (m/s)
r	parameter in equation 3.3.5 (L/mg)

The dispersion function, d_{disp}, is often set as a product of the fluid velocity and a continuous function (Burger et al., 2011):

$$d_{disp}(z) = \begin{cases} \alpha_1 Q_f \cdot exp\left(\frac{-z^2/\left(\alpha_2 Q_f\right)^2}{1-|z|/\left(\alpha_2 Q_f\right)}\right) & for \; |z| < \alpha_2 Q_f \\ 0 & for \; |z| \geq \alpha_2 Q_f \end{cases} \tag{3.3.6}$$

where the parameters α_1 and α_2 are greater than zero. One of the idealising assumptions is that the suspended solids/water mixture follows the bulk flows in the outlet pipes.

Table 3.3: Parameters to be implemented into gPROMS for the clarification unit (Burger et al., 2012).

Description	Parameter	Value
Height of clarification zone (m)	Top	-1
Depth of thickening zone (m)	Bottom	3
Cross-sectional area (m^2)	A	400
Maximum concentration (mg/L)	c_{max}	20×10^3
Settling velocity of a single particle in unbounded fluid (m/s)	v_0	3.47
Parameter in equation for fbk (L/mg)	r	0.37×10^{-3}
Parameter in dispersion coefficient (m^{-1})	α_1	2.3×10^{-3}
Parameter in dispersion coefficient (h/m^2)	α_2	2.5×10^{-3}
Concentration at feed inlet (mg/L)	$cmhn_f$	4.5×10^3
Feed volumetric flowrate (L/h)	Q_f	230×10^3
Underflow volumetric flowrate (L/h)	Q_u	100×10^3

This means that as the suspended solids/water mixture leaves the SST, it cannot return (Burger et al., 2011); thus suggesting:

$$d_{disp}(z) \begin{cases} = 0 & for\ z \leq Top\ and\ z \geq Bottom \\ \geq 0 & for\ Top < z < Bottom \end{cases} \tag{3.3.7}$$

3.3.3 Model simulation and validation

In this section, the clarification model derived above will be simulated in gPROMS. Various assumptions were made in the development of this model. The simulation results produced from this model are evaluated in the following section. First, the models will be validated against literature and then the limitations of the models will be tested through a sensitivity analysis.

Model parameters

Burger et al. (2012) tested their convection-dispersion-compression model with parameters that will currently be used for model validation. Table 3.3 shows the values of the model parameters for the simulation.

Model validation and sensitivity analysis

In solving the equations, as a function of time and height solution discontinuities are expected to occur. This can be interpreted physically as the sediment interface or sludge blanket height that can also be observed in experiments (Li and Stenstrom, 2014). The use of the Godunov approach was initially proposed by Jeppsson and Diehl (1996); in this approach, the concentration related to each grid point at a given time point is calculated as the average of an analytical solution that originates from piecewise constant initial data at the preceding time point. The details of how this is implemented to simulate this model can be found in Appendix C.

The literature case study simulated to validate the model in this work can be in found Figures 3.6a and 3.6b. The simulation begins at steady state for the first 5 hours and then a step increase is imposed on the feed volumetric flowrate changing the value to 360×10^3 L/hr, the feed concentration is decreased by 10% and the underflow volumetric flowrate is kept constant. This change is kept for 15 hours after which all variables are returned to steady state. Burger et al. (2012) incorporates compression into their model which has an affect on the second step change imposed on the system. In Figures 3.6a and 3.6b, there is a gradual decreases in concentration to steady state between t = 20 hrs to t = 48 hrs. This is, however, not observed in Figure 3.6c as the model in Figures 3.6a and 3.6b incorporates compression conditions into the system.

Between t = 0 hr to t = 20 hrs, Figure 3.6c shows a trend to represent the formation of a sludge blanket; this is formed approximately one metre from the bottom of the tank and there is an increase in solids concentration the closer to the bottom of the tank as the suspended solids start to settle there. However, with the omission of the sediment compression function, the dynamic simulation results for the gPROMS clarifier model presented here and from Burger et al. (2012) are in good agreement, as the model is still able to represent the phenomena occurring in the sedimentation clarification unit.

To test the limitations of the model, a sensitivity analysis is conducted to check the robustness of the model with regards to the number of discretised points. As the sludge blanket is formed with discontinuous behaviour, this would mean that the discretisation model and detail will have an affect on the overall representation of the model.

Sensitivity study: Effect of layer number on the system

The simulations are performed for three different cases with 10, 20 and 30 grid points/layers using the same parameters presented in Table 3.3. Figure 3.7 shows that the predictions

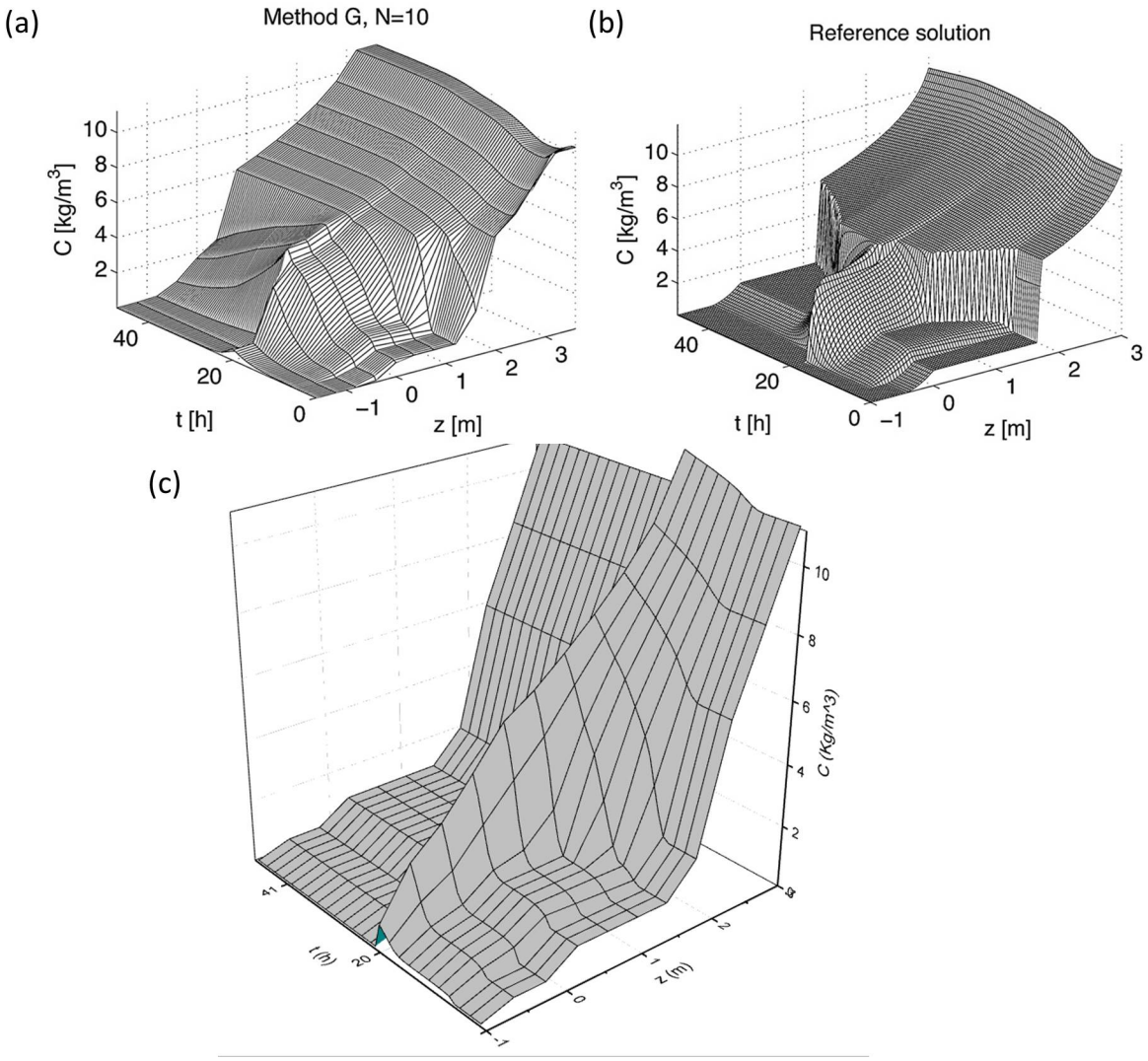


Figure 3.6: A dynamic simulation of the convection-diffusion clarifier model starting at steady state with the parameters found in Table 3.3.
a) literature simulation with 10 discretised points (Burger et al., 2012).
b) literature reference simulation, both are reproduced from literature with permission (Burger et al., 2012).
c) simulation using the model shown in Equation 3.3.1 with 10 discretised points.

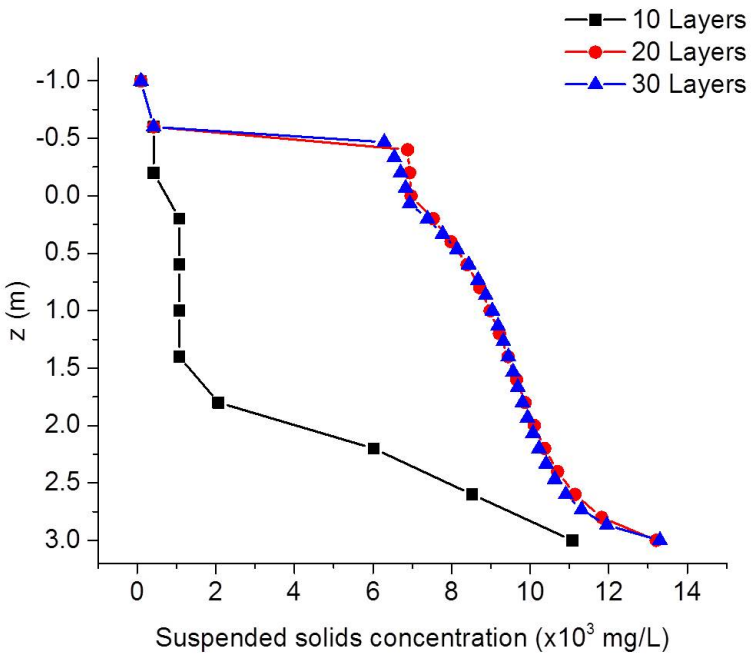


Figure 3.7: A steady state simulation of the sedimentation clarification unit using the parameters in Table 3.3. The concentration profile of different discretisation levels: 10, 20 and 30 are shown.

diverge with differences in the sludge blanket level and the underflow concentration. Except for the case of 10 layers, the difference between the concentrations calculated with the other layers is not too large. This shows that 10 layers is clearly not enough to accurately predict the suspended solids concentration as it underpredicts the concentration within the thickening zone.

3.3.4 Concluding remarks

The primary objective of modelling a one-dimensional sedimentation clarification unit was to investigate the suspended solid settling characteristics, such as suspended solids concentration and height of sludge blanket formed at the bottom of the unit. Most of the focus in this section has been placed on a sedimentation clarification unit as the development of a predictive model can be obtained. Dissolved air flotation is another commonly used clarification unit; however, obtaining an accurate predictive one dimensional model of the process unit is quite complex due to the presence of a large number of empirical parameters. Developing a detailed model of dissolved air flotation is out of the scope for this work.

The mathematical model developed in Section 3.3.2 was used to simulate suspended solids concentration within the clarification unit. The limitations and sensitivity of the model were tested to see what could be improved. The comparison in Figure 3.6 demonstrates a reasonable agreement between literature results and the simulated gPROMS clarification model developed in this work. It can be concluded from this preliminary study that this model is capable of predicting the sludge blanket height and settling time to an acceptable degree but further work, such as around the compression function, would be needed to make it more robust.

3.4 Modelling of filtration

In this section, a model is being proposed to simulate a two-stage hypothesis of the phenomena occurring within the rapid gravity filtration process. This model considers the attachment and detachment of suspended particle deposits onto a porous medium.

3.4.1 Unit principle

The purpose of filtration is the removal of solid particles from the water by passing the solid/water mixture through a porous medium or other suitable material to capture the solid particles whilst allowing the water to pass through, thus achieving the required quality of filtered water. This unit is usually the third physical unit in the clean water treatment process and is often the last line of defense to removal floc and colloidal particles from entering the water distribution by their retention in the porous medium. A porous medium is a solid matrix containing voids which interconnect to enable the fluid flow through the medium at a low speed. The media thereby retains most of the solid matter within the pore structure.

3.4.2 Model development

As explained in Chapter 2, mathematical modelling of filtration can be divided into two sub-categories: macroscopic (deals with the cumulative collection of deposits) and microscopic (considers the size of the individual particle as well as the number of particles).

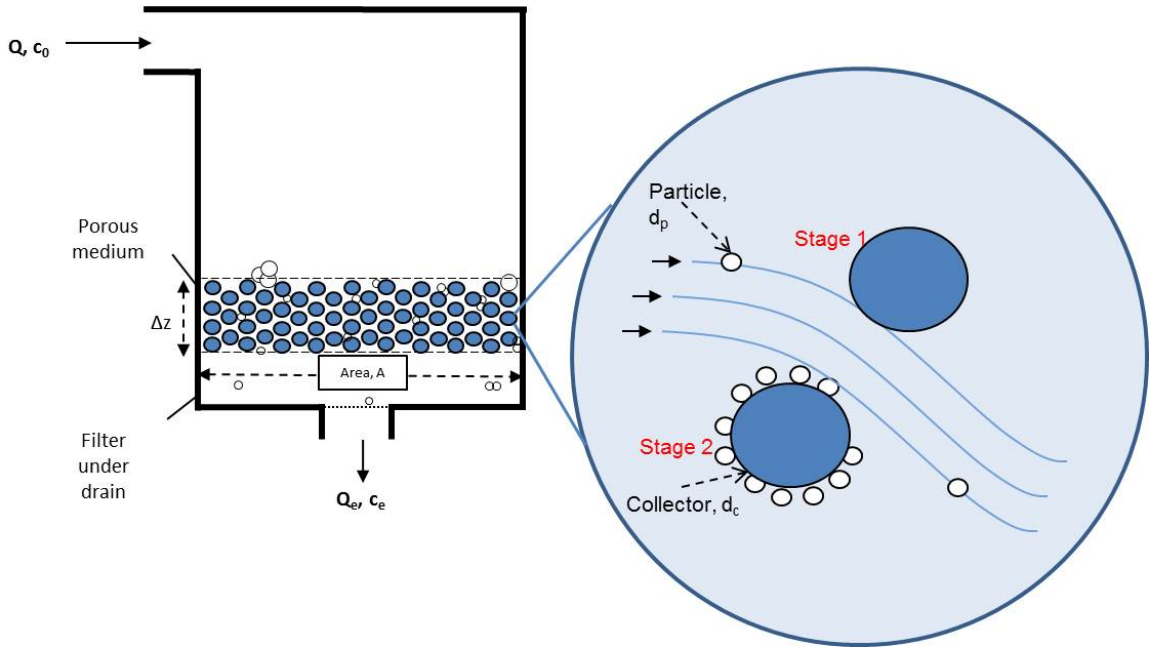


Figure 3.8: Schematic of rapid gravity filtration unit.

Macroscopic modelling

The macroscopic conservation equation can be derived by observing the phenomena affecting the water flow and deposition of suspended solids passing through a down-flow or up-flow granular depth filter with initial porosity, ε_0, under constant flow rate or pressure drop conditions. Consider a porous medium element of depth, Δz, and area, A (as shown in Figure 3.8), which contains:

- a volume $A\sigma\Delta z$ of retained particles
- a volume $A\varepsilon c\Delta z$ of moving particles entrained by the liquid
- a deposit of real volume $A\beta\sigma\Delta z$ imprisoned by the retained particles

where

σ	specific deposit expressed in terms of the ratio of the volume of deposited material over the differential volume under consideration (mg/L)
c	concentration of suspended solid particles within the zone (mg/L)
ε	porosity of clogged bed/filter medium (ε=ε_0 - $\beta\sigma$) (-)
z	distance (depth) measured from the inlet of the filter (m)
β	inverse of compactness (actual volume of deposit/compacted volume of deposit) (-)

Following the model created by Han et al. (2008), a two-stage hypothesis is a developed to represent the entire rapid gravity filtration process (as shown in Figure 3.8):

Stage 1: Suspended solid particles begin depositing outside of the filter grains. The particles that deposited previously start to serve as additional collector sites to enhance further attachment of suspended particles. During this time period, detachment of deposited particles does not occur until the specific deposit reaches a critical specific deposit, σ_c. This assumption is consistent with experiments carried out by Ison and Ives (1969). The authors demonstrate over several hours of filtration, the experiments show that clay deposits accumulated onto the grain, and were then partially detached by arrival of further suspended particles. Thus, proving that detachment of particles during filtration is an occurring phenomenon when substantial amounts of deposit are present.

Stage 2: During this stage detachment starts to occur. This is due mainly an increase of the hydraulic shear forces with an increased interstitial velocity within the free space of the filter media. At the second stage, both deposition and detachment occurs.

The general material balance of particles can be written as:

$$accumulation\,rate\; = (flow\,in)\; -\; (flow\,out)$$

or

$$\frac{\partial\left[A\left(\sigma+\varepsilon c\right)\right]}{\partial t}+\frac{\partial\left(Auc-AD_z\frac{\partial c}{\partial z}\right)}{\partial z}=0 \tag{3.4.1}$$

where

Aσ	volume of particles retained in a unit depth filter (m^2.mg/L)
Aεc	volume of particles in motion entrained by liquid in a unit depth filter (m^2.mg/L)
Auc	particle flow entrained by the fluid (mg/s)
D_z	dispersion coefficient in water (m^2/s)
-AD_z (∂c/∂z)	diffusional flux of particles (m^4/s)
ε_0	clean bed porosity (-)

The assumptions used when deriving the model are:

- Axial dispersion is assumed negligible which is true for small particle sizes.
- Filtration takes place throughout the entire filter and no macroscopic transverse mass or flow variations take place within the zone under consideration.

- The velocity of suspension is constant throughout the filter.

Under these assumptions, the material balance of particles in a differential volume of the filter is written as:

$$\left(\frac{\partial\left(\sigma+\varepsilon c\right)}{\partial t}\right)_z + v_s\left(\frac{\partial c}{\partial z}\right)_t = 0 \tag{3.4.2}$$

where v_s is the filtration velocity and ε is the porosity of the filter media. The porosity of the filter, ε, varies with time and with the specific deposit due to particle deposition on grain surfaces, altering the morphology of the void space of the porous medium (Skouras et al., 2011). This variation can be expressed as:

$$\varepsilon = \varepsilon_0 - \frac{\sigma}{1-\varepsilon_d} \tag{3.4.3}$$

where ε_d is the porosity of the deposits. At early stages of filtration, the porosity is nearly constant, and Equations 3.4.2 and 3.4.3 can be rewritten as:

$$v_s\frac{\partial c}{\partial z} + \varepsilon_0\frac{\partial c}{\partial t} + \frac{\partial \sigma}{\partial t} = 0 \tag{3.4.4}$$

For a homogeneous filter, ε_0 is constant, and τ_f can be estimated from the expression (Skouras et al., 2011):

$$\tau_f = t - \varepsilon_0\frac{z}{u} \tag{3.4.5}$$

where τ_f is the time elapsed before a given amount of the suspended solids reaches the depth z. The difference between t and τ_f is usually negligible (Han et al., 2008). Then, Equation 3.4.4 can be written as:

$$u\frac{\partial c}{\partial z} + \frac{\partial \sigma}{\partial t} = 0 \tag{3.4.6}$$

The rate of particle deposition can be written in terms of the specific deposit, σ, or the particle concentration, c. The basic granular filtration equation proposed in 1937 by Iwaki, which was later experimentally verified by Ison and Ives (1969), is as follows:

$$-\frac{\partial c}{\partial z} = \lambda c \tag{3.4.7}$$

where λ is the filter coefficient. Combining Equation 3.4.7 and Equation 3.4.6 gives:

$$\frac{\partial \sigma}{\partial t} = \lambda u c \tag{3.4.8}$$

The governing parameters of the macroscopic model, the filter coefficient, λ, and the specific deposit, σ, are implicit functions of the physical and chemical characteristics such as attachment and transport efficiency between particles and to the filter, of the suspended solids and filter medium, as well as of filtration velocity, u. The parameters vary with time and filter depth during the filtration process. In order to predict the concentration profile, the value of the filter coefficient λ must first be estimated by Equation 3.4.11 utilising microscopic modelling, which can be found later in this section.

Two stage hypothesis

The two stage hypothesis which is applied to rapid gravity filtration focuses in the microscopic approach. Within *Stage 1*, suspended solids begin depositing onto the filter grains. During this stage, the detachment of deposited suspended solids doesn't occur as the filter grain is not over saturated; therefore, the attraction is still there.

Deposition rates for stage 1

Assuming that filter grains are perfect spheres of diameter, d_c, the number of collectors, N_c, in the differential volume with a height, ∂z, and a cross-sectional area, A, can be calculated (Tien, 1989):

$$N_c = \frac{6\left(1-\varepsilon_0\right) A \partial z}{\pi d_c^3} \tag{3.4.9}$$

By definition the single collector removal efficiency η as the ratio of particle deposition rate on the collector to the rate of particle flow towards the collector (Crittenden et al., 2012):

$$\frac{3}{2}\eta\left(1-\varepsilon_0\right)\frac{u}{d_c} c A \partial z = -\left(uA\right)\partial c \tag{3.4.10}$$

Combining Equations 3.4.7 and 3.4.10 gives:

$$\lambda = \frac{3}{2}\frac{\left(1-\varepsilon_0\right)\eta}{d_c} \tag{3.4.11}$$

O'Melia and Ali (1978) suggested during the ripening stage, the actual collector consists of a filter grain and an associated number of particles deposited on it that also serve as collectors, and the removal efficiency of the single collector was calculated by (Han et al., 2008):

$$\eta = \alpha\eta_0 + N\alpha_p\eta_p\left(\frac{d_p}{d_c}\right)^2 \tag{3.4.12}$$

and

$$N = \alpha\eta_0\beta\left(\frac{3}{2\,x\,(1000\,\times\,\rho_p)}\frac{d_c^2}{d_p^3}\right)u\int_0^t c\partial t \tag{3.4.13}$$

where

η	single collector removal efficiency (-)
η_0	single collector contact efficiency in the clean filter bed (-)
η_p	single deposited particle contact efficiency (-)
α	particle/filter grain attachment coefficients (-)
α_p	particle/particle attachment coefficients (-)
β	factor of particles deposited directly onto the filter grain which can act as additional collectors (-)
ρ_p	suspended solid density (mg/L)
d_c	collector diameter (m)
d_p	particle diameter (m)
N	number of deposited particles per filter grain which acts as additional collectors (-)

Obtaining particle/filter grain transport efficiency in the clean filter

The particle/filter grain transport efficiency in the clean filter, η_0, can be calculated from a correlation developed by Rajagopalan and Tien (1976):

$$\eta_0 = 4A_s^{1/3}Pe^{-2/3} + A_sN_{LO}^{1/8}N_R^{15/8} + 3.38\,x\,10^{-3}A_sN_G^{1.2}N_R^{-0.4} \tag{3.4.14}$$

where

$$A_s = \frac{1\,(1-p^5)}{w} \tag{3.4.15}$$

$$w = 2 - 3p + 3p^5 - 2p^6 \tag{3.4.16}$$

$$p = (1-\varepsilon)^{1/3} \tag{3.4.17}$$

The deposition rate at the first stage of the filtration can be obtained by combining Equations 3.4.7, 3.4.6, 3.4.11, 3.4.12 and 3.4.13.

$$\frac{\partial \sigma}{\partial t} = \frac{3}{2}\frac{(1-\varepsilon)}{d_c}\alpha\eta_0 \left[1 + \alpha_p\eta_p\beta\left(\frac{3}{2\,x\,(1000\,x\,\rho_p)}\frac{d_c^2}{d_p^3}\right) u\int_0^t c\partial t\right] uc\;\sigma \leq \sigma_c \qquad (3.4.18)$$

Deposition rates for stage 2

When the specific deposit is greater than the critical value, σ_c, the detachment of deposited particles from filter grains is assumed to occur in the filtration process and the second stage begins. At the second stage, both deposition and detachment are assumed to occur simultaneously. This is due mainly an increase of the hydraulic shear forces with an increased interstitial velocity within the free space of the filter media. The deposition rate at the second stage of filtration can be described by the following equation, which assumes the detachment rate is proportional to the relative specific deposit (σ - σ_c) rather than the absolute specific deposit σ. A few researchers have assumed this to describe the detachment rate (Adin and Rebhun, 1974; Harvey and Garabedian, 1991; Han et al., 2008):

$$\frac{\partial \sigma}{\partial t} = \frac{3}{2}\frac{(1-\varepsilon)}{d_c}\left[\alpha\eta_0 + \alpha_p\eta_p\beta\left(\frac{d_p}{d_c}\right)^2 N\right] uc - \varpi J\,(\sigma - \sigma_c)\;\; \sigma > \sigma_c \qquad (3.4.19)$$

where

$$N = \alpha\eta_0\beta\left(\frac{3}{2\,x\,(1000\,x\,\rho_p)}\frac{d_c^2}{d_p^3}\right)\int_0^{t_c} uc\partial t + \int_{t_c}^{t}\frac{1}{1000\,x\,\rho_p\,(1-\varepsilon_0)}\left(\frac{d_c}{d_p}\right)^3\frac{\partial\sigma}{\partial t}\partial t \qquad (3.4.20)$$

N is an associated number of deposited particles which are served as additional collectors for a single filter grain and J is the hydraulic gradient. The first term and the second term on the right side of Equation 3.4.19 describe the number of deposited particles at the first and second stages, respectively. Han et al. (2008) states that experimental data has suggested that the detachment coefficient, ϖ, is described as a function of filtration flow rate using the following equation:

$$\varpi = \varpi_0 u^{1.75} \qquad (3.4.21)$$

ϖ_0 is a constant for a specific filtration system and would be determined experimentally for industrial applications.

Headloss through the filter column

Headloss in a filter bed is an important factor for the filter bed conditions, and can be used as an indicator to start filter washing. Assuming a constant filtration flow rate u, the deposition of suspended solids σ, on the surface of a filter media causes clogging. This results in a reduction in permeability. O'Melia and Ali (1978) suggested that permeability is inversely proportional to the square of the inter-facial surface area in the filter (Han et al., 2008). The hydraulic gradient within a clogged filter can be expressed as:

$$J = J_0 \left(1 + \frac{\gamma}{\rho_p}\sigma\right)^2 \tag{3.4.22}$$

where γ is an empirical parameter which is relates the flow rate, clean filter bed porosity, filter grain size, and the particle surface area-to-volume ratio. From experimental data in the literature (Yao et al., 1971), γ was proposed to be expressed as:

$$\gamma = \gamma_0 u^{-0.55} \tag{3.4.23}$$

where γ_0 is a constant for specific filtration system. Combining Equation 3.4.22 and Equation 3.4.23 gives:

$$J = J_0 \left(1 + \frac{\gamma_0}{\rho_p}u^{-0.55}\sigma\right)^2 \tag{3.4.24}$$

Therefore, the headloss through the filter can be calculated by:

$$h = J_0 \int_0^L \left(1 + \frac{\gamma_0}{\rho_p}u^{-0.55}\sigma\right)^2 \partial z \tag{3.4.25}$$

The hydraulic gradient in the clean filter bed J_0 can be experimentally obtained or calculated by the Carmen-Kozany equation.

$$J_0 = \frac{h_0}{L} \tag{3.4.26}$$

Initial and Boundary Conditions

For filtration with a clean filter, the initial conditions states that the concentration along the space in the column, c(z) is equal to the inlet concentration c_{in} and the specific deposit, σ, onto the media is 0. The boundary condition states that for the filtration time, the concentration at the inlet height, c(z = 0) is equal to the initial concentration,c_{in}:

$$c = c_{in},\ \sigma = 0 \quad for \quad z \geq 0,\ t = 0$$
$$c = c_{in} \quad for \quad z = 0,\ t > 0 \tag{3.4.27}$$

3.4.3 Model simulation and validation

In this section, a model has been proposed to simulate suspended solids concentration and specific deposit profiles within the filter in time and space. Various assumptions were made in the development of this model. The simulation results produced from this model are evaluated in the following section. First, the model will be validated by comparing with the literature sources and then the limitations of the model will be tested.

Model Parameters

The model requires model parameters α, α_p, η_p, β, ϖ_0, σ_c and γ_0 to be determined. However, since α_p, η_p, and β appear as a group in the model, they can be treated as a single parameter (Han et al., 2008). Han et al. (2008) state thatα values can be calculated from the experimental data for clean or initial filter bed particle removal and that the value of α_p, η_p, and β is estimated by best fitting experimental data with the calculated values of particle removal efficiency at the ripening stage in the proposed model. The values of ϖ_0 and σ_c can be estimated by particle removal in the breakthrough stage. Headloss coefficient γ_0 is determined by best fitting experimental results with the simulated headloss profile in the proposed filtration model. Table 3.4 show the values of the model parameters for the simulation (Han et al., 2008).

Model validation and sensitivity analysis

The filtration model is simulated to determine concentration and specific deposit profiles of suspended solids within the filter column, with a duration of 24 hrs. The case study will aid the understanding of what occurs within the filter column during filtration. In the simulation, the filter column with a depth of 0.9 m has 100 discretised layers using the backward finite element method. Han et al. (2008) state values of model parameters

Table 3.4: Parameters to be implemented in gPROMS for the rapid gravity filtration unit (Han et al., 2008).

Description	**Parameters**	**Value**
Filter bed depth (m)	L	0.9
In-fluent particle concentration ($^{mg}/_{L}$)	c_{in}	6
Superficial velocity ($^{m}/_{h}$)	u	5
Clean grain diameter (m)	d_c	0.8 $\times 10^{-3}$
Particle diameter (m)	d_p	4 $\times 10^{-6}$
Porosity (-)	ε_0	0.4
Particle/filter grain attachment efficiency (-)	α	0.9
Single parameter (-)	α_p, η_p, β	0.9
Detachment coefficient constant (-)	ϖ_0	200
Transitional specific deposit ($^{mg}/_{L}$)	σ_c	300
Particle density ($^{mg}/_{L}$)	ρ_p	1350 x 10^3
Constant parameter (-)	γ_0	30
Clean headloss (m)	h_0	0.4

that were intentionally chosen to make breakthrough[4] take place significantly, so that the proposed filtration model can be assessed.

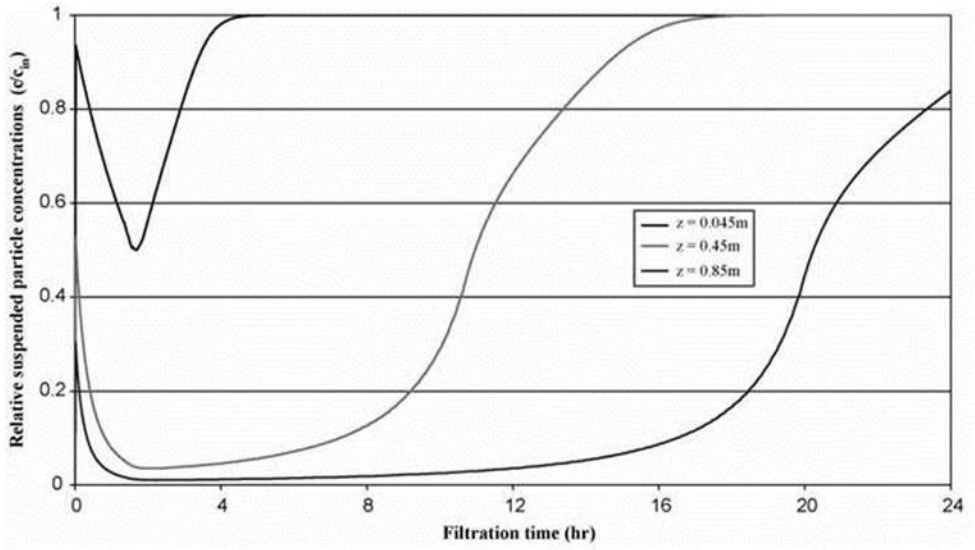
Figure 3.9a (Han et al., 2008) and Figure 3.9b (this work) represent the changes in suspended solids concentration with filtration time at 3 different positions in space (z = 0.045 m, z = 0.45 m and z = 0.85 m). These positions are reflective of the top, middle and bottom of the tank respectively. The figures show the suspended solids concentration in the upper layer (z = 0.045 m) is high during filtration and the breakthrough stage occurs quickly. As we move down the filter column, there is a delay in occurrence of the breakthrough stage and the suspended particle concentrations in the working stage continuously decreases. The model is able to be used to represent the phenomena occurring in the filtration unit due to a comparison between Figure 3.9a and Figure 3.9b which shows they are in good agreement.

To test the limitations of the model, a sensitivity analysis is conducted to:

1. Test the relationship between effluent suspended solids concentration and headloss through the filter column to confirm the importance of headloss and to see if it can be used as an indicator for back-wash within this model. This is informative for purposes as it can aid in the identification of influential parameters by quantifying

[4]Reminder: Breakthrough is the point at which the filter grains are oversaturated with suspended solid deposits; thus the efficiency decreases and suspended solids concentration increases as the suspended solids detach from the grain.

(a)



(b)

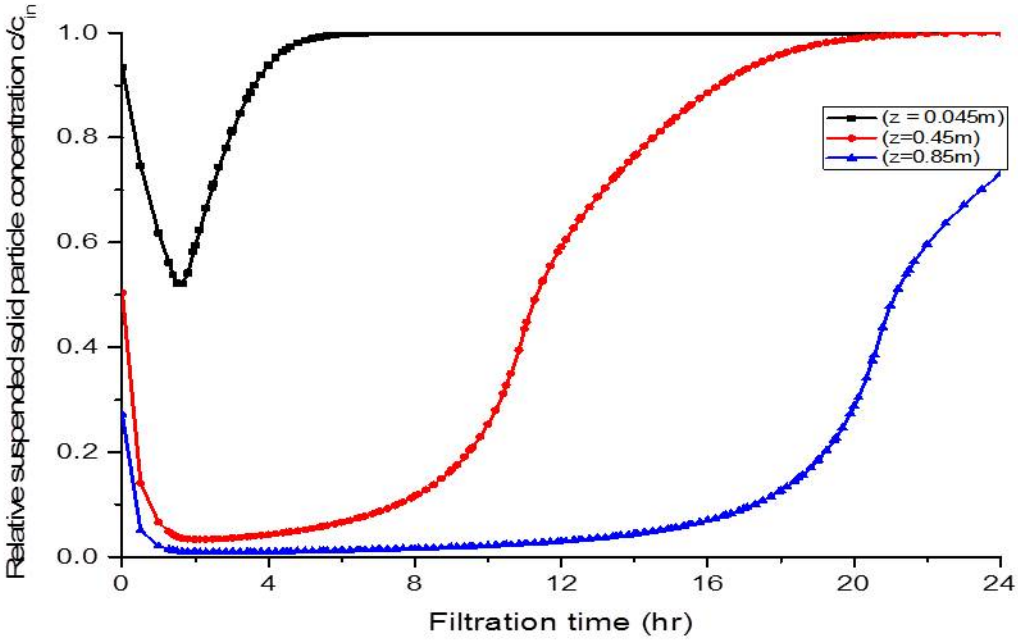


Figure 3.9: The changes in relative suspended particle concentration with filtration time at 3 different positions in space (z = 0.045 m, z = 0.45 m and z = 0.85 m). The filter column has a depth of 0.9m has been simulated with 100 discretised layers.
a) shows the graph reproduced with permissions from literature (Han et al., 2008).
b) show the graph obtained from modelling in gPROMS.

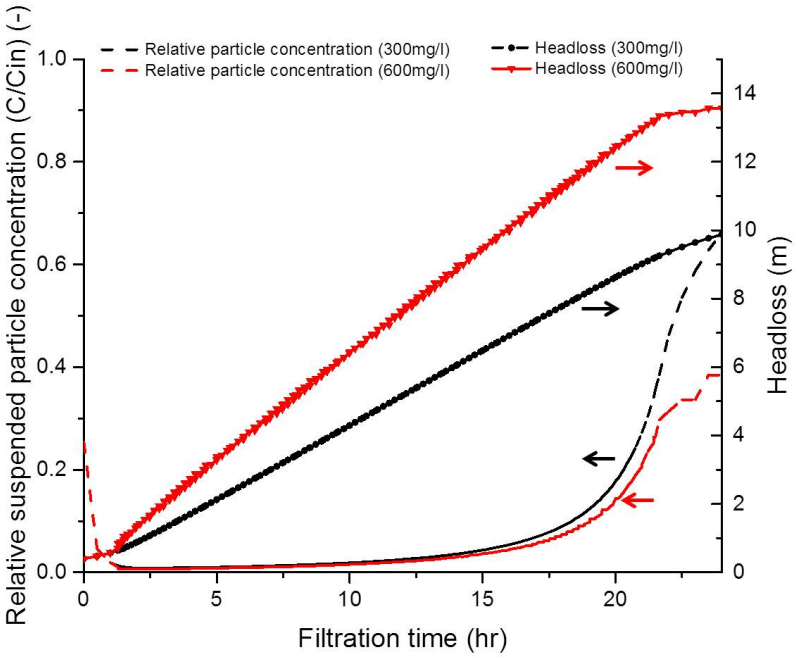


Figure 3.10: Relative effluent suspended solids concentration and headloss through the filter column during the filtration. The values of the transitional specific deposit value σ_c, is changed from 300 $^{mg}/_{L}$ (black) to 600 $^{mg}/_{L}$ (red).

the individual contribution of the uncertain parameters to the model output uncertainty.

2. Test the effect of flowrate on filter separation capability as change in flowrate can occur due to changes propagating from upstream.

Sensitivity study 1: Effluent particle concentration and headloss through the filter column

Figure 3.10 shows the effluent suspended solids concentration profile with filtration time. The values of the critical specific deposit value σ_c, is changed from 300 $^{mg}/_{L}$ to 600 $^{mg}/_{L}$ as this indicates at which point the second stage approach, where detachment occurs simultaneous with attachment, becomes active. The simulated results demonstrate a expected pattern of the effluent suspended solids concentration, which describes the ripening, working and breakthrough stages. The increase in the critical specific deposit value results in an increase in the effluent concentration and an increase in the working stage area. This may be attributed to increasing the unit of the saturated specific deposit, and enables more time for stage one to occur so particle detachment is not

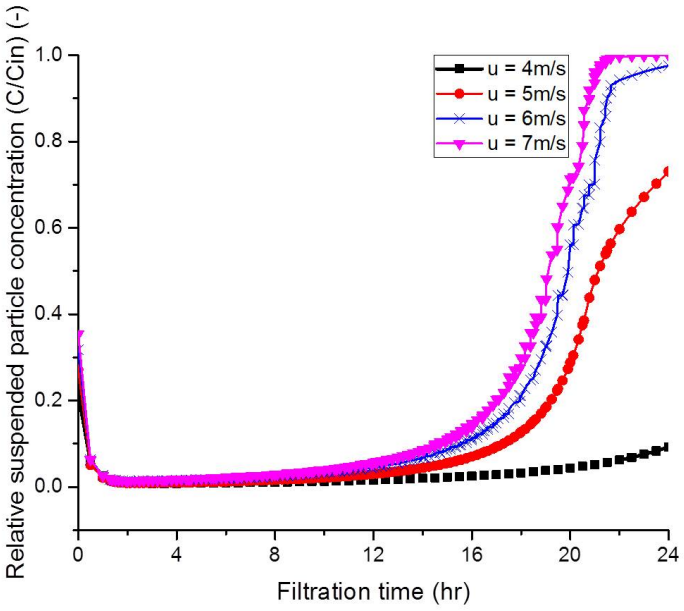


Figure 3.11: The effect of flow rates (4 m/s, 5 m/s, 6 m/s and 7 m/s) on relative effluent suspended solids concentration.

taken into account at this stage. The estimated parameters for this model are important features as varying them has an effect on the results. The figure also shows headloss through the filter increases with filtration time. The headloss of filter media initially increases and then starts to slow down over time, which is due to most of the filter has being saturated. This agreement can also be seen with the corresponding relative suspended solids effluent concentration showing the head loss would also be a good indicator of back-washing time.

Sensitivity study: Effect of flowrate on filter separation capability

Four different flow rates (4 m/s, 5 m/s, 6 m/s and 7 m/s) were chosen to simulate how suspended solids effluent concentrations effect the ability to remove suspended solids from water within the filter. Figure 3.11 shows that the effluent suspended solids concentration significantly increase with increase in flow rate; this may be as a result of the increase in flowrate enhancing the detachment of already deposited particles from the filter grains due to increased velocity, as described in the filtration model. The saturated specific deposit decreases with the increase in flow rate, which agrees with findings in literature.

3.4.4 Concluding remarks

The primary objective of the this study was to investigate the particle removal behaviour of filters under realistic operating conditions and to simulate a model based on literature. Numerous models to predict the removal efficiency in deep bed filtration at initial and transient stages have been examined in the past (Rajagopalan and Tien, 1976). However, research is still being conducted to develop a model that can describe the entire filter cycle to an excellent standard incorporating back-washing. The inclusion of back-wash is out of the scope for this work; however, a detailed discussion is provided in Chapter 6.

The mathematical model derived in Section 3.4.2 was used to simulate a two-stage filtration model developed by Han et al. (2008). An objective of this study was a simulation of a filtration model to test the limitations and to see what can be improved. A comparison demonstrated a reasonable agreement between literature results and the simulated gPROMS filtration model. It can be concluded from this study that this model is capable of predicting particle removal and headloss during rapid gravity filtration to a certain degree but further work, such as incorporating the back-washing system into the model, is needed to make it more robust.

3.5 General discussion of model development

In this chapter, physical processes from clean water treatment works, namely coagulation/flocculation, clarification, and filtration units, are simulated. The detailed models are validated, where possible, with literature data before a sensitivity analysis is conducted. Some are modelled with alternative methods of operation, such as rapid mixing and flocculation in chambers for the coagulation/flocculation process.

Coagulation and flocculation models have been developed in literature originating from Smoluchowski's equation which deals with the surface chemical effects in a simplistic manner. This leads to a poor understanding of the interactions between the chemicals, the coagulant dose and the primary particles, which leaves a scope for future work. The models utilised in this study from the Argaman-Kaufman flocculation model, for both a rapid mixing unit and a series of flocculation occurring in chambers, and the dissolved air flotation model relies on empirical relationships to identify parameters needed.

The model representing the sedimentation clarification unit was able to accurately portray the phenomena predicted to occur within the unit in real life settings. The main limitation with the model is neglecting a compression function which can add another dimension to the model; however adding a compression function to the model increases the computation complexity of the model for little reward, especially with the creation of surrogate models, which will be discussed in a later chapter. This model will be used for scenario analysis (especially the effect of an additional sludge settling unit) and will play an important role in clean water treatment modelling. The inlet to this unit is water from the underflow outlet and enables the collection of water from the sludge, which can be recycled to join the pipeline before entering the coagulation and flocculation unit (simulations of these connected units can be seen in Chapter 4).

The filtration model successfully simulated the three sub-stages occurring in filtration enabling an accurate representation of the phenomena occurring so for further improvement the incorporation of a predictive back-wash model will strengthen the applicability to a complete water treatment plant model.

One shortcoming with the models shown in this chapter is due to the fact they are all modelled individually, "ideal" conditions are often assumed which will have an effect on the predicted concentration, once the units have been combined to make a complete clean water treatment model. Another shortcoming is that due to the nature of the process models, empirical parameters are needed for accurate simulation of a process on a specific site, which requires experiments or historical data to find empirical relationships. However, this means there will be an indication of where to explore experimentally and thus, provides useful information for innovation.

3.6 Conclusion

With drinking water standards becoming more rigorous, mathematical models will become an important tool to assess clean water plant performance (Van Hulle et al., 2006). Simulation is a useful tool and this chapter focuses on the use of numerical simulation for the dynamic modelling of processes. One of the main problems with the existing work on dynamic modelling water treatment processes individually is a lack of understanding as to how these models fit together to develop a complete water treatment plant. The knowledge and understanding of the individual units gained can direct the efforts in the production of robust complete water treatment plant models.

The biggest limitation with this modelling is that some pilot scale experiments will need to be carried out in order to have accurate data for some parameters needed; however, this means that there will be an indication of where to explore experimentally and thus, accelerates the process development in order to help optimise the overall process.

Chapter 4 shows the simulation of a complete clean water treatment work. As the water industry is traditional in its approach and utilises process operators to run the day-to-day operation of the water treatment plants, the use of detailed dynamic mathematical models may introduce an added complexity and therefore, models that can represent similar phenomena occurring in a simpler manner may be utilised more frequently. In Chapter 5, there will be the development of surrogate models from the individual detailed dynamic models presented in this chapter and will be used to show how simpler surrogate models can represent the phenomena occurring in the detailed models.

Chapter 4

Complete model of clean water treatment

To shift the operation of drinking water treatment plants from experience driven to knowledge based, a model-based approach is shown to be effective. This chapter considers an overall mathematical model of a clean water treatment work based on individual processing unit models developed and verified in Chapter 3. The first principles modelling based approach has proven useful for: (1) increasing the understanding of the process by providing a more informative method for exploring how different processing units are affected by sequential events, and (2) enabling the ability for a variety of scenarios to be tested out, which can enhance the process design stage depending on the raw water source available. Several scenarios are presented which illustrate the capabilities of the overall model to predict the propagation of disturbances or changes through out the plant.

4.1 Introduction

The process of purifying water is often conducted in a large water treatment plant where environmental changes can occur and will be detected late in the process. Traditionally, black box models, which are based on historical data, have been used to predict the

response to these changes in the system. The incorporation of white box models, that describe the physical process mathematically, will lead the industry into a more proactive approach. Mathematical models can be utilised to simulate operation of a clean water treatment work to predict the behaviour of the individual treatment processes under changing conditions; thus, giving companies who adopt this approach a competitive edge.

By combining the individual detailed models shown in Chapter 3, a novel use of a mechanistic modelling approach to generate individual models of different types of clean water treatment process units will be demonstrated. The main objective is the development of a complete mathematical model of an entire water treatment plant, which will benefit the industry as simulations can be used as risk mitigation by simulating feedback responses to proposed changes in the work. This enables a wider view on how changes in one processing unit will affect the treatment process as a whole. An additional benefit of complete water treatment model is the ability to run scenario based analysis, which enables the development of an optimal water treatment work. This will also enhance the understanding of the flow and concentration behaviour within the clean water treatment work.

4.2 Unit configurations

Generally, an accurate mathematical model can enable quick and efficient investigation and screening of different design and operating alternatives. The plant considered in this work consists of the main physical processing steps typically available on a conventional water treatment plant; a coagulation/flocculation unit, a clarification unit, a filtration unit and a sludge settling unit. For each of the processing steps, there are several alternative unit operation that can be used in the overall plant. The technology choice and the number of corresponding units of each processing step to place in parallel, affect the overall water output quality.

4.2.1 Integration of units

In Chapter 3, detailed mathematical models for the individual treatment processes were presented. In order to combine these individual models into a model of a complete treatment plant that represents industrial situations, connections between each unit

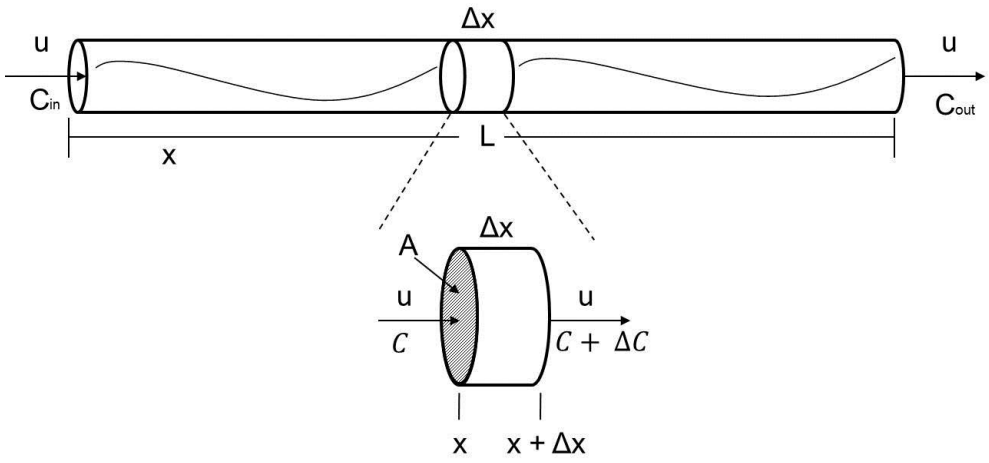


Figure 4.1: Illustration of plug flow reactor model.

are needed. In a conventional water treatment plant, the main processing units are connected by pipes or troughs. In this work, these are described by simple non-reacting plug flow models. The transient material balance for flow in a plug flow unit or pipe, as illustrated in Figure 4.1, can be written as:

$$\underset{(accumulation)}{A_c x \tfrac{\delta c}{\delta t}} = \underset{(in)}{uA_c c \mid_x} - \underset{(out)}{\left[uA_c c + \delta\left(uA_c c\right)\right] \mid_{x+\Delta x}} \tag{4.2.1}$$

or

$$\frac{\delta c}{\delta t} = -\frac{\delta(uc)}{\delta x} \tag{4.2.2}$$

where A is the cross-sectional area of the tube. If u = constant, then:

$$\frac{\delta c}{\delta t} = -u\frac{\delta c}{\delta x} \tag{4.2.3}$$

Equation 4.2.3 will be used to simulate the pipeline connections when there is no change in the flowrate between the processing units; otherwise Equation 4.2.1 will be used. The outlet concentration from the individual processing unit models are equated to the inlet concentration of the "pipeline" model. In reality, if there is a change in flowrate, a pump would be used, but Equation 4.2.1 will enable the model to consider a change and implement it accordingly. This flow rate will flow along the length of the pipeline then the effluent concentration from the pipeline is equated to the inlet concentration and flow for the following unit, as illustrated in Figure 4.2.

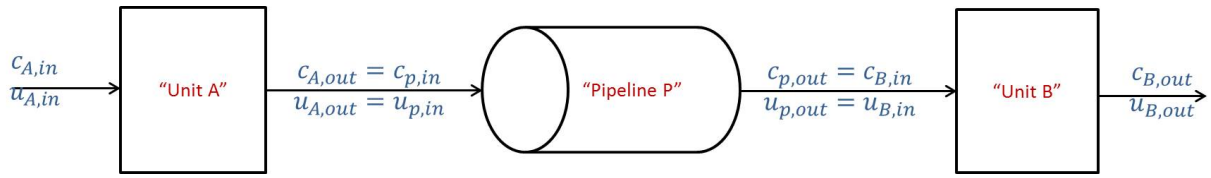


Figure 4.2: Illustration of the individual mathematical model connections with the pipeline model.

4.3 Overall plant performance

To demonstrate the applicability of the overall plant model, several illustrative scenarios will be presented that consider the impact of a disturbance propagating through the plant. As discussed in Chapter 1, the type of raw water entering a clean water treatment plant will have an impact on the degree of efficiency for suspended solid removal through out the system. The key information is that surface water (upland water) has higher suspended solid concentration due to the fact they have contact with mineral deposits in the soil and groundwater (lowland water) has a lower suspended solids concentration as these waters are found in underground aquifers so that many of the microorganisms and suspended solids have to pass through solids and rock which act as a filter. Three illustrative scenarios have been investigated to test the impact of using a mixture of raw water sources on the overall clean water treatment plant. The first scenario considers a blend of raw water sources from surface water and groundwater that have been stored in a reservoir during the summer months. The second scenario considers the same raw water inlets but they are stored in a reservoir over winter months as the expected suspended solids concentration will be different during these times. These two scenarios are based around a clean water treatment configuration that does not account for a sludge settling tank with recycled water. The third scenario takes this additional unit into account and considers multiple units in parallel. Different configurations have been presented and comparisons on the suspended solids concentration for the given scenarios will be shown.

4.3.1 Scenario 1

Figure 4.3 shows the overall plant configuration considered for Scenarios 1 and 2, and Table 4.1 shows the plant data. This scenario considers 24 hrs of operation for a water treatment plant which utilises both raw water from a nearby river and groundwater that has been stored in a reservoir within the summer season. The first change imposed after

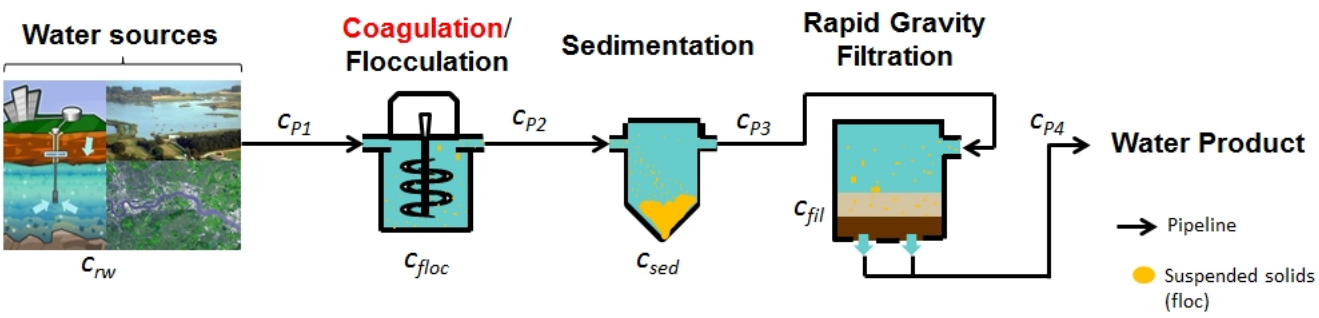


Figure 4.3: Illustrative flowsheet of a conventional clean water treatment work that will be used in the simulations for Scenario 1 and 2. The physical processes are labelled in black and the chemical processes are named in red.

5 hours of operation is a decrease in the river water inlet due to larger debris being stuck in the pre-screens and it is assumed that this will lead to a proportional increase in the raw water inlet from the groundwater source. This will decreases the overall suspended solids concentration by 10% as groundwater has less suspended solids than surface water (Binnie and Kimber, 2009). Overall there, is a decrease in the suspended solids concentration in the inlet water. There is usually a water demand increase in the warmer summer months; keeping the first change in mind, the second change imposed is a simultaneous 30% overall increase in the flowrate from the reservoir and a further 20% decrease in the suspended solids concentration. Suspended solids in water settle with gravity and as these raw waters are stored in a reservoir, the amount of suspended solids in the influent water is reduced.

Results and discussion

It can be seen from Figure 4.4 that the imposed changes in the inlet raw water concentration propagates through the whole process. Figures 4.4a, 4.4c, 4.4e, and 4.4g represent the suspended solids concentration within the pipelines between each of the water treatment processing steps, and Figures 4.4b, 4.4d, 4.4f represent the suspended solids concentration in the processing steps. Figure 4.4a shows the step changes within the initial raw water inlet pipeline. Initially, the suspended solids concentration is at steady state, after which a 10% decrease in suspended solids concentration in the raw water inlet is imposed for a duration of 11 hours, followed by an additional simultaneous change for a further 20% decrease in suspended solids concentration and a 30% increase in inlet flowrate. Figure 4.4b represents an equilibrium of suspended solids

Table 4.1: Plant data for Scenarios 1 - 3 (initial suspended solids concentration for Scenarios 1 and 2 is 6 mg/L and for Scenario 3 the initial suspended solids concentration is 4500 mg/L).

Pipelines			**Coagulation/Flocculation** (Argaman, 1971)		
C_{n0}	Initial primary particle concentration (mg/L)	6* 4500**	K_A	Collision constant (-)	1.8 x 10^{-5}
V_u	Velocity (m/s)	0.003	K_B	Break-up constant (s)	0.8 x 10^{-7}
A	Area (m^2)	20	G	Velocity Gradient (s^{-1})	20
L	Length (m)	10***	L	Length (m)	6
Clarification (Burger and Concha, 1998)			**Filtration** (Han et al., 2008)		
H	Height of clarification zone (m)	-1	L	Filter bed depth (m)	0.9
B	Depth of thickening zone (m)	3	d_c	Clean grain diameter (m)	0.8 x 10^{-3}
A	Area (m^2)	400	d_p	Particle diameter (m)	4 x 10^{-6}
C_{max}	Maximum concentration (mg/L)	7.5	ε_0	Porosity (-)	0.4
v_0	Settling velocity of a single particle in unbounded fluid (m/s)	3.47	α	Particle/filter grain attachment efficiency (-)	0.9
r	Parameter in equation for fbk (L/mg)	9.64 x 10^{-4}	α_p, η_p, β	Single parameter (-)	0.9
α_1	Parameter in equation for fbk (m^{-1})	0.0023	ϖ_0	Detachment coefficient constant (-)	200
α_2	Parameter in dispersion coefficient (s/m^2)	6.9 x 10^{-7}	σ_c	Critical specific deposit ($^{mg}/_{L}$)	300
Q_u	Underflow volumetric flowrate (m^3/s)	0.4 * Q_f	ρ_p	Particle density ($^{mg}/_{L}$)	1350 x 10^3
			γ_0	Constant (-)	30
			h_0	Clean headloss (m)	0.4

*Initial suspended solids concentration for Scenarios 1 and 2

**Initial suspended solids concentration for Scenario 3

***An average of pipeline distance for water treatment works (DEFRA, 2014)

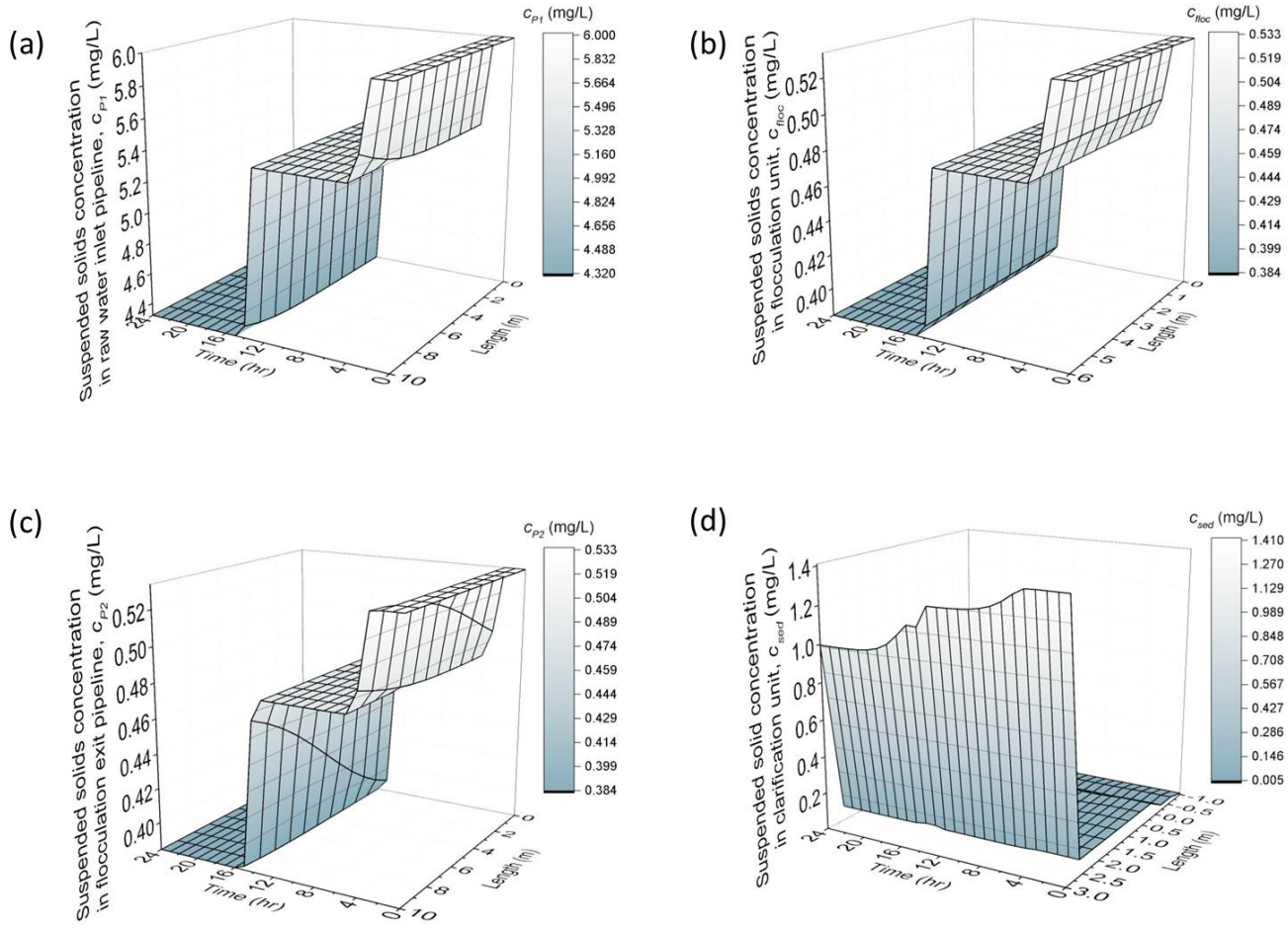


Figure 4.4: Scenario 1 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours. The simulation begins at steady state, a step change of a 10% decrease in suspended solids concentration in the raw water inlet for a duration of 11 hours, then another step change for a further 20% decrease in suspended solids concentration and a 30% increase in inlet flowrate imposed.
a) Shows the suspended solids concentration (mg/L) in the raw water inlet pipeline.
b) Shows the suspended solids concentration (mg/L) in the flocculation unit.
c) Shows the suspended solids concentration (mg/L) in the flocculation unit exit pipeline.
d) Shows the suspended solids concentration (mg/L) in the clarification unit.

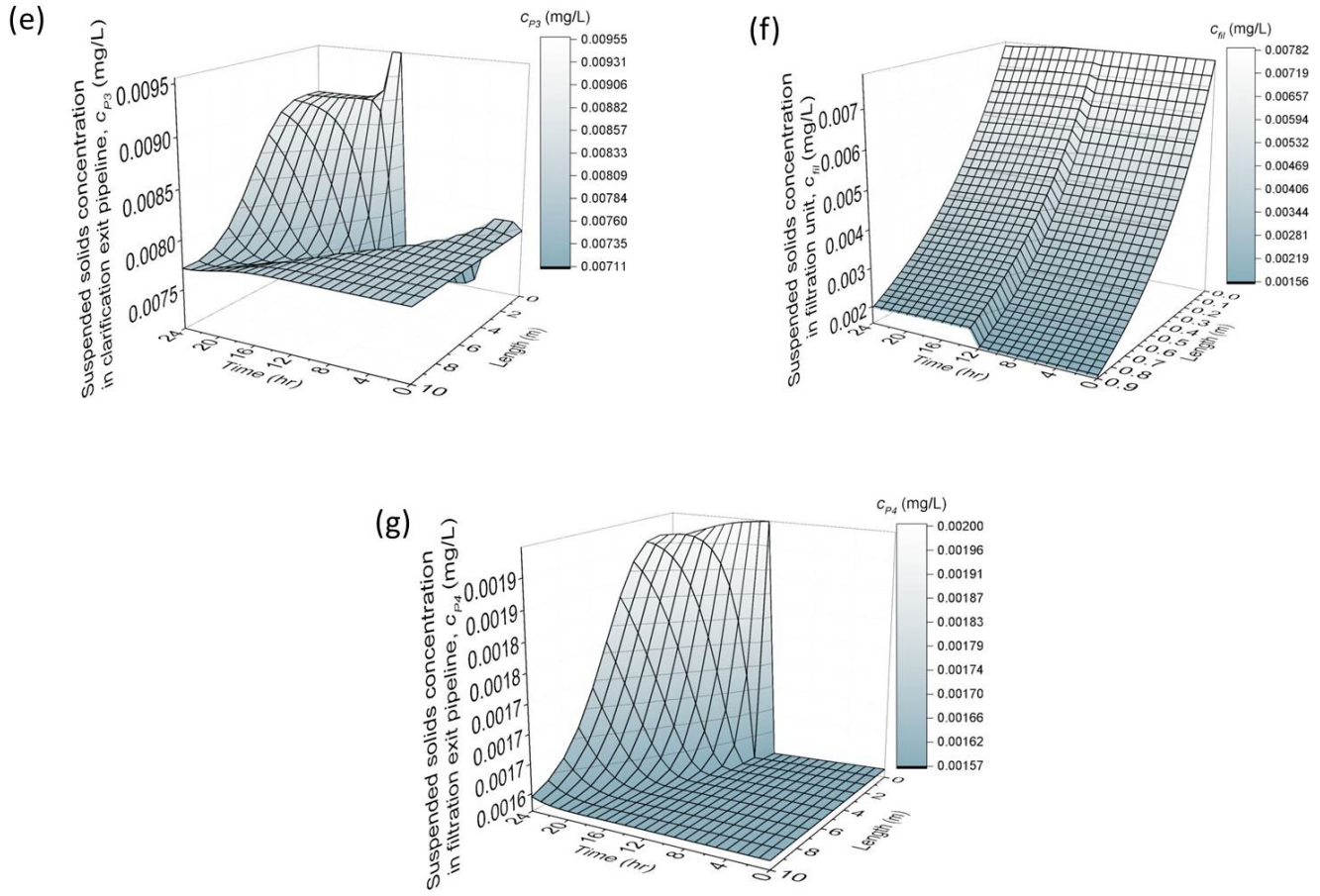


Figure 4.4 continued: Scenario 1 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours. The simulation begins at steady state, a step change of a 10% decrease in suspended solids concentration in the raw water inlet for a duration of 11 hours, then another step change for a further 20% decrease in suspended solids concentration and a 30% increase in inlet flowrate imposed.
e) Shows the suspended solids concentration (mg/L) in the clarification unit exit pipeline.
f) Shows the suspended solids concentration (mg/L) in the filtration unit.
g) Shows the suspended solids concentration (mg/L) in the filtration unit exit pipeline.

concentration between the primary and secondary (flocs) particle phases. There is an initial decrease in the concentration of flocs being formed due to the decrease of the raw water inlet suspended solids concentration, which leads to a second order change in the clarification unit (Figure 4.4d) as can be seen by the collection of suspended solids concentration in bottom of the tank (axial position 3 m). As there are less flocs being formed, there are fewer suspended solids settling in the clarification unit, as can also be seen from the decrease in the concentration of particles settling in the clarification unit, which eventually reaches a new steady state. Within the filtration unit (Figure 4.4f), there is a steady increase in suspended solids concentration: this is due to the assumption (Han et al., 2008) that the filtration unit is used after back-wash, which enables a greater deposition of particles onto the surface, and with this scenario, the filtration unit remains in the ripening stage.

With the second imposed change of 20% decrease in suspended solids concentration and a 30% increase in inlet flowrate propagating through the system, it is evident that even with the further decrease in the suspended solids concentration, the increased velocity affects the suspended solids concentration that is carried through the process, as can be seen in the pipeline exiting the flocculation unit (Figure 4.4c), clarification (Figure 4.4e) and filtration unit (Figure 4.4g). It is important to note that a decrease in raw water inlet concentration can have a negative impact on the water purity if the number of primary particles entering is not sufficient to create flocs in the coagulation/flocculation unit, in which case these smaller particles will go through to the clarification unit. As there are more small suspended solids-to-floc ratio, the small particles will not settle to sludge and may pass through to the filtration unit. In theory, this can make the filtration unit saturate at a faster rate (Fitzpatrick, 1998), leading to cloudy water being sent to consumer taps. The impact of the second change particularly affected the clarification unit (Figure 4.4d), as the flocculation/coagulation unit relies on the primary concentration of particles to form flocs and the clarification unit uses the weight of the flocs as a form of separation.

4.3.2 Scenario 2

This scenario considers 24 hrs of operation of a water treatment plant that utilises raw water from a nearby river and groundwater that has been stored in a reservoir within the winter season. The first change imposed (at 5 hours) is an increase in the raw water suspended solids concentration due to early rainfall. Parsons and Jefferson

(2006) state that with continual rainfall, the raw water turbidity and suspended solids concentration increases significantly by approximately 40%. The second change (at 16 hours) is an increase in water demand so the raw water flowrate from the reservoir is increased by 20% (to accommodate for the demand) with an accompanying 10% increase in suspended solids concentration. The increase in the suspended solids concentration is to account for the additional raw water turbidity and suspended solids concentration due to the raw water being used in combination with the highly turbid rain water.

Results and discussion

It can be seen from Figure 4.5 that the imposed changes in the inlet raw water concentration propagates through the whole process. Figures 4.5a, 4.5c, 4.5e, and 4.5g represent the suspended solids concentration within the pipelines between each of the water treatment processing steps and Figures 4.5b, 4.5d, 4.5f represent the suspended solids concentration in the processing steps. Figure 4.5a shows the step changes within the initial raw water inlet pipeline; initially, the simulations begin at initial steady state, after which a 40% increase in suspended solids concentration in the raw water inlet for a duration of 11 hours is imposed and then another additional change for a further 10% increase in suspended solids concentration and a 20% increase in inlet flowrate occurs. The flocculation graph in Figure 4.5b represents an equilibrium of suspended solids concentration between the primary and secondary (flocs) particle phases. There is a substantial increase in the concentration of flocs being formed due to the decrease of the raw water inlet suspended solids concentration, which leads to a second order change in the clarification unit (Figure 4.5d) as can be seen by the collection of suspended solids concentration at the bottom of the tank (axial position 3 m). The impact of rainfall means the underflow from the clarification unit will have an increase in suspended solids concentration, and with this increase the sludge height may to increase with the increasing suspended solids concentration settling, which can contribute to a higher concentration of suspended solids in the effluent pipe. Within the filtration unit (Figure 4.5f), there is a gradual increase in concentration: this is once again due to the assumption that the filtration unit is used after back-wash. The slight suspended solids concentration increase, indicates the beginning of the breakthrough stage, and as a result the increased suspended solids concentration and velocity enables the suspensions to escape with effluent waters more easily. Moreover, in this scenario (and evident in Scenario 1) the filtration unit is not hugely impacted by the imposed changes. This is due to the majority of the suspended solids concentration being removed in the

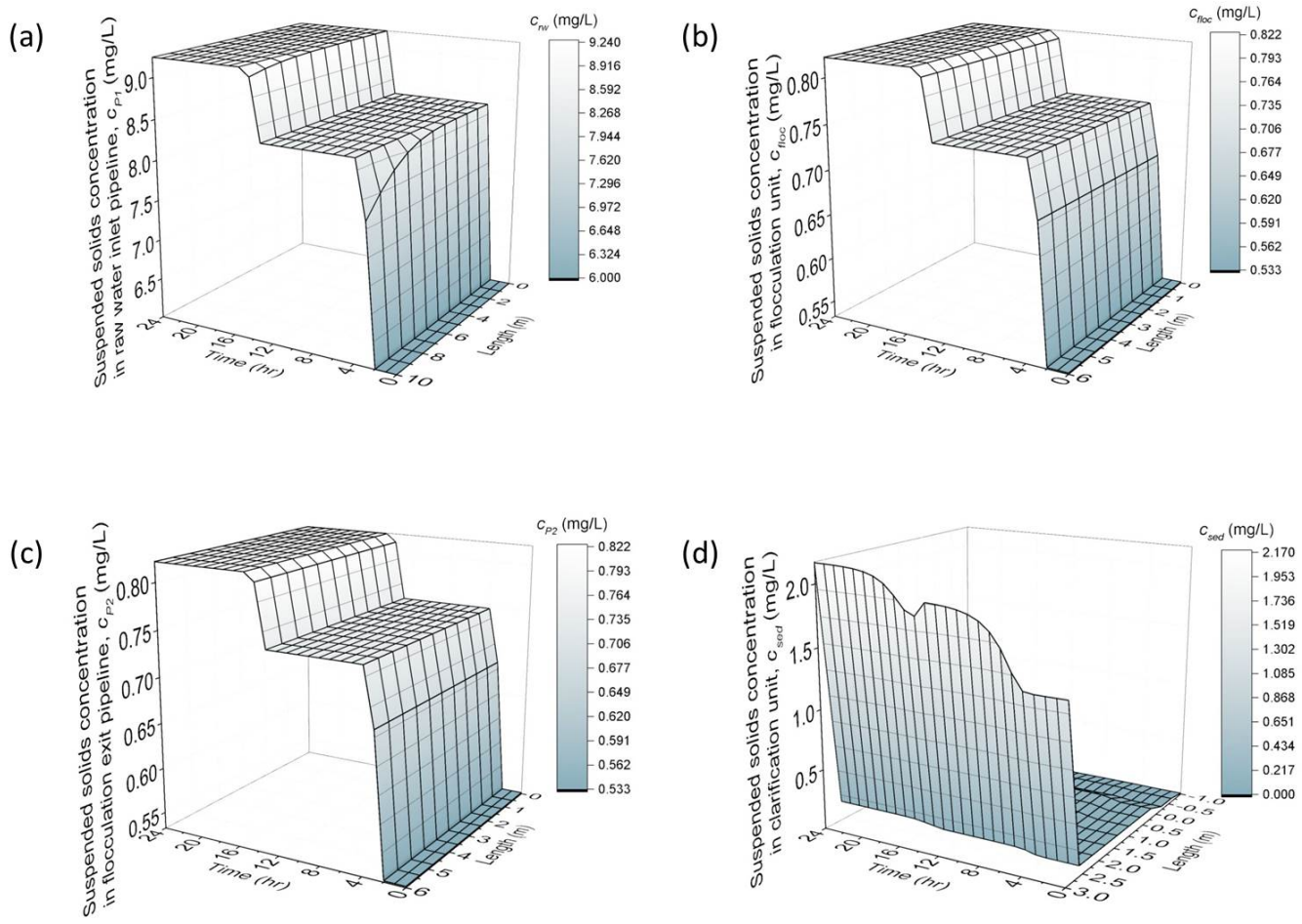


Figure 4.5: Scenario 2 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours. The simulation begins at steady state, a step change of a 40% increase in suspended solids concentration in the raw water inlet for a duration of 11 hours, then another step change for a further 10% increase in suspended solids concentration and a 20% increase in inlet flowrate imposed.
a) Shows the suspended solids concentration (mg/L) in the raw water inlet pipeline.
b) Shows the suspended solids concentration (mg/L) in the flocculation unit.
c) Shows the suspended solids concentration (mg/L) in the flocculation unit exit pipeline.
d) Shows the suspended solids concentration (mg/L) in the clarification unit.

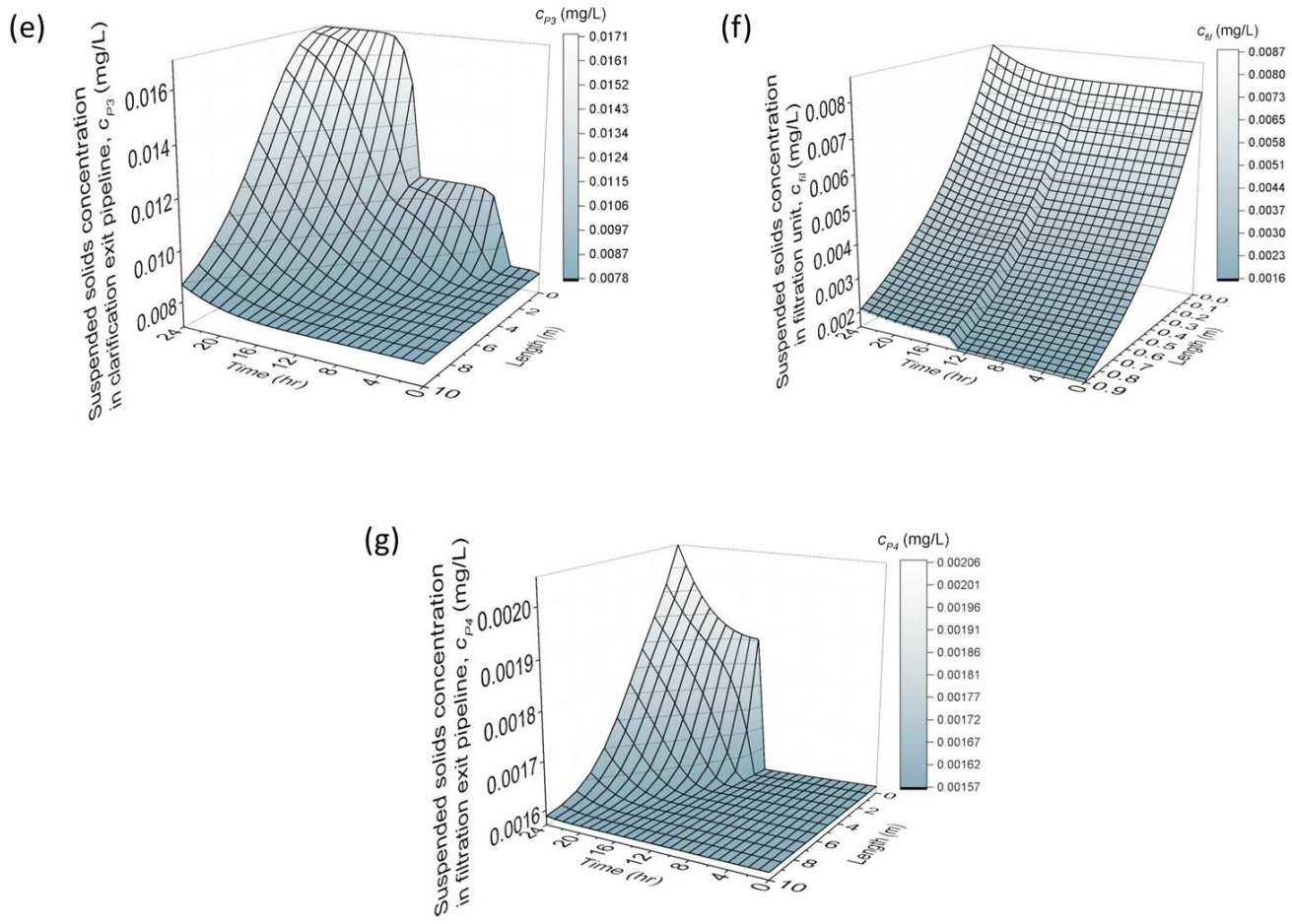


Figure 4.5 continued: Scenario 2 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours. The simulation begins at steady state, a step change of a 40% increase in suspended solids concentration in the raw water inlet for a duration of 11 hours, then another step change for a further 10% increase in suspended solids concentration and a 20% increase in inlet flowrate imposed.
e) Shows the suspended solids concentration (mg/L) in the clarification unit exit pipeline.
f) Shows the suspended solids concentration (mg/L) in the filtration unit.
g) Shows the suspended solids concentration (mg/L) in the filtration unit exit pipeline.

underflow within the clarification unit before this final physical removal unit. The increased suspended solids concentration means there is more flocs formed that can be separated by weight within the clarification unit.

With the second imposed change of 10% increase in suspended solids concentration and a 20% increase in inlet flowrate propagating through the system, it is evident that even with the further increase in the suspended solids concentration, the increased velocity affects the suspended solids concentration that is carried through the process as can be seen in the pipeline exiting the flocculation unit (Figure 4.5c), clarification (Figure 4.5e) and filtration unit (Figure 4.5g). The impact of the second change greatly effects all the units, which means more attention to the water quality is needed in winter, which mimics industrial practise (Binnie and Kimber, 2009).

4.3.3 Scenario 3

This scenario considers the configurations shown in Figure 4.6a and Figure 4.6b. There are two main alterations compared to the original plant configuration in Scenario 1 and 2: i) the addition of a sludge recycle stream, which is a unit that can often be found in a clean water treatment process, and ii) the addition of multiple units for the clarification and filtration processes. The recycle stream is incorporated after the sludge settling unit where the effluent water from this unit is returned to the flocculation unit as the water contains chemical coagulants and can therefore undergo further floc formation. In a clean water treatment plant, multiple process units are normally used. Using multiple units has benefits; for instance, parallel operations of the processing units will eliminate the constraint of continuous operations making it safer and easier for maintenance, replacement or upgrades to be made without the need for plant shut-down. The addition of multiple smaller scale units may reduce costs as they can be sized to maximise their technical performance rather than being preselected for only large-volume processing (Binnie and Kimber, 2009; Crittenden et al., 2012). A comparison between the configuration of single and multiple processing units and the addition of the sludge recycle stream will be examined with an illustrative scenario where an imposed step change of a 20% decrease in suspended solids concentration after 12 hours will occur.

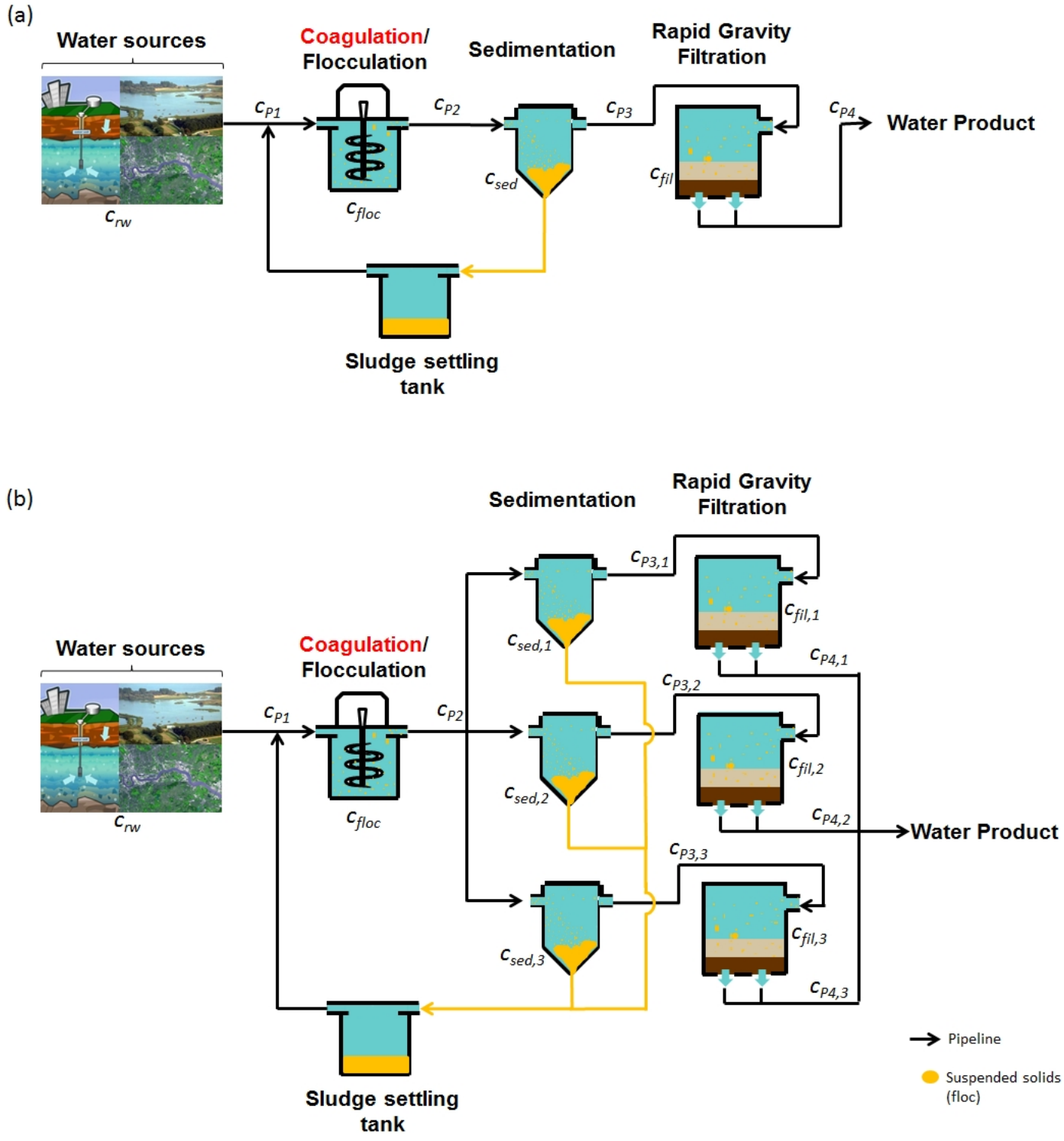


Figure 4.6: Illustrative flowsheet of a conventional clean water treatment work that will be used in the simulations for scenario 3 incorporating a sludge recycle unit. The physical processes are labelled in black and the chemical processes are named in red.
a) Single processing units.
b) Expansion of Figure 4.6a incorporating multiple processing units in parallel for clarification and filtration.

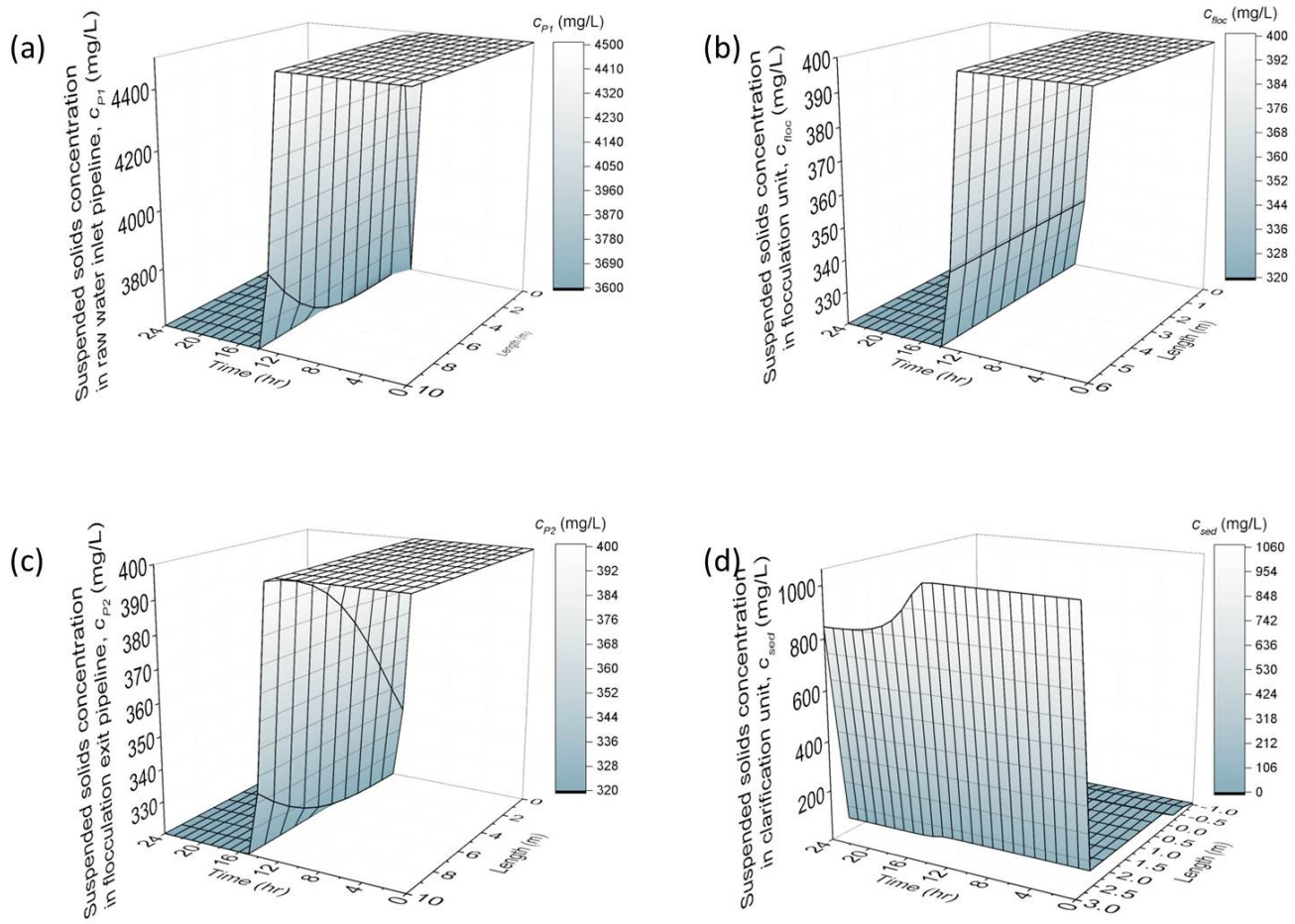


Figure 4.7: Scenario 3 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours, incorporating a sludge recycling unit (as shown in Figure 4.6). The simulation begins at steady state, and then a step change of a 20% decrease in suspended solids concentration in the raw water inlet after 12 hours.
a) Shows the suspended solids concentration (mg/L) in the raw water inlet pipeline.
b) Shows the suspended solids concentration (mg/L) in the flocculation unit.
c) Shows the suspended solids concentration (mg/L) in the flocculation unit exit pipeline.
d) Shows the suspended solids concentration (mg/L) in the clarification unit

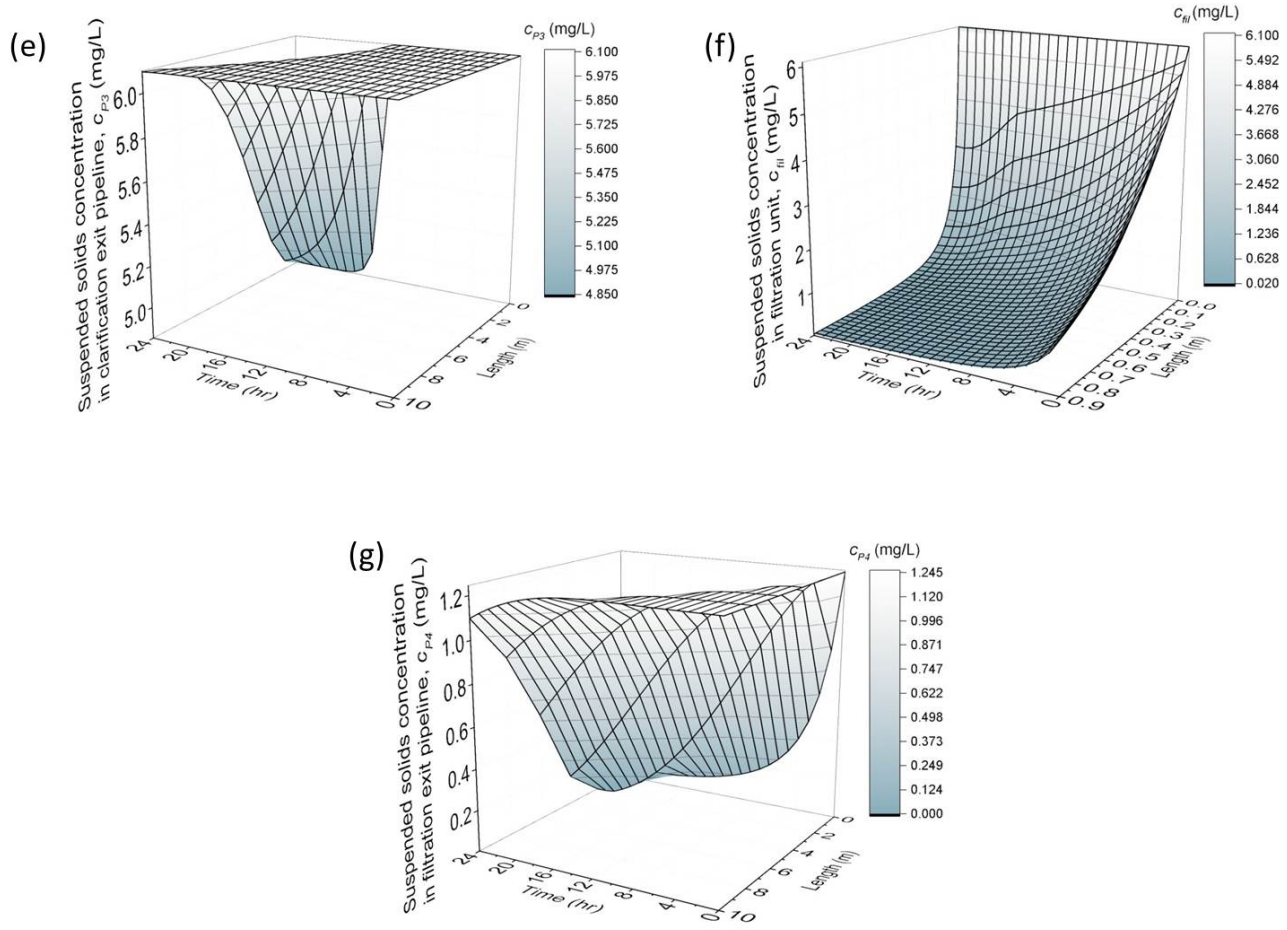


Figure 4.7 continued: Scenario 3 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours, incorporating a sludge recycling unit (as shown in Figure 4.6). The simulation begins at steady state, and then a step change of a 20% decrease in suspended solids concentration in the raw water inlet after 12 hours.
e) Shows the suspended solids concentration (mg/L) in the clarification unit exit pipeline.
f) Shows the suspended solids concentration (mg/L) in the filtration unit.
g) Shows the suspended solids concentration (mg/L) in the filtration unit exit pipeline.

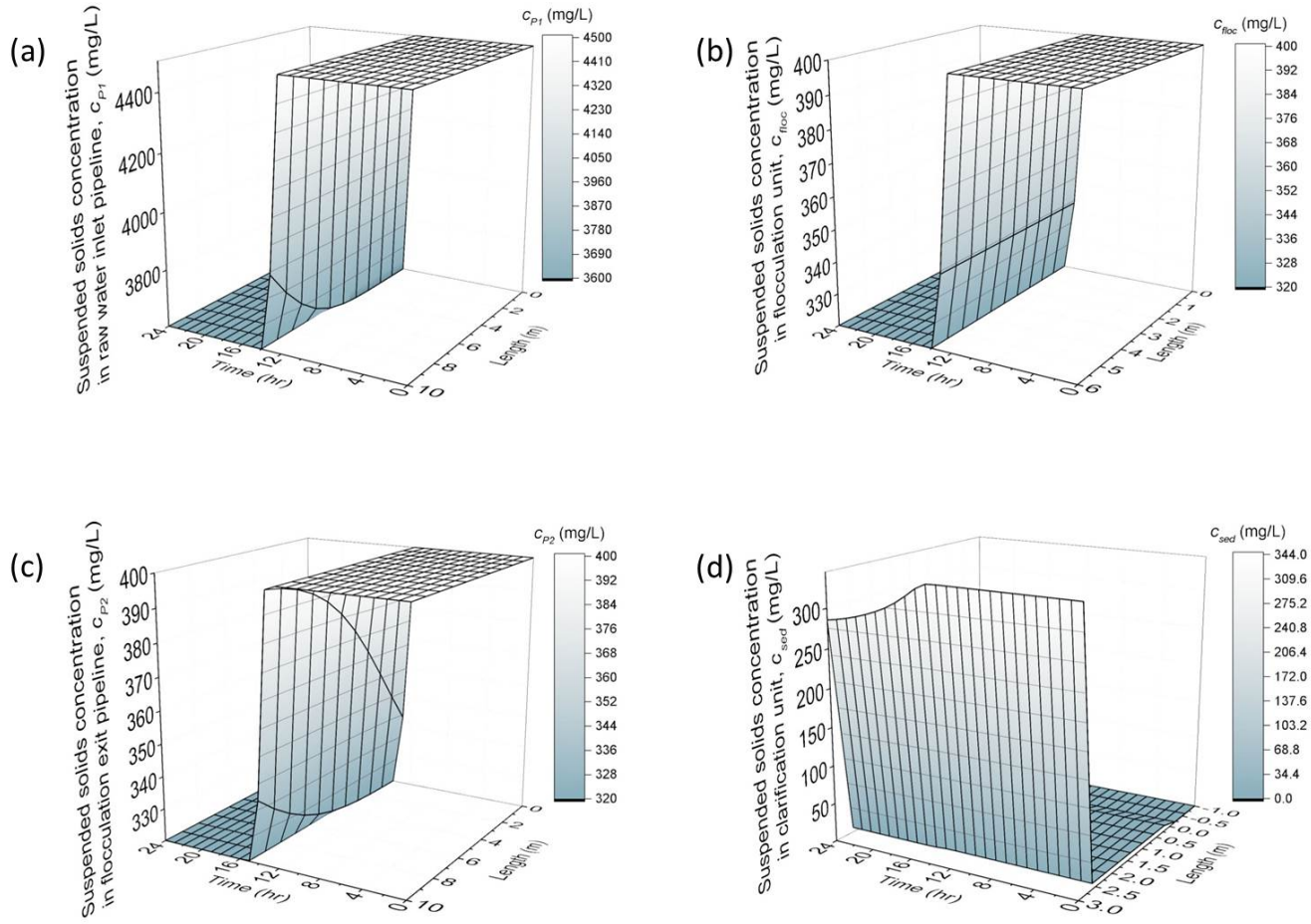


Figure 4.8: Scenario 3 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours, incorporating multiple processing units for clarification and filtration incorporating a sludge recycle unit (as shown in Figure 4.6b). The simulation begins at steady state, and then a step change of a 20% decrease in suspended solids concentration in the raw water inlet after 12 hours.
a) Shows the suspended solids concentration (mg/L) in the raw water inlet pipeline.
b) Shows the suspended solids concentration (mg/L) in the flocculation unit.
c) Shows the suspended solids concentration (mg/L) in the flocculation unit exit pipeline.
d) Shows the suspended solids concentration (mg/L) in the clarification unit.

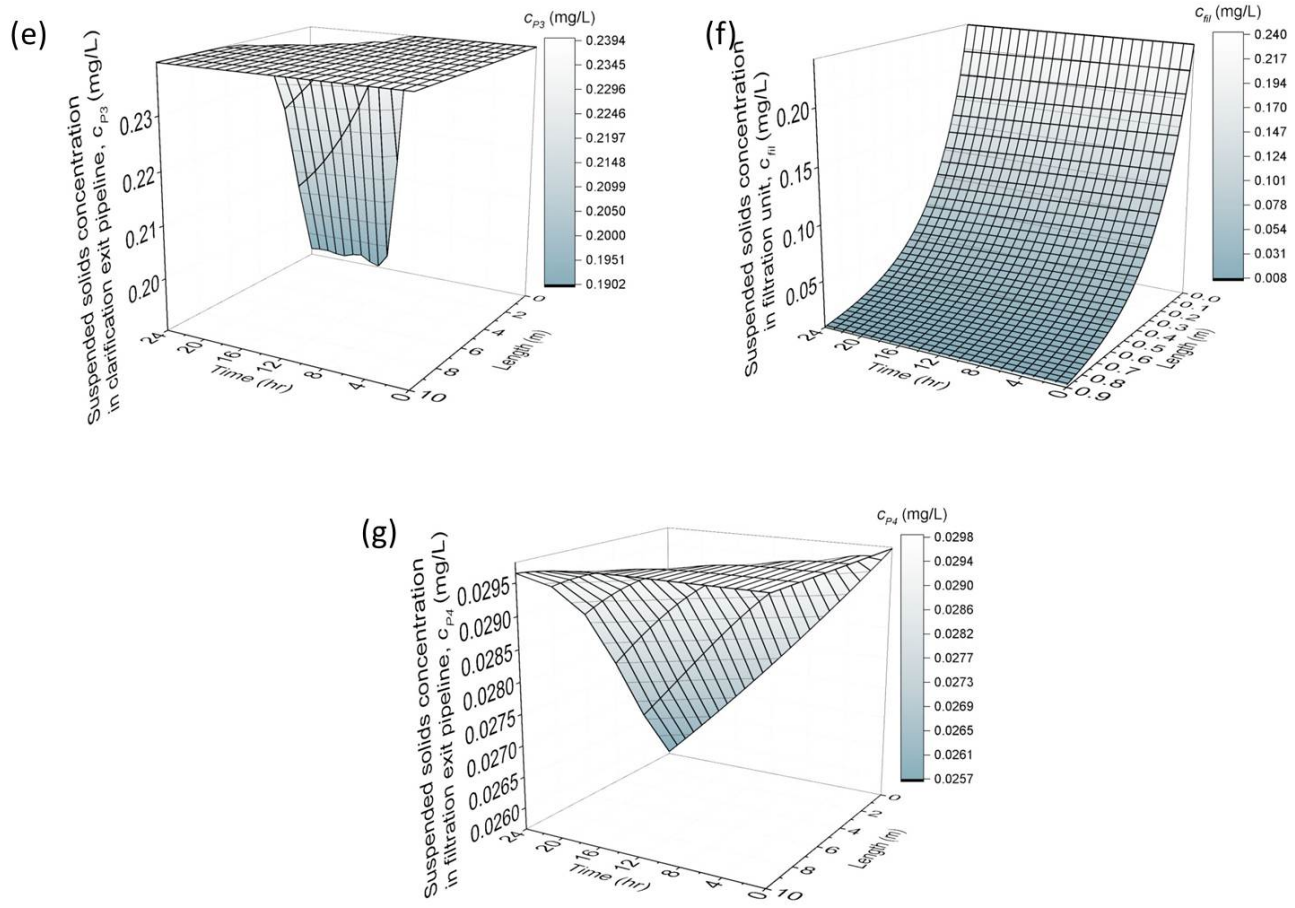


Figure 4.8 continued: Scenario 3 - Concentration of suspended solids (mg/L) in each unit of an overall plant over the course of 24 hours, incorporating multiple processing units for clarification and filtration incorporating a sludge recycle unit (as shown in Figure 4.6b). The simulation begins at steady state, and then a step change of a 20% decrease in suspended solids concentration in the raw water inlet after 12 hours.
e) Shows the suspended solids concentration (mg/L) in the clarification unit exit pipeline.
f) Shows the suspended solids concentration (mg/L) in the filtration unit.
g) Shows the suspended solids concentration (mg/L) in the filtration unit exit pipeline.

Results and discussion

Figure 4.7 shows the propagation of an imposed step change of a 20% decrease in suspended solids concentration through a clean water treatment plant with a single unit configuration (as shown in Figure 4.6a) whilst Figure 4.8 shows the propagation through a multiple unit configuration (as show in Figure 4.6b). The coagulation/flocculation unit is singular in both scenarios and the resulting concentration and propagation through this unit is the same however the units following show some interesting results. Figure 4.6b assumes that the flow is split equally by the number of units, in this case 3 units; however this might not necessarily be the case in real life as the pipelines connecting units are not in ideal conditions. The first observation to note is that with the use of multiple units, the concentration exiting each unit (Figure 4.8c, 4.8e, 4.8g) is substantially decreased; this implies that the area for these units can be made smaller, which in reality would make the units easier to manage. The addition of multiple units also indicates there is a decrease in suspended solids concentration in the underflow leaving from a single clarification unit to the sludge stream, which may aid in the prevention of pipe blockage due to an overflow of suspended solids being concentrated in one unit.

Focusing on the concentration of suspended solids particles exiting the clarification unit (Figure 4.8e), the amount of suspended solids that leaves each of the clarification units is shown to be significantly smaller than the amount that leaves in Figure 4.7e. This has an effect on the behaviour of the filtration unit, in the sense that when there is a single filtration unit, there is an indication that the unit is beginning to enter the "working" stage as there is a returning curve around t = 4 hrs. However, this phenomenon is not present in Figure 4.8f, meaning that the filtration system would be able to last for a longer time period without the need for a back-wash to clean the filters. The final exit suspended solids concentration (Figure 4.8g) is also lower in the multiple configuration system by a magnitude of 10 and this suggests the reduced concentration and flow demands when using multiple units the areas can be increased which may lead to significant saving in the overall capital costs of a new infrastructure.

4.4 Computational statistics

All three scenarios were simulated using gPROMS 4.2 (Process Systems Enterprise, 2014) on a Dell OptiPlex 990MT workstation with 3.1 GHz processor, 4GB RAM and

Table 4.2: Computational statistics of clean water treatment Scenarios 1 - 3.

	Without sludge recycle	
	Scenario 1	Scenario 2
Variables	926	926
Equations	1200	1200
CPU Time (s)	0.87 (14% system time)	0.58 (11% system time)

	With sludge recycle (Scenario 3)	
	Single *unit flowsheet*	***Multiple*** *unit flowsheet*
Variables	1010	2665
Equations	1286	3371
CPU Time (s)	1.48 (13% system time)	13.84 (87% system time)

Windows 7 64-bit operating system. The computational statistics of all three scenarios are shown in Table 4.2. Scenarios 1 and 2 have the same number of variables and equations as the only change are the numerical values of the proposed step changes. Scenario 1 has a larger CPU time (0.87 s) than Scenario 2 (0.58 s) and this difference can be attributed to the simulation accounting for the second step change in Scenario 1 which incorporates both a decrease in suspended solids concentration with an increase in the flowrate. Many large scale water treatment plants include at least one recycle stream for water recovery. When a recycle is included in the single unit model the time to find an optimal solution is 1.48 seconds. The increased CPU when a recycle stream is added is expected additional equations and variables have been added. The addition of a recycle stream is not the only increase in CPU, additional units in parallel also increase the computational time needed.

4.5 Conclusion

This chapter has presented an overall mathematical model of a clean water treatment plant by combining together models of individual processing units which have been previously studied in isolation. The detailed models developed in Chapter 3 have been combined in order to simulate an overall conventional clean water treatment model. The overall model can be used at an early stage of process development for design purposes as a training tool for plant operators, or to investigate the consequences of changes in the plant.

It has been demonstrated that the developed model is able to predict the behaviours of

the plant following an imposed changes in the raw water suspended solids concentration. Three different scenarios were presented with three alternative clean water treatment configurations; namely, single processing units, multiple processing units and the addition of a sludge recycle stream. The scenarios presented considered a blend of raw water sources from surface water and groundwater that have been stored in a reservoir during both the summer and winter months, each with varying step changes imposed. The changes, when imposed, were successfully propagated through the clean water treatment process simulation. For a model like this to be fully utilised, it needs to be operator friendly, and the detailed mathematical models shown so far are complex and the simulations require specialist software and computational capabilities. With this in mind, the next chapter addresses the development of simpler, or "surrogate" models, which are easier to use and require less sophisticated solution methods.

Chapter 5

Surrogate models for process integration

In this chapter, the development of novel surrogate models from detailed mathematical models will be discussed for the process units considered in previous chapters. A major benefit of surrogate modelling is simplistic models that can be implemented in the water treatment process. Detailed models are complex and require specialist knowledge in computational tools that surrogate models will overcome. After the development of the surrogate models, their ability to predict mechanistic trends will be verified against the detailed models developed in chapter 3.

5.1 Introduction

Chapter 3 presented detailed dynamic mathematical models for a number of individual water treatment processes. These are complex models based fundamental knowledge and are only concerned with the phenomena occurring within the individual process units. Linking these dynamic models together into an overall plant model increased the complexity. This resulted in a challenging equation system which could prove difficult for operators to use on a water treatment plant. This can be resolved through the use of simplified surrogate models that are generated by the detailed models but with less complexity which will therefore reduce the computational expertises and time needed.

5.2 Surrogate modelling

Surrogate models, developed through regression analysis, are black box models which are generated from data either sourced experimentally or obtained from a highly-accurate and computationally expensive models. Regression analysis predicts continuous output or response variables from various independent input variables by approximating their functional relationship (Yang et al., 2016). Surrogate models built with a large number of data points are generally more accurate than models with a reduced number of data points, due to limited information. The surrogate models built with less data points are able to predict output variables from relevant input variables without providing details of the complex mechanisms (Box and Draper, 1987; Davis and Ierapetritou, 2008; Bai et al., 2014); however, bias results may be produced with a surrogate model built from approximate information. It is more beneficial to have an understanding of the true underlying functional relationship with variables that is offered by detailed models. If detailed computationally expensive simulations are replaced with approximate mathematical models, then much more data points can be generated through repeated simulations. With simpler functions, regression analysis is able to approximate the overall system behaviour whilst preserving the desired level of accuracy (Caballero and Grossmann, 2008; Henao and Maravelias, 2010, 2011; Beck et al., 2012).

In literature, several regression analysis methodologies exist, including: Kriging (Kleijnen and Beers, 2004; Kleijnen, 2009), Radial Basis Functions (RBF) (Sarimveis et al., 2004), Multivariate Adaptive Regression Splines (MARS) (Friedman, 1991), and Support Vector Regression (SVR) (Smola, 2004; Levis and Papageorgiou, 2005; Forrester and Keane, 2009).

The two most common methods utilised in water quality modelling are artificial neutral networks (ANN) (Zhang and Stanley, 1999; Raman and Sunilkumar, 1995; Hamed et al., 2004; Cordoba et al., 2014) and polynomial response surface (linear and multi-variable linear regression) (Sadiq and Rodriguez, 2004; Chenini and Khemiri, 2009). The main difference between these two methods is that ANN creates mapping sequences between input and output datasets obtained from the process. The mapping between the input and outputs is achieved using historical data to train the network, which is utilised to create the architecture required to predict process outputs for any data that is not used as the training set. ANNs require a larger dataset to benefit from its optimisation, if enough data is not provided then irrespective of the existing non-linearities, linear regression model may be better adjusted. These two methodologies will summarised briefly before the selected method is discussed in detail.

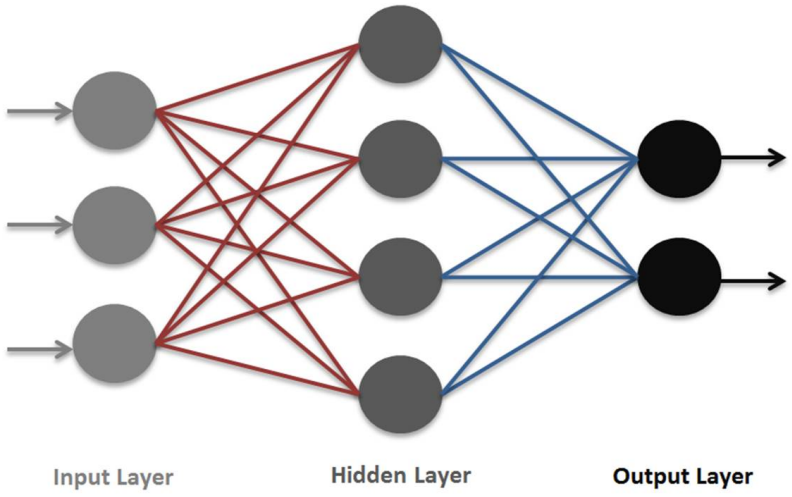


Figure 5.1: Typical structure of a feedforward artificial neural network (ANN).

5.2.1 Artificial neural network

An artificial neutral network (ANN) is a developed mathematical model or algorithm that is inspired by the operations of the biological nervous system (biological neural networks) (Hill et al., 1994). In other words, patterns are found in data utilising the functioning of neutral networks as non-linear statistical data modelling tools used to model complex relationships between inputs and outputs. Generally, in the learning phase, an ANN is adaptive and can change its structure based on external or internal information that flows through the network. Ultimately, knowledge is gained by the network through a learning process and the interconnections between the elements of the network store the knowledge (Gernaey et al., 2004). When there is a lot of training data available, ANN are especially useful for function-approximating problems (Gevrey et al., 2003). Trained with sufficient data, ANN can sufficiently describe multivariate systems with non-linear dynamics (Dua, 2010).

The general format for an ANN structure is presented in Figure 5.1, which shows a typical feedforward ANN. The relationships between the input layer, the hidden layer and the output layer are connected with weighted links and the nodes have biases, both of these aspects represent the system parameters (Prasad and Bequette, 2003). The ANN receives information through the input layer; this information is processed and sent to the hidden layer. Computationally, the hidden layer processes the information further and this data is sent to the output layer which provides the information of the process system. Generally, the nodes in the input layer receive information from the training/validation datasets, whilst the nodes in the hidden and output layers receive

information directly from the nodes in the preceding layer of the network. Within the wastewater sector, ANN has been used to describe the biochemical processes in the biological wastewater treatment (Hamoda et al., 1999; Gontarski et al., 2000; Mjalli et al., 2007).

5.2.2 Polynomial response surface methodology

Response surface methodology (RSM) is a series of mathematical and statistical techniques that are useful for developing, improving and optimising different processes (Gunst, 1996). It identifies polynomial equations that can describe the relationship between input (independent variables) and output (response) data. RSM was initially developed to model responses of experiments (Box and Draper, 1987), it was then further developed to numerical experiment modelling (Toropov and Markine, 1996). The application of RSM to design optimisation is aimed at reducing computational costings of expensive analysis methods (e.g. finite element method or CFD analysis) in addition to their associated numerical noise (Khayet et al., 2008). In general, the structure of the relationship between the independent variables and the response is unknown.

The end goal of RSM is to find a suitable approximation to the true functional relationship between dependent and independent variables. The most common forms are low-order polynomials (first or second-order), where second-order models are usually sufficient to reflect the data and trends of more complex models as they are very flexible and can easily estimate the parameters using the least-square method. The general governing equation for a second-order multiple polynomial regression model is:

$$Z = \beta_0 + \beta_i x_i + \beta_j x_j + \beta_{ii} x_i^2 + \beta_{jj} x_j^2 + \beta_{ij} x_i x_j \tag{5.2.1}$$

Where:

Z	predicted response
β_0	constant coefficient
β_i	linear interaction coefficient
β_{ii} , β_{ij}	quadratic interaction coefficients
x_i, x_j	input variables influencing predicted response Z

The main purposes of these types of models are (Draper, 1997):

1. To establish an approximate relationship between Y and x_1,x_2,...,x_k that can be used to predict response values for given settings of input variables, Y_i.

2. To determine the level of significance of the factors with levels represented by x_1,x_2,...,x_k.

3. To determine the optimum settings of x_1,x_2,...,x_k that result in the maximum or minimum response over a certain region of interest.

The method of least squares is typically used to estimate the regression coefficients, β, in a multi-linear regression model. It is simpler to solve Equation 5.2.1 in matrix notation which is given by (Draper, 1997):

$$\beta = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_k \end{bmatrix} \quad Z = \begin{bmatrix} Z_1 \\ \vdots \\ Z_n \end{bmatrix} \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \begin{matrix} \\ \\ \\ \\ \\ \\ \end{matrix} \begin{matrix} \forall i = 1...k \\ \forall j = 1...n \end{matrix} \tag{5.2.2}$$

In general, β is a $k\times 1$ vector of the regression coefficients, Z is an $n\times 1$ vector of the observations and X is an $n\times k$ model matrix consisting of the expanded independent variables. Thus, Equation 5.2.1 may be expressed as (Edgar et al., 1989):

$$X^T X\beta = X^T Z$$

when re-arranged the least-squares estimator of β can be written as (Edgar et al., 1989):

$$\beta = \left(X^T X\right)^{-1} X^T Z$$

In scalar notation, the fitted model is:

$$Z = \beta_0 + \sum_{i=1}^{K} \beta_i x_i + \sum_{i<j} \beta_{ij} x_i x_j + \sum_{i=1}^{K} \beta_{ii} x_i^2 \tag{5.2.3}$$

5.2.3 Full factorial design

Factorial designs can be used for fitting first- and second-order models. The accuracy of the approximation and the time taken to construct the response surface is largely

influenced by the choice of the design of experiments (Montgomery, 1997). In this work, the factorial design strategy will be used to transform the detailed mathematical models into quadratic surrogate models. From previous chapters, influential variables are identified for the various detailed process models. Within the factorial design strategy, the design variables are varied together instead of focusing on each one individually.

To build an approximation model to capture k design variables, the upper and lower bounds of each design variables need to be defined to create the desired range. This is followed by discretisation of the desired range, two and three levels are more commonly used. Two levels (called 2^k full factorial) require the ranges to be defined by only the lower and upper bounds whilst three levels (also known as 3^k full factorial) include mid-points. The development of a quadratic response surface model in k variables requires three levels so that the interaction coefficients can be estimated and the model will be able to fit curved response functions (Montgomery, 1997), as will be considered in this work.

For simultaneous optimisation using response surface modelling, each input variable, Y_i, and normalised variable, x_i, must have a low, centre and high value assigned to each goal. For a goal of maximum, the desirability curve is given by:

$$x_i = \left[\frac{Y_i - Y_{Low_i}}{Y_{High_i} - Y_{Low_i}}\right], \quad Y_{Low_i} \leq Y_i \leq Y_{High_i} \quad \forall i = 1...k \tag{5.2.4}$$

For a goal of centre, the desirability curve is given by:

$$x_i = \left[\frac{Y_i - Y_{Centre_i}}{Y_{Centre_i} - Y_{Low_i}}\right], \quad \begin{matrix} Y_{Low_i} \leq Y_i \leq Y_{Centre_i} \\ Y_{Centre_i} \leq Y_i \leq Y_{High_i} \end{matrix} \quad \forall i = 1...k \tag{5.2.5}$$

or

$$x_i = \left[\frac{Y_i - Y_{Centre_i}}{Y_{High_i} - Y_{Centre_i}}\right], \quad \begin{matrix} Y_{Low_i} \leq Y_i \leq Y_{Centre_i} \\ Y_{Centre_i} \leq Y_i \leq Y_{High_i} \end{matrix} \quad \forall i = 1...k \tag{5.2.6}$$

For a goal of minimum, the desirability curve is given by:

$$x_i = \left[\frac{Y_{High_i} - Y_i}{Y_{High_i} - Y_{Low_i}}\right], \quad Y_{Low_i} \leq Y_i \leq Y_{High_i} \quad \forall i = 1...k \tag{5.2.7}$$

Draper (1997) and Montgomery (1997) presented a methodology to develop surrogate models from data provided.

1. The number of runs required to ensure all the combination of variables, k, and

levels, n, are considered can be calculated by:

$$No.\,runs = n^k \tag{5.2.8}$$

2. Develop a coded matrix X, where all the levels (low, centre and high) are represented by -1, 0 and 1, respectively.

3. Use the detailed mathematical models to determine a value for Z, for a given set of independent variables, k.

4. Determine the transpose matrix, X^T, and calculate $(\mathrm{X}^T\mathrm{X})^{-1}$.

5. Calculate the transpose matrix, X^T multiplied by Z, $(\mathrm{X}^T\mathrm{Z})$.

6. Solve for the least squares estimator of β.

In the next section, the methodology detailed above is used to develop the surrogate models for calculating the effluent suspended solids concentration in each of the processing units considered in Chapter 3. The polynomial response surface methodology will be used as the limitation with the using ANN in this work is the lack of sufficient plant data to create an adequate system. The developed surrogate models will be tested against the detailed models within the desired range, between the low and high goals, to validate their use by checking the accuracy of the fit utilising parity plots, and values outside of the desired range to explore how these models will react.

5.3 Coagulation-flocculation surrogate model

In Chapter 3, two detailed mathematical models were developed in sub-section 3.2.2 to represent the unit processes of rapid mixing and flocculation in chambers/compartments for the coagulation/flocculation process.

Rapid Mixing

In this section, a surrogate model will be developed which links two key variables to the effluent suspended solids concentration. The sensitivity analysis conducted in sub-section 3.2.2 showed that the suspended solids concentration in the rapid mixing

unit was affected by the inlet (primary) suspended solids concentration and the speed at which suspended solids were mixed. Using Equation 5.2.1, the polynomial equation will take on the form:

$$c_{floc,RM} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \tag{5.3.1}$$

where

$c_{Floc,RM}$	output effluent suspended solids concentration, (mg/L)
x_1	normalised initial suspended solids, (mg/L)
x_2	normalised velocity gradient, (s^{-1})

As explained in sub-section 5.2.2, the two factors, x_1 and x_2, will be explored at three different levels (low, centre and high) with the goal of finding an average desirability range. By using Equation 5.2.5, the following expressions will be used to determine the factors for each variable, e.g.:

$$x_1 = \left[\frac{c_0 - c_{0_{centre}}}{c_{0_{centre}} - c_{0_{low}}}\right] \tag{5.3.2}$$

$$x_2 = \left[\frac{G - G_{centre}}{G_{centre} - G_{low}}\right] \tag{5.3.3}$$

where

c_0	initial suspended solids values used in detailed model, (mg/L)
G	velocity gradient values used in detailed model, (s^{-1})

Utilising the methodology detailed in Section 5.2.2, Equation 5.2.8 shows there are 9 simulations needed in order to have all combinations. Table 5.1 presents the typical ranges of operation that were considered to ensure the level of accuracy, and the justifications for the choices.

Once these variables were specified, the detailed models were simulated with the different combinations of variable values to obtain an effluent suspended solids concentration. Formulas programmed into Microsoft Excel are then utilised to develop the surrogate models using steps 2 to 7. Table 5.2 presents the numerical values for the least squares estimator, β, for coagulation/flocculation via rapid mixing. The values are provided as both "unlogged" and "logged"[1] due to a log scale making it easy to compare values that cover a large range.

[1]For ease of interpretation, the logarithmic transformation of models in the text are referred to as *"logged"* and the regular model notation is referred to as *"unlogged"*.

Table 5.1: Desirability curve ranges presented for coagulation/flocculation via rapid mixing as normalised and normal units of measurement for Equations 5.3.2 and 5.3.3, along with justifications for the ranges considered.

	Coded factor level			
Variable	**Low (-1)**	**Centre (0)**	**High (1)**	**Justification**
Initial suspended solids, c_0 (mg/L)	10	30	50	Raw water turbidity in the UK varies from 5 NTU (units for turbidity) in the lowlands to 22 NTU in the uplands (Parsons and Jefferson, 2006). Edzwald (2011) and Hannouche et al. (2011) state an assumption that there is a proportional link between NTU and total suspended solids; as discussed in Chapter 2, this relationship is linear. The authors also state that there is a constant multiplier in different water sources which generally remains in the region of 0.7 to 2.3, e.g. if theory states a particular water source will have a concentration of 22 mg/L, it is likely the to be in the range of 15.4 - 52.9 3mg/L. It is better to over design a treatment unit and assume there is more suspended solids in the water, therefore, the upper limit of 2.3 will be taken.
Velocity gradient, G (s^{-1})	5	25	45	Crittenden et al. (2012) state that a horizontal shaft paddle is commonly used in industrial practice and the velocity gradients are typically within this range.

Table 5.2: Surrogate model β parameters for coagulation/flocculation via rapid mixing.

	$c_{Floc,RM}$	$\log c_{Floc,RM}$
β_0	3.33	0.524
β_1	2.22	0.350
β_2	2.67	0.478
β_{11}	4.44×10^{-16}	-0.129
β_{22}	8.88×10^{-16}	-0.222
β_{12}	1.78	-0.001

The regression equation developed for coagulation/flocculation via rapid mixing, expressed as the "unlogged" and "logged" values of $c_{Floc,RM}$ are:

$$c_{Floc,RM} = 3.33 + 2.22x_1 + 2.67x_2 + 4.44 \times 10^{-16}x_1^2 + 8.88 \times 10^{-16}x_2^2 + 1.78x_1x_2 \quad (5.3.4)$$

$$logc_{Floc,RM} = 0.524 + 0.35x_1 + 0.478x_2 - 0.129x_1^2 - 0.222x_2^2 - 0.001x_1x_2 \quad (5.3.5)$$

The validation and sensitivity analysis of the equations above to predict the effluent concentration, $c_{Floc,RM}$, will be presented in Section 5.3.1.

Flocculation in chambers/compartments

For the coagulation/flocculation unit, an alternative unit operation has been developed for performance comparison. The rapid mixing unit occurs in a reactor whilst this flocculation unit takes place in compartments in series. In this section, a surrogate model will be developed which links four key variables to the effluent suspended solids concentration. The sensitivity analysis conducted in sub-section 3.2.2 showed that the suspended solids concentration in the flocculation unit was affected not only by the inlet (primary) suspended solids concentration and the speed at which these suspended solids were mixed but also the number of compartments and the time spent in the compartments (residence time). Using Equation 5.2.1, the polynomial equation will take on the form:

$$\begin{aligned} c_{floc,COM} = \; & \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \beta_{44}x_4^2 \\ & + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 \end{aligned} \quad (5.3.6)$$

where

$c_{Floc,COM}$	effluent suspended solids concentration, (mg/L)
x_1	normalised initial suspended solids concentration values used in detailed model, (mg/L)
x_2	normalised velocity gradient values used in detailed model, (s^{-1})
x_3	normalised number of compartments values used in detailed model, (-)
x_4	normalised residence time values used in detailed model, (s)

The four factors, x_1, x_2, x_3 and x_4 will be explored at three different levels (low, centre and high) with the goal of finding an average desirability range. By using Equation

5.2.5, the following equations will be used to determine the factors for each variable, i.e.:

$$x_1 = \left[\frac{c_0 - c_{0_{centre}}}{c_{0_{centre}} - c_{0_{low}}}\right] \tag{5.3.7}$$

$$x_2 = \left[\frac{G - G_{centre}}{G_{centre} - G_{low}}\right] \tag{5.3.8}$$

$$x_3 = \left[\frac{m - m_{centre}}{m_{centre} - m_{low}}\right] \tag{5.3.9}$$

$$x_4 = \left[\frac{\tau - \tau_{centre}}{\tau_{centre} - \tau_{low}}\right] \tag{5.3.10}$$

where

- c_0 initial suspended solids concentration, (mg/L)
- G velocity gradient, (s^{-1})
- m number of compartments, (-)
- τ residence time, (s)

Utilising the methodology detailed in Section 5.2.2, Equation 5.2.8 shows there are 81 simulations needed in order to have all combinations. Table 5.3 presents the typical ranges of operation that were considered to ensure the level of accuracy, and the justifications for the choices.

Once these variables are specified, the detailed models are simulated with the different combinations of variable values to obtain an effluent suspended solids concentration. As with rapid mixing, the formulae was programmed in Microsoft Excel then utilised to develop the surrogate models from steps 2 to 7. Table 5.4 presents the numerical values for the least squares estimator, β, for coagulation/flocculation via flocculation in chambers/compartments.

The regression equation developed for flocculation via flocculation chambers/compartments,

Table 5.3: Desirability curve ranges for coagulation/flocculation via flocculation chambers/compartments presented as input units of measurement for Equations 5.3.7 to 5.3.10, along with justifications for the ranges considered.

	Coded factor level			
Variable	**Low (-1)**	**Centre (0)**	**High (1)**	**Justification**
Initial suspended solids, c_0 (mg/L)	10	30	50	Same justification as in Table 5.1
Velocity gradient, G (s^{-1})	5	25	45	Same justification as in Table 5.1
Number of compart-ment s, m (-)	3	5	7	In industry, typically flocculation of this nature typically has multiple compartments, and baffles are often used to separate these compartments, It is assumed that the range of compartments in series typically between 3 and 7 (Hendricks, 2006).
Residence time, τ (s)	1200	2100	3000	Crittenden et al. (2012) state that a horizontal shaft paddle is commonly used in industrial practice and the residence time is typically within this range.

Table 5.4: Surrogate model β parameters for coagulation/flocculation via flocculation chambers/compartments.

	$c_{Floc,COM}$	$\log c_{Floc,COM}$
β_0	68.8	1.85
β_1	51.9	0.349
β_2	45.4	0.254
β_3	7.05	0.0238
β_4	29.01	0.131
β_{11}	-0.167	-0.128
β_{22}	10.7	-0.0246
β_{33}	-2.12	-0.009
β_{44}	5.24	0.0053
β_{12}	30.2	-4E-05
β_{13}	4.59	-0.0007
β_{14}	19.3	3.3E-05
β_{23}	8.91	0.0259
β_{24}	29.4	0.0927
β_{34}	6.49	0.0146

expressed as the "unlogged" and "logged" values of $c_{Floc,COM}$ are:

$$\begin{aligned} c_{Floc,COM} = \; & = 68.8 + 59.9x_1 + 45.4x_2 + 7.05x_3 + 29.01x_4 - 0.167x_1^2 + 10.7x_2^2 \\ & -2.12x_3^2 + 5.24x_4^2 + 30.2x_1x_2 + 4.59x_1x_3 + 19.3x_1x_4 + 8.91x_2x_3 \\ & +29.4x_2x_4 + 6.49x_3x_4 \end{aligned} \tag{5.3.11}$$

$$\begin{aligned} logc_{Floc,COM} = \; & 1.85 + 0.349x_1 + 0.254x_2 + 0.0238x_3 + 0.131x_4 - 0.128x_1^2 \\ & -0.0246x_2^2 - 0.009x_3^2 - 0.005x_4^2 + 3.5 \times 10^{-5}x_1x_2 - 0.00072x_1x_3 \\ & +3.32E-05x_1x_4 + 0.0259x_2x_3 + 0.0927x_2x_4 + 0.0146x_3x_4 \end{aligned} \tag{5.3.12}$$

The validation and sensitivity analysis of the equations above to predict the effluent concentration, $C_{Floc,COM}$, will be presented in Section 5.3.1.

5.3.1 Results and validation

In this section, the surrogate model developed for the coagulation/flocculation unit via rapid mixing and in chambers/compartments is verified and the response values are analysed.

Rapid mixing

The regression coefficient, R^2, is the statistical measure of how well the regression line approximates the data points and here the R^2 value compares the detailed model response with the surrogate model response. By plotting this data, the order of the relationship between the computational requirement and the number of equations can be obtained. With both the "logged", $logc_{Floc,RM}$, and the "unlogged", $c_{Floc,RM}$, data, the model fit is very good with a R^2 value of 99.9% meaning that either surrogate model (in the "logged" or "unlogged" form) can describe the process behaviour within the variable bounds almost as well as the detailed model for the same data set.

Figure 5.2 presents the predicted response for the effluent suspended solids concentration using the surrogate model against the effluent suspended solids concentration determined by the detailed model. In agreement with the R^2 coefficient, for both the "logged" and "unlogged" model, the surrogate model's predictive capacity seem to be a very good fit as shown by the almost linear plot and the data points laying close the x=y line.

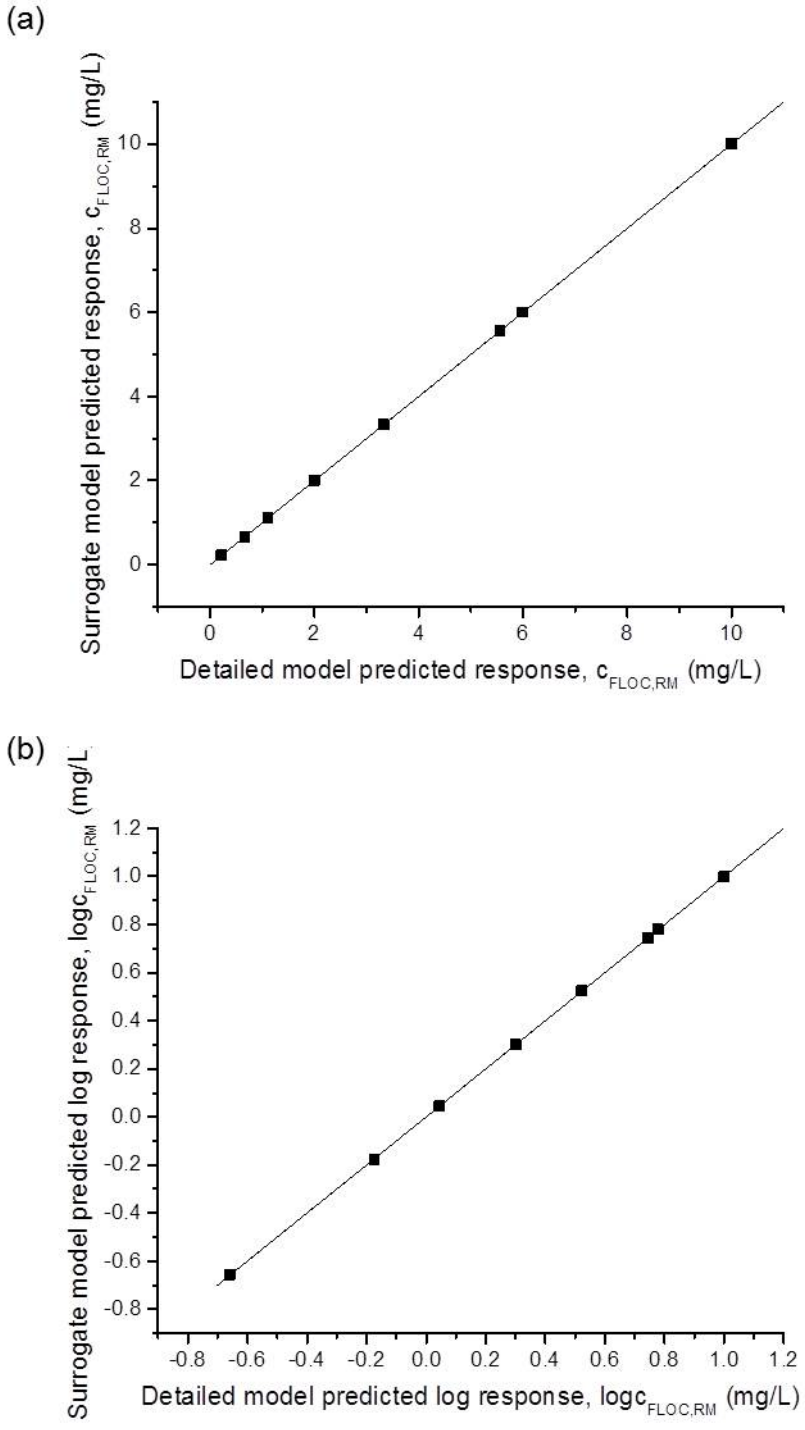


Figure 5.2: Rapid mixing: surrogate versus detailed modelling responses for effluent concentration for a) normal model responses and b)"logged" model responses. The dashed line represent the x=y line on a parity plot.

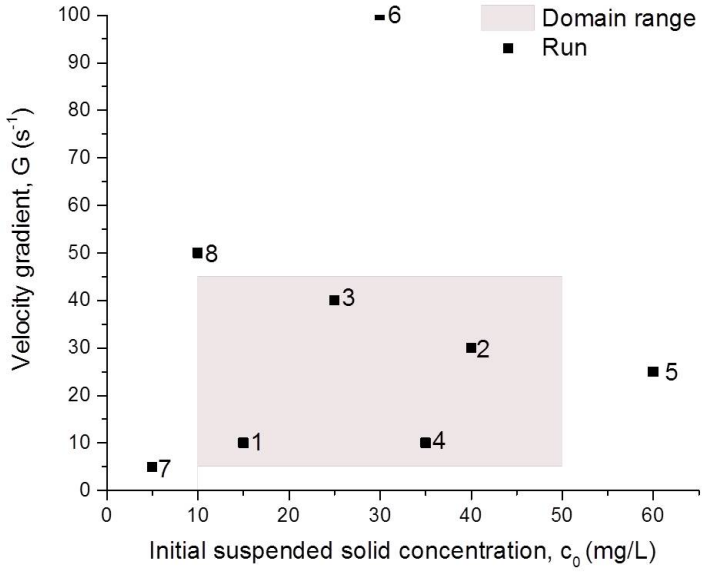


Figure 5.3: Coagulation/flocculation via rapid mixing: 2D graphical domain representation of the ranges for the variables and the data used for verification in Table 5.5.

Although, the surrogate models are able to accurately fit data from the detailed model this, however, does not necessarily mean that the models are able to predict other mechanistic trends as the surrogate models were fitted within a specific range of variables (Caballero and Grossmann, 2008; Henao and Maravelias, 2011). The surrogate models were verified against the detailed rapid mixing model, with variable values inside and outside of the ranges considered in Table 5.1.

Eight different runs (four inside the range and four outside the range) are simulated by both the detailed and surrogate models in order to compare the effluent suspended solids concentration predicted. Figure 5.3 represents graphically the range in which the surrogate model is fitted and Table 5.5 provides the data used for the verification of the surrogate model. Inside of the prediction range, the four runs (1-4) show that the "unlogged" surrogate model produces a small error when compared with the detailed model; however, when the "logged" detailed model is compared with the "logged" surrogate model there is a bigger error. This shows that the "logged" surrogate model is not as reliable within the prediction range even though the R^2 value is the same. From Table 5.5, it can be seen that the "logged" model does not predict as accurately as the "unlogged" response values, instead it under/over predicts the effluent suspended solids concentration.

Table 5.5: Verification of effluent suspended solids concentration derived from "logged" and "unlogged" surrogate model for coagulation/flocculation via rapid mixing against the detailed model.

			Normal			LOG		
Run	c_0 (mg/L)	**G** (s^{-1})	**Detailed** $c_{Floc,RM}$ (mg/L)	**Surrogate** $c_{Floc,RM}$ (mg/L)	**Error** %	**Detailed** $c_{Floc,RM}$ (mg/L)	**Surrogate** $c_{Floc,RM}$ (mg/L)	**Error** %
Inside prediction range ($10 \leq c_0 \leq 50$ **and** $5 \leq G \leq 45$)								
1	15	10	0.67	0.665	0.65	-0.17	-0.29	70
2	40	30	5.33	5.338	0.07	0.73	0.77	6.21
3	25	40	4.44	4.44	0.09	0.65	0.66	2.16
4	35	10	1.56	1.555	0.38	0.19	0.12	36
Outside prediction range ($c_0 < 10$, $c_0 > 50$ **and** $G < 5$, $G > 45$)								
5	60	25	6.67	6.668	0.03	0.82	0.76	7.94
6	30	100	13.3	13.33	0.25	1.12	-0.81	28
7	5	5	0.11	0.109	0.57	-0.96	-0.82	14.8
8	10	50	2.22	2.224	0.07	0.35	0.29	14.7

This is further shown when observing the response values produced outside of the prediction range where each run represents one variable being out of the range. Four runs simulated outside of the prediction range to observe how the models will react when faced with a variety of variables both inside and outside of the desired ranges:

- Run 5: the initial suspended solids concentration, c_0, is higher than the range.
- Run 6: the velocity gradient, G, is more than 200% bigger than the top of the range.
- Run 7: the initial suspended solids concentration, c_0, is lower then the desired range
- Run 8: the velocity gradient, G, is lower then the desired range.

The largest error (70%) is predicted with the "logged" models especially during Run 1; however, the "unlogged" model is still able to predict to a good extent the response outside of the prediction range. For this run, both of the variables, c_0 and G, are near the lower boundary which shows the “logged” model is not able to accurately predict in this range. From analysing Figure 5.2, it can be seen the “logged” suspended solids concentration value for the detailed model (-0.17 mg/L) and surrogate model (-0.29

Table 5.6: Verification of effluent suspended solids concentration derived from "logged" and "unlogged" surrogate model for flocculation via flocculation in chambers/compartments against the detailed model.

					Normal			LOG		
Run	c_0 (mg/L)	**G** (s^{-1})	**m** (-)	τ (s)	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %
Inside prediction range ($10 \leq c_0 \leq 50$, $5 \leq G \leq 45$, $3 \leq m \leq 7$ **and** $1200 \leq \tau \leq 3000$)										
1	30	20	5	1500	49.6	46	7.21	1.69	1.7	0.59
2	40	30	4	2000	100.4	99.5	0.92	2	2	0.69
3	15	20	5	1500	24.8	22.4	9.75	1.39	1.38	1.63
4	50	10	6	1800	68.4	62.5	8.6	1.84	1.84	0.15
Outside prediction range ($c_0 < 10$, $c_0 > 50$, $G < 5$, $G > 45$, $m < 3$, $m > 7$ **and** $\tau < 1200$, $\tau > 3000$)										
5	5	50	2	3600	25.2	74	193.2	1.4	1.74	24.23
6	30	50	2	3600	151.4	218	43.98	2.18	2.38	9.16
7	30	40	2	3600	128.5	166.9	29.82	2.11	2.22	5.25
8	30	40	5	3600	221.7	208.5	5.97	2.35	2.34	0.19

mg/L) are in a sparse area of data points on the line of best fit. This will contribute to the inaccuracy in the value predicted.

Flocculation in chambers/compartments

In this section, the surrogate model developed for the coagulation/flocculation unit via flocculation in chambers/compartments is verified and the response values are analysed. The regression coefficient, R^2, compares the detailed model response with the surrogate model response and it showed the "logged" model, $\log c_{Floc,COM}$, will provide a better prediction of process behaviour within the variable bounds than the "unlogged" model, $c_{Floc,COM}$, with R^2 values of 99.8% and 95.9%, respectively.

Figure 5.4 presents the predicted response for the effluent suspended solids concentration using the surrogate model against the effluent suspended solids concentration determined by the detailed model. The R^2 value suggests that although both models might provide satisfactory predictions, the model fitted to "logged" data maybe be more accurate as the graph for the "logged" data is more linear and the data points laying close the x=y line.

Figure 5.4 show that the surrogate models are able to accurately fit data from the detailed model. Table 5.6 provides the data for the verification of the surrogate model,

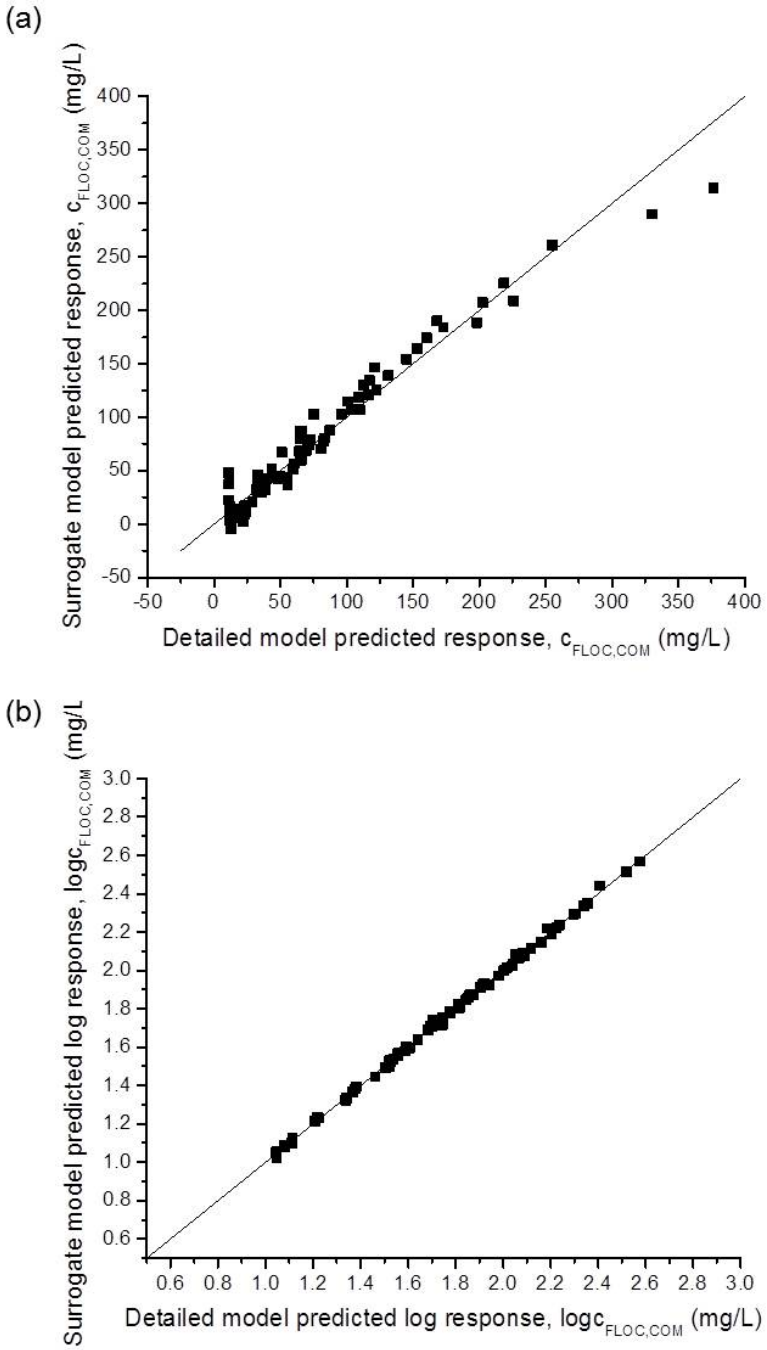


Figure 5.4: Flocculation in compartments: surrogate versus detailed modelling responses for effluent concentration for a) normal model responses and b)"logged" model responses. The dashed line represent the x=y line on a parity plot.

the domain for the variable used will not be shown as it is not possible to visualise this here in 4D. Inside of the prediction range, the four runs show that the "logged" surrogate model produces a smaller error when compared with the detailed model response; whilst the "unlogged" data seems to be under predicting the effluent suspended solids concentration. This is in agreement with the R^2 coefficient value, which shows the "unlogged" data to have a weaker fit. There are four runs simulated (results shown in Table 5.6) for outside of the prediction range to see how the models will react when faced with a variety of variables both inside and outside of the desired ranges:

- Run 5: None of the variables are within the desired range.
- Run 6: one variable (initial suspended solids concentration, c_0) is within the desired range whilst three variables (velocity gradient, G, number of compartments, m, and residence time, τ) are outside of the range.
- Run 7: two variables (initial suspended solids concentration, c_0, and velocity gradient, G) are within the desired range whilst two variables (number of compartments, m, and residence time, τ) are outside of the range.
- Run 8: three variables (initial suspended solids concentration, c_0, velocity gradient, G, number of compartments, m) are within the desired range whilst one variables (residence time, τ) is outside of the range.

The responses produced by the "logged" model provides a more linear trend and has a smaller error. The "logged" model was more accurately able to predict the suspended solids concentration within the desired range, showing that the more variables that are outside of the range the bigger the numerical error.

For runs 1 - 3, the "logged" model over-predicts the suspended solids concentration by up to 25% when all the variables are outside of the desired range but then slightly under predicts when there only one variable is outside of the desired range. The issue of over-predicting the effluent suspended solids by this amount is not compromising as it will lead to an over designed system, i.e. a system which has a larger capacity than a smaller, under designed system (Amirtharajah et al., 1991; Bratby, 1980; McConnachie et al., 1999).

The largest error is predicted during Run 5 operating outside of the desired range, where the error for the “logged” model is 24% and “unlogged” model is 193.2%. This run has no variables operating within the range and it has an affect one the model’s ability to accurately predict a response.

5.3.2 Concluding remarks

The primary objective of the study in this section was the development of surrogate models for the coagulation/flocculation unit, which are able to accurately predict the effluent suspended solids concentration. There are two alternative processing units that have been developed (in Chapter 3) into surrogate models: namely, flocculation via rapid mixing and flocculation occurring in a series of chambers/compartments. The models were developed in both "logged" and "unlogged" form, where the "logged" form is to respond to any skewed results, i.e. any points that are much larger/smaller than the bulk of the data. Although, the value of R^2 coefficient was close for both alternatives, the numerical errors during the verification revealed which form of the model ("logged" or "unlogged") was the best to use. For flocculation via rapid mixing, the "logged" and "unlogged" models produced a similar R^2 coefficient, with Figure 5.2 showing that the models were a good fit. However, when the sensitivity of the models were analysed with numerical values inside and outside of the desired ranges, it was clear that the "unlogged" model was superior as the absolute errors between the surrogate model prediction and the detailed model response were smaller. For flocculation occurring in a series of chambers/compartments, by taking the logarithm of the response of the detailed model, there is an increase in the models predictive capacity, the correlation is highly linear and the predicted values fit very closely to the actual model values. With this in mind, the "logged" surrogate model for flocculation occurring in a series of chambers/compartments will be used.

5.4 Clarification surrogate model

In Chapter 3, one detailed mathematical model is developed to represent a sedimentation unit within the clarification process.

Sedimentation clarification

In this section, a surrogate model will be developed which links three key variables to the effluent suspended solids concentration. The variables considered are the inlet suspended solids concentration, c_0, which is affected by the feed volumetric flowrate, Q_f, and the inlet feed position, L_f due to the settling of the suspended solids. The height at

which sludge blanket settles will impact on the effluent suspended solids concentration. Using Equation 5.2.1, the polynomial equation will take on the form:

$$\begin{aligned} c_{Clar,eff/und} = \quad & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 \\ & + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 \end{aligned} \tag{5.4.1}$$

where

$c_{Clar,eff}$	effluent suspended solids concentration from overflow, (mg/L)
$c_{Clar,und}$	effluent suspended solids concentration from underflow, (mg/L)
x_1	normalised initial suspended solids, (mg/L)
x_2	normalised feed volumetric flowrate, (m^3/s)
x_3	normalised inlet feed position from bottom, (m)

The three factors, x_1, x_2 and x_3 will be explored at three different levels (low, centre and high) with the goal of finding an average desirability range. By using Equation 5.2.5, the following will be used to determine the factors for each variable:

$$x_1 = \left[\frac{c_0 - c_{0_{centre}}}{c_{0_{centre}} - c_{0_{low}}} \right] \tag{5.4.2}$$

$$x_2 = \left[\frac{Q_f - Q_{f_{centre}}}{Q_{f_{centre}} - Q_{f_{low}}} \right] \tag{5.4.3}$$

$$x_3 = \left[\frac{L_f - L_{f_{centre}}}{L_{f_{centre}} - L_{f_{low}}} \right] \tag{5.4.4}$$

where

c_0	initial suspended solids concentration value used in detailed model, (mg/L)
Q_f	feed volumetric flowrate value used in detailed model, (L/s)
L_f	inlet feed position from bottom value used in detailed model, (m)

Utilising the methodology detailed in Section 5.2.2, there are 27 simulations needed in order to have all combinations. Table 5.7 presents the typical ranges of operation that were considered to ensure the level of accuracy and the justifications for the choices.

Once these variables are specified, the detailed models are simulated with the different combinations of variable values to obtain an effluent suspended solids concentration. Microsoft Excel is then employed to develop the surrogate models using steps 2 to 7. Table 5.8 presents the numerical values for the least square estimator, β, for the

Table 5.7: Desirability curve ranges for clarification presented as coded and uncoded units of measurement for equations 5.4.2 to 5.4.4, along with justifications for the ranges considered.

	Coded factor level			
Variable	**Low (-1)**	**Centre (0)**	**High (1)**	**Justification**
Initial suspended solids, c_0 (mg/L)	5	77.5	150	A range of 5 to 150 mg/L was considered for c_0 to account for any changes in the inlet suspended solids concentration water source (Binnie and Kimber, 2009).
Feed volumetric flowrate, Q_f (L/s)	64	82	100	A range of 0.64 to 100 L/s was considered as higher flowrate will lead to poor efficiency of removal due to flocs breaking back up because of the collisions occurring (Argaman, 1971).
Inlet feed position from bottom, L_f (m)	3	2	1	Typical values in industry vary from 1m from bottom of the tank to 1m from the top of the tank (Crittenden et al., 2012). This is especially useful for the sedimentation clarification unit when being utilised in the sludge collecting recycle unit. It should be noted that the detailed model assumed an absolute depth of 4m.

Table 5.8: Surrogate model β parameters for effluent suspended solids concentration in clarification via sedimentation.

	$c_{Clar,eff}$	$\log c_{Clar,eff}$
β_0	0.407	-0.45
β_1	0.711	0.745
β_2	0.341	0.331
β_3	-0.883	-0.935
β_{11}	0.00437	-0.456
β_{22}	0.0546	-0.019
β_{33}	0.468	-0.236
β_{12}	0.319	-0.00737
β_{13}	-0.828	0.00497
β_{23}	-0.305	0.139

effluent suspended solids concentration leaving in the overflow from the sedimentation clarification unit.

The regression equation developed for clarification via sedimentation, expressed as for the "unlogged" and "logged" values of $c_{Clar,eff}$ are:

$$\begin{aligned} c_{Clar,eff} = \; & 0.497 + 0.711x_1 + 0.34x_2 - 0.883x_3 + 0.00437x_1^2 + 0.0546x_2^2 \\ & +0.468x_3^2 + 0.319x_1x_2 - 0.828x_1x_3 - 0.305x_2x_3 \end{aligned} \tag{5.4.5}$$

$$\begin{aligned} logc_{Clar,eff} = \; & -0.45 + 0.745x_1 + 0.3431x_2 - 0.935x_3 - 0.456x_1^2 - 0.0191x_2^2 \\ & -0.236x_3^2 - 0.00737x_1x_2 + 0.00497x_1x_3 - 0.139x_2x_3 \end{aligned} \tag{5.4.6}$$

Within the sedimentation clarification unit, the suspended solids concentration in the effluent is not the only concentration of interest. The suspended solids concentration leaving as sludge in the underflow, $c_{Clar,und}$, is also important due to the recycle stream. This recycle takes the underflow suspended solids concentration to a sludge settler unit, the sludge is concentrated in a sedimentation clarifying unit and the effluent suspended solids from this sludge unit is recycled into the water treatment process. This stream is mixed with the raw water inlet before the coagulation/flocculation processing unit (as shown in Figure 4.6).

The regression equation developed for underflow suspended solids concentration in the clarification via sedimentation, can be expressed as the “unlogged” and “logged” values of $c_{Clar,und}$:

$$\begin{aligned} c_{Clar,und} = \; & 208.2 + 187.8x_1 + 1.99x_2 - 1.93x_3 + 0.0339x_1^2 + 0.767x_2^2 \\ & -12.03x_3^2 + 1.87x_1x_2 - 1.81x_1x_3 + 4.05x_2x_3 \end{aligned} \tag{5.4.7}$$

$$\begin{aligned} logc_{Clar,und} = \; & 2.32 + 0.739x_1 + 0.00376x_2 - 0.00418x_3 - 0.452x_1^2 + 0.00113x_2^2 \\ & -0.0526x_3^2 + 5.15 \times 10^{-5}x_1x_2 + 3.54 \times 10^{-5}x_1x_3 + 0.00889x_2x_3 \end{aligned} \tag{5.4.8}$$

Table 5.9 presents the numerical values for the least square estimator, β, for the effluent suspended solids concentration leaving in the underflow from the sedimentation clarification unit.

The validation and sensitivity analysis of the equations above to predict the underflow concentration, $c_{Clar,und}$, and effluent concentration, $c_{Clar,eff}$, will be presented in Section 5.4.1.

Table 5.9: Surrogate model β parameters for underflow suspended solids concentration in clarification via sedimentation.

	$c_{Clar,und}$	$\log c_{Clar,und}$
β_0	208.25	2.32
β_1	187.82	0.739
β_2	1.99	0.0038
β_3	-1.93	-0.0042
β_{11}	0.034	-0.452
β_{22}	0.767	0.0011
β_{33}	-12.03	-0.025
β_{12}	1.86	5.15×10^{-5}
β_{13}	-1.81	3.54×10^{-5}
β_{23}	4.05	0.0089

5.4.1 Results and validation

In this section, the surrogate model developed for the clarification unit via sedimentation is verified and the response values are analysed. There were two responses considered for this unit the effluent suspended solids concentration, $c_{Clar,eff}$, which leaves this unit and continues into the filtration unit and the underflow suspended solids concentration, $c_{Clar,und}$, which leaves with a high concentration of suspended solids from the bottom of the tank and into a sludge collection unit.

Focusing on the surrogate model for the effluent suspended solids concentration, $c_{Clar,eff}$, the values of the regression coefficient, R^2, shows the "logged" model, $\log c_{Clar,eff}$, will provide a better prediction of process behaviour within the variable bounds than the "unlogged" model, $c_{Clar,eff}$, with R^2 values of 99.8% and 96.1%, respectively.

Figure 5.5 presents the predicted response for the effluent suspended solids concentration using the surrogate model against the effluent suspended solids concentration determined by the detailed model. For both the "logged" and "unlogged" model, the surrogate model's predictive capacity seem to be a very good fit as shown by the graphs; however, the graph for the "logged" data is more linear as the "unlogged" model has an uneven distribution of data points between 0 - 0.5 mg/L. The R^2 value suggests that although both models might provide accurate predictions, the model fitted to "logged" data is more slightly accurate along the desired range. Figure 5.5 shows that the surrogate models are able to fit data from the detailed model. The models were verified against the detailed clarification models, developed in Sub-section 3.3.2, with variable values inside and outside of the ranges considered in Table 5.7. Within the

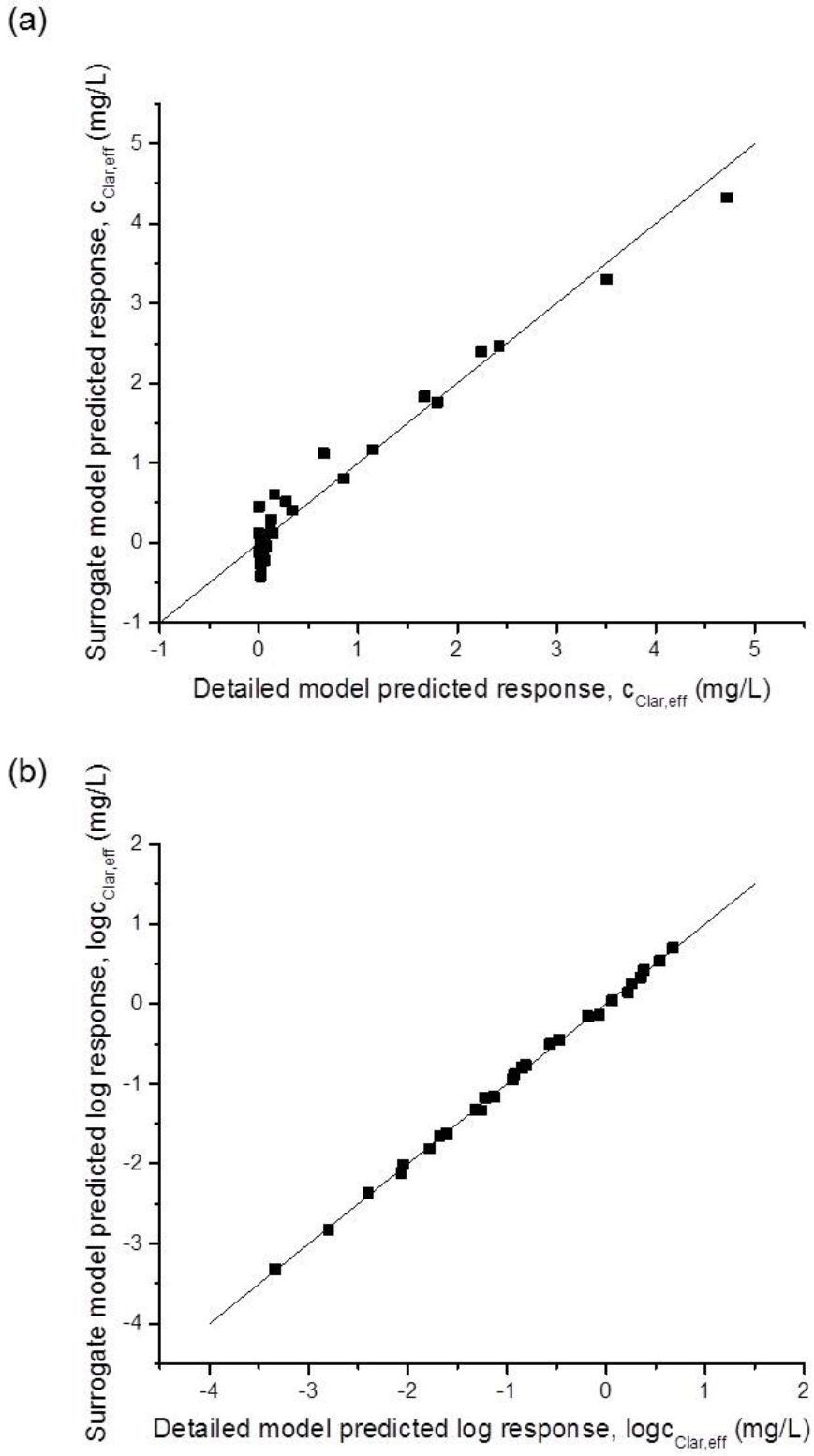


Figure 5.5: Sedimentation clarification: surrogate versus detailed modelling responses for effluent suspended solids concentration for a) normal model responses and b)"logged" model responses. The dashed line represent the x=y line on a parity plot.

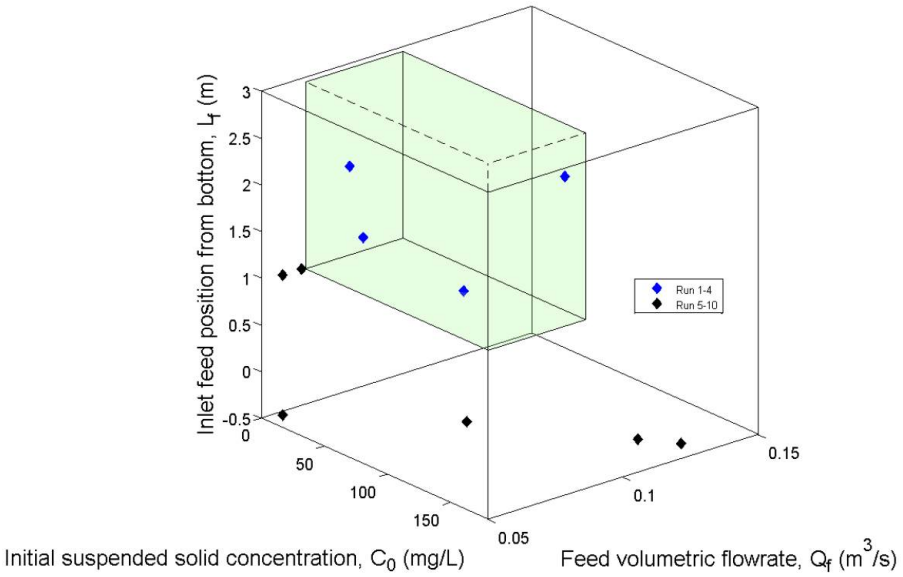


Figure 5.6: Clarification: 3D graphical domain representation of the ranges for the runs within the ranges (blue dots) and outside of the ranges (black dots) and the data used for verification in Tables 5.10 and 5.11.

desired range, Run 2 for the logged model presents a large error, for this run the feed volumetric flowrate is near the lower range (69 L/s) and this shows a limitation in the surrogate model's behaviour when the variables approach the lower boundaries. Within the clarification unit, the flowrate plays an important role as the speed can affect the settling behaviour within the unit (Takacs et al., 1991).

Ten different runs (four inside the range and six outside the range) are simulated with both the detailed and surrogate models to compare the effluent suspended solids concentration predicted. Figure 5.6 represents graphically the range in which the surrogate model will be fitted and Table 5.10 provides the data for the verification of the surrogate model. Inside of the prediction range, runs 1-4 generally show the "logged" surrogate model produces a small error when compared with the detailed model. The "logged" model also has a smaller error when compared with the "unlogged" model, especially between 0-0.5 mg/L where there responses cluster and are not part of the linear path. This could lead to an over or underestimation of the suspended solids concentration. The inaccuracy of the "unlogged" model is further exacerbated when observing the response values produced outside the prediction range. The six runs simulated (results shown in Table 5.10) for outside of the prediction range to see how the models will react when faced with a variety of variables both inside and outside of the desired ranges:

- Run 5: None of the variables are within the desired range,.
- Run 6: one variable (inlet feed position, L_f) is within the desired range whilst two variables (initial suspended solids concentration, c_0, and feed volumetric flowrate, Q_f) are outside of the range.
- Run 7: two variables (inlet feed position, L_f, and feed volumetric flowrate, Q_f) are within the desired range whilst one variable (initial suspended solids concentration, c_0) is outside of the range.
- Run 8: one variable (initial suspended solids concentration, c_0) is within the desired range whilst two variables (inlet feed position, L_f, and feed volumetric flowrate, Q_f) are outside of the range.
- Run 9: two variables (initial suspended solids concentration, c_0 and feed volumetric flowrate, Q_f) are within the desired range whilst one variable (inlet feed position, L_f) is outside of the range.
- Run 10: one variable (initial suspended solids concentration, c_0) is within the desired range whilst two variables (inlet feed position, L_f, and feed volumetric flowrate, Q_f) are outside of the range.

The responses produced by the "logged" model were able to more accurately predict within the desired range (maximum error 43% - run 2); however, for "unlogged" model, the responses predicted when operating near the lower boundaries of the variables up to 6796.8% error (run 3), presented large errors. The location of the inlet feed position is within the sludge blanket and this will drastically change the effluent suspended solids concentration. Within the desired range, the surrogate model over predicted the effluent suspended solids concentration whilst outside the desired range it was under predicted. The detailed model for the sedimentation unit describes the relationship between the variables as a single source feed mechanism to the clarifier (Burger et al., 2011; Torfs et al., 2015), where convective flux function, F, influences the movement of the suspended solids concentration. The surrogate model is unable to accurately predict the complexity of this phenomena when the initial suspended solids concentration, c_0 and feed volumetric flowrate, Q_f, are near their upper or lower boundaries.

Focusing on the surrogate model for the underflow suspended solids concentration, $C_{Clar,und}$, the R^2 coefficient for the "logged" and "unlogged" model are 99.9% and 99.6% respectively. Figure 5.7 presents the predicted response for the underflow suspended

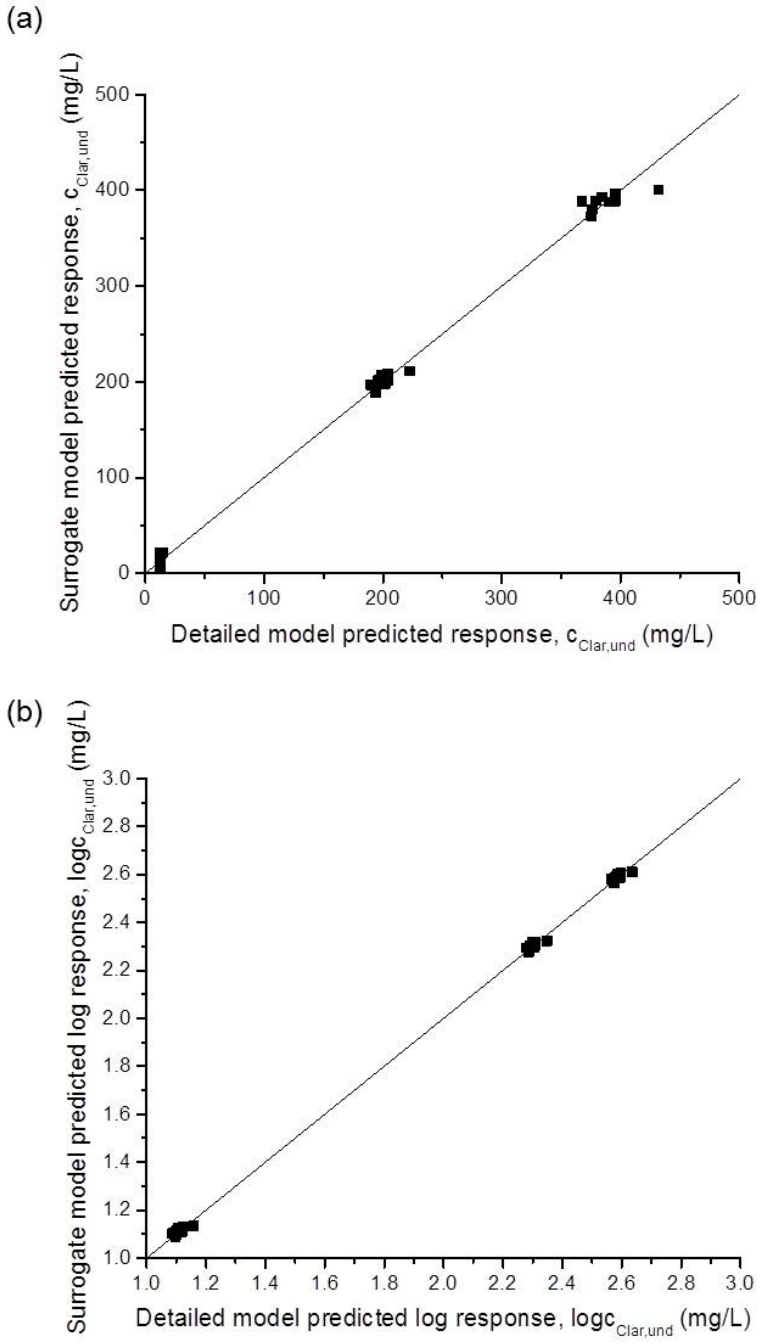


Figure 5.7: Sedimentation clarification: surrogate versus detailed modelling responses for underflow suspended solids concentration for a) normal model responses and b) "logged" model responses. The dashed line represent the x=y line on a parity plot.

Table 5.10: Verification of effluent suspended solids concentration derived from "logged" and "unlogged" surrogate model for clarification via sedimentation against the detailed model.

				Normal			LOG		
Run	c_0 (mg/L)	$\mathbf{Q}_f$ (m^3/s)	$\mathbf{L}_f$ (m)	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %
Inside prediction range ($5 \leq c_0 \leq 150$, $0.0064 \leq Q_f \leq 0.1$, **and** $1 \leq L_f \leq 3$)									
1	80	0.0875	1	0.48	0.55	13	-0.32	-0.33	2.58
2	40	0.069	1.5	0.058	-0.059	3.51	-1.24	-1.77	43.3
3	10	0.078	2	0.0024	0.17	6796.8	-2.61	-2.83	8.14
4	140	0.097	2.5	0.033	-0.145	338.7	-1.48	-1.64	10.4
Outside prediction range ($c_0 < 5$, $c_0 > 150$, $Q_f < 0.0064$, $Q_f > 0.1$, **and** $L_f < 1$, $L_f > 3$)									
5	4	0.056	-0.5	0.043	0.23	442	-1.37	-1.02	25.03
6	4	0.056	1	0.0046	-0.22	4624	-2.34	-2.21	5.48
7	4	0.063	1	0.0072	-0.27	3674	-2.14	-2.03	5.2
8	140	0.14	-0.75	5.92	9.42	59.2	0.77	0.82	6.72
9	120	0.07	0	2.09	2.11	0.91	0.32	0.39	20.8
10	170	0.11	-0.25	5.43	6.45	18.5	0.74	0.74	0.49

solids concentration using the surrogate model against the underflow suspended solids concentration determined by the detailed model. For both the "logged" and "unlogged" versions of the model, the surrogate models show a strong linear trend; however, the data points cluster up in three specific areas and this is associated with whether the initial suspended solids concentration has been given a low, centre or high numerical number. This is a reflection of industrial water treatment practices, as it is expected the underflow flow suspended solids concentration will have the highest concentration of suspended solids which is due for removal via a sludge collector (Jeppsson and Diehl, 1996; Ramin et al., 2014). The R^2 value suggests that although both models might provide accurate predictions. Moreover, the model fitted to "logged" data is more slightly accurate along the desired operating range (R^2_{log}= 99.9% and R^2_{unlog}= 99.6%).

Figure 5.7 show that the surrogate models are able to predict the phenomena from the detailed model. Figure 5.6 represents graphically the range in which the surrogate model will be fitted and Table 5.11 provides the data for the verification of the surrogate model. Inside of the prediction range, the four runs show that the "unlogged" surrogate model generally produces a smaller error when compared with the detailed model (run 1 - 3: 0.72% - 19.6%); when compared with the "logged" model there is a larger error (run 1 - 3: 0.35% - 13.8%). There is a large error predicted for run 4 for both the “logged” and “unlogged” model, the three variables c_0, Q_f and L_f are near the upper boundary

Table 5.11: Verification of underflow suspended solids concentration derived from "logged" and "unlogged" surrogate model for clarification via sedimentation against the detailed model.

				Normal			LOG		
Run	c_0 (mg/L)	$\mathbf{Q_f}$ (m^3/s)	$\mathbf{L_f}$ (m)	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %
Inside prediction range ($5 \leq c_0 \leq 150$, $0.0064 \leq Q_f \leq 0.1$, **and** $1 \leq L_f \leq 3$)									
1	80	0.0875	1	217	215.4	0.72	2.34	2.34	0.35
2	40	0.069	1.5	102	105.9	3.88	2	1.8	10.3
3	10	0.078	2	25	20	19.6	1.4	1.2	13.8
4	140	0.097	2.5	61	346.6	467.7	1.79	2.57	44
Outside prediction range ($c_0 < 5$, $c_0 > 150$, $Q_f < 0.0064$, $Q_f > 0.1$, **and** $L_f < 1$, $L_f > 3$)									
5	4	0.056	-0.5	9.9	1.32	86.7	0.99	1.07	7.4
6	4	0.056	1	10.2	19.4	89.9	1.01	1.1	9.28
7	4	0.063	1	10.3	18.5	80	1.01	1.1	8.9
8	140	0.14	-0.75	248.6	336	35.2	2.4	2.5	5.34
9	120	0.07	0	317	310.3	1.9	2.5	2.57	3.14
10	170	0.11	-0.25	352	435	23.7	2.51	2.5	2.5

within the desired range; however, Figure 5.7 shows the linear fit and predicted response will lay in an area that has no predicted points near it. This shows a limitation of this surrogate model.

With the R^2 value for the "logged" model being 99.9%, it can be interpreted as the "logged" model is a better fit; however, further investigation shows that it is not as accurate within the desired range. There are six runs simulated for outside of the prediction range (with the same values as explained for the model above) to see how both the detailed and surrogate models will react when faced with a variety of variables both inside and outside of the desired ranges. These six runs are in agreement the findings within the desired range and shows that the "unlogged" model is able to accurately predict the values when the initial suspended solid concentration and inlet volumetric flow rate are within the desired range.

5.4.2 Concluding remarks

The primary objective of this study is the development of surrogate models (from detailed models developed in Chapter 3), for the clarification unit, which are able to accurately predict the effluent suspended solids concentration. For the clarification via

sedimentation, two responses are predicted; the effluent suspended solids concentration, $c_{Clar,eff}$, and the underflow suspended solids concentration, $c_{Clar,und}$. The surrogate models can be used in either a "logged" or "unlogged" form and eventhough the R^2 coefficients were close for both alternatives, the numerical errors during the verification revealed which for was the best to use. For predicting the effluent suspended solids concentration, $c_{Clar,eff}$, there is a discrepancy between the R^2 coefficient for the "logged" and "unlogged" model with the "logged" data being closer to one, where R^2 of one indicates the regression line perfectly fits the data. As shown in Figure 5.7, the "logged" model has a stronger linear fit and from analysing the model sensitivities with the numerical values inside and outside of the desired ranges, it was reconfirmed that the "logged" model is the more accurate model to use as the absolute errors between the surrogate model prediction and the detailed model response was smaller. For predicting the underflow suspended solids concentration, $c_{Clar,und}$, the "logged" and "unlogged" model produced a similar R^2 values, despite the grouping of the responses into three distinct regions (low, centre and high). By logging the response of the detailed model, there is an increase in the models predictive capacity, due to the highly linear correlation and the predicted values fit very closely to the detailed model values. The surrogate model for predicting the underflow suspended solids concentration, $c_{Clar,und}$, will be the models based on "logged" data.

5.5 Filtration surrogate model

In Chapter 3, one detailed mathematical model is developed to represent the rapid gravity filtration process unit for the filtration processing step.

Rapid gravity filtration

In this section, a surrogate model will be developed which links three key variables to the effluent suspended solids concentration at the filtration breakthrough stage. This is affected by the initial suspended solids concentration, the filtration velocity and the depth of the unit. This model simplification allows for easier optimisation of the complete conventional clean water treatment process. Using Equation 5.2.2, the polynomial equation will take on the form:

$$c_{Fil} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 \quad (5.5.1)$$

where

c_{Fil}	effluent suspended solids concentration, (mg/L)
x_1	normalised initial suspended solids, (mg/L)
x_2	normalised filtration velocity (m/s)
x_3	normalised filter bed depth, (m)

The three factors, x_1, x_2 and $x_3$will be explored at three different levels (low, centre and high) with the goal of finding an average desirability range. By using Equation 5.2.5, the following will be used to determine the factors for each variable:

$$x_1 = \left[\frac{c_0 - c_{0_{centre}}}{c_{0_{centre}} - c_{0_{low}}} \right] \quad (5.5.2)$$

$$x_2 = \left[\frac{u - u_{centre}}{u_{centre} - u_{low}} \right] \quad (5.5.3)$$

$$x_3 = \left[\frac{L - L_{centre}}{L_{centre} - L_{low}} \right] \quad (5.5.4)$$

where

c_0	initial suspended solids, (mg/L)
u	filtration velocity (m/s)
L	filter bed depth, (m)

Utilising the methodology detailed in Section 5.2.2, 27 simulations are needed in order to have all combinations. Table 5.12 presents the typical ranges of operation that were considered to ensure the level of accuracy, and the justifications for the choices.

Once these variables are set values, the detailed models are simulated with the different combinations of variable values to obtain an effluent suspended solids concentration. Microsoft Excel is then utilised to develop the surrogate models from steps 2 to 7. Table 5.13 presents the numerical values for the least squares estimator, β, for the effluent suspended solids concentration leaving filtration unit. The regression equation developed for the "unlogged" and "logged" values of c_{Fil} are:

$$c_{fil} = 0.129 + 0.136 x_1 + 0.444 x_2 - 0.16 x_3 - 0.018 x_1^2 - 0.011 x_2^2 + 0.0948 x_3^2 + 0.0392 x_1 x_2 - 0.138 x_1 x_3 - 0.0297 x_2 x_3 \quad (5.5.5)$$

Table 5.12: Desirability curve ranges for filtration presented as coded and uncoded units of measurement for equations 5.5.2 to 5.5.4, along with justifications for the ranges considered.

	Coded factor level			
Variable	**Low (-1)**	**Centre (0)**	**High (1)**	**Justification**
Initial suspended solids, c_0 (mg/L)	0.5	3.25	6	The range 0.5 to 6 mg/L is considered for c_0 as the influent suspended solids concentration should be of high enough quality to extend the life of the filter bed.
Filtration velocity (m/s)	0.0014	0.0028	0.0042	Regulatory limits usually defines the maximum filtration rate. This is due to higher filtration rates leading to poorer removal efficiency. In the UK, 5 to 15m/h is commonly used (Parsons and Jefferson, 2006).
Filter bed depth, (m)	0.6	1.2	1.8	The values typically used in industry often varies from 0.6m to 1.8m. This excludes the additional height required for backwashing (Crittenden et al., 2012), which is not considered in this work.

Table 5.13: β parameters that have been determined to be utilised in the surrogate model equation for effluent concentration in filtration.

	c_{fil}	**Log**c_{fil}
β_0	0.13	-0.87
β_1	0.14	0.44
β_2	0.044	0.13
β_3	-0.16	-0.43
β_{11}	-0.018	-0.28
β_{22}	-0.011	-0.07
β_{33}	0.095	0.058
β_{12}	0.039	0.035
β_{13}	-0.14	-0.086
β_{23}	-0.029	0.039

$$\begin{aligned} logc_{fil} = \quad & -0.867 + 0.436x_1 + 0.132x_2 - 0.43x_3 - 0.284x_1^2 - 0.071x_2^2 \\ & +0.058x_3^2 + 0.0355x_1x_2 - 0.0857x_1x_3 + 0.0391x_2x_3 \end{aligned} \tag{5.5.6}$$

The validation and sensitivity analysis of the equations above to predict the effluent concentration, c_{Fil}, will be presented in Section 5.5.1.

5.5.1 Results and validation

In this section, the surrogate model developed for the rapid gravity filtration unit is verified and the response values are analysed. The R^2 shows the "logged" model has a better fit than the "logged" model with values of 99.7% and 96.8%, respectively.

Figure 5.8 presents the predicted response for the effluent suspended solids concentration using the surrogate model against the effluent suspended solids concentration determined by the detailed model. For both the "logged" and "unlogged" model, the surrogate model's predictive capacity seem to be a very good fit as shown by the graphs; however, the graph for the "logged" data is more linear. The R^2 value suggests that although both models might provide accurate predictions, the model fitted to "logged" data is more accurate as the "unlogged" data has a cluster of data points at the lower level of suspended solids concentration (as shown in Figure 5.8).

The models were verified with variable values inside and outside of the ranges considered in Table 5.12. Figure 5.9 represents graphically the range in which the surrogate model will be fitted. Table 5.14 provides the data for the verification of the surrogate model. Inside of the prediction range, the four runs show that generally the "logged" surrogate model predicts a smaller error when compared with the detailed model response and this is in agreement with the R^2 coefficient value that shows the "unlogged" data to have a weaker fit.

There are six runs simulated for outside of the prediction range to see how the models will react when faced with a variety of variables both inside and outside of the desired ranges:

- Run 5: None of the variables are within the desired range.
- Run 6: one variable (filter bed depth, L) is within the desired range whilst two variables (initial suspended solids concentration, c_0, and filtration velocity, u) are outside of the range.

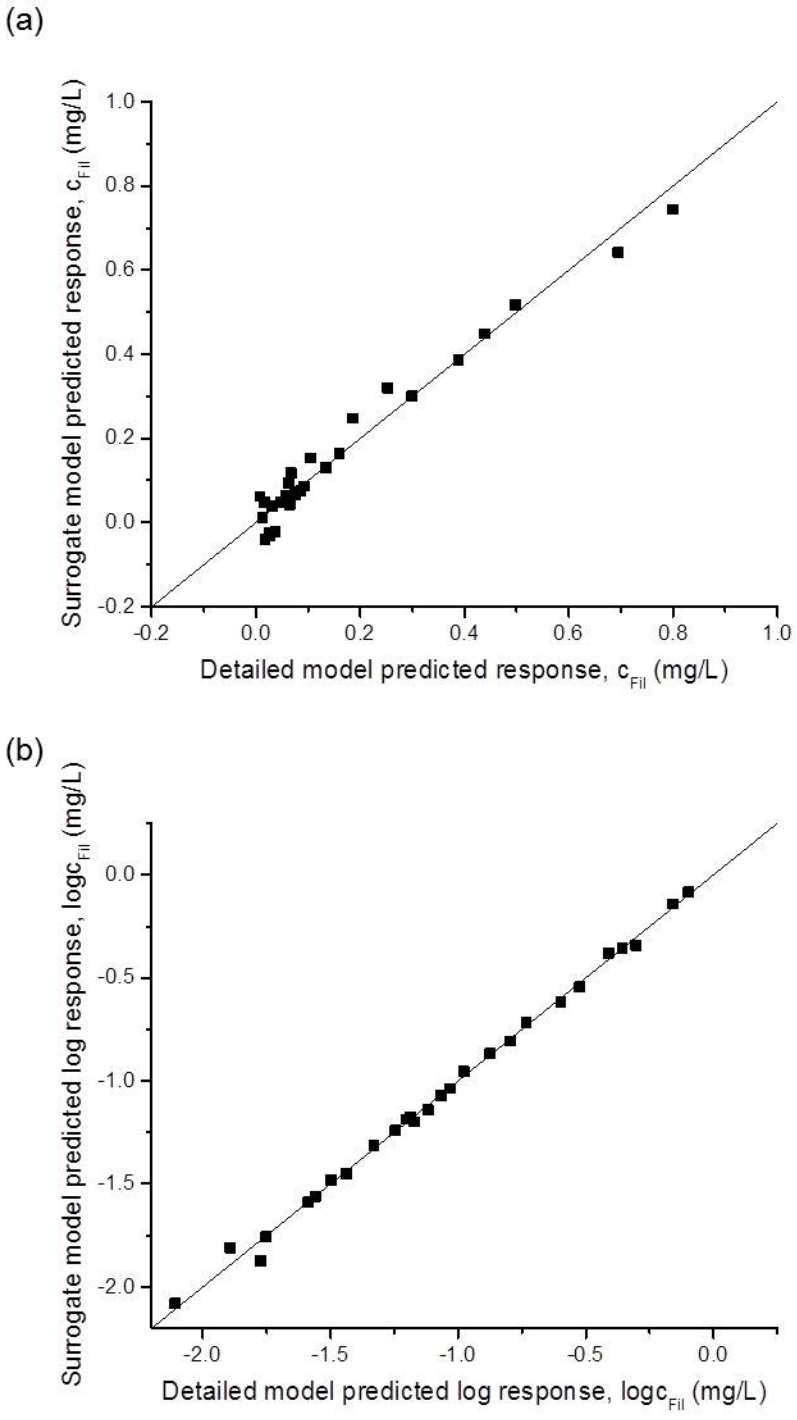


Figure 5.8: Filtration: surrogate versus detailed modelling responses for effluent suspended solids concentration for a) normal model responses and b) "logged" model responses. The dashed line represent the x=y line on a parity plot.

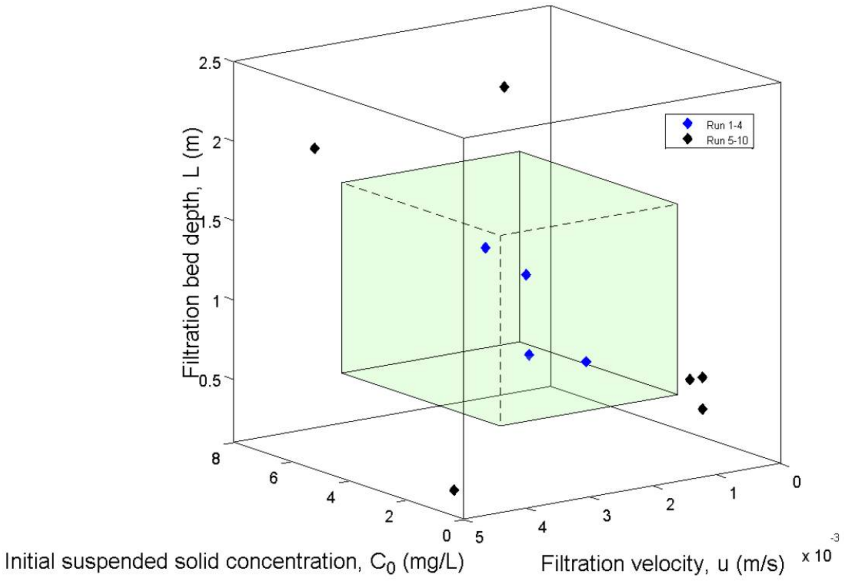


Figure 5.9: Filtration: 3D graphical domain representation of the ranges for the runs within the ranges (blue dots) and outside of the ranges (black dots) and the data used for verification in Table 5.14.

- Run 7: two variables (filter bed depth, L, and filtration velocity, u) are within the desired range whilst one variable (initial suspended solids concentration, c_0) is outside of the range.
- Run 8: None of the variables are within the desired range.
- Run 9: one variable (initial suspended solids concentration, c_0) is within the desired range whilst two variables (filtration velocity, u and filter bed depth, L) are outside of the range.
- Run 10: two variables (initial suspended solids concentration, c_0 and filtration velocity, u) are within the desired range whilst one variable (filter bed depth, L) is outside of the range.

This sensitivity study further shows that the "unlogged" model is not accurate enough and has a poor prediction of values inside and outside of the desired range. The "logged" model has a slight under prediction of the effluent suspended solids concentration and although these values are small, the filtration unit itself has very low effluent concentration so a small error is significant.

Table 5.14: Verification of effluent suspended solids concentration derived from "logged" and "unlogged" surrogate model for filtration via rapid gravity filtration against detailed models.

				Normal			LOG		
Run	c_0 (mg/L)	$\mathbf{Q}_f$ (m^3/s)	$\mathbf{L}_f$ (m)	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %	**Detailed** $c_{Floc,COM}$ (mg/L)	**Surrogate** $c_{Floc,COM}$ (mg/L)	**Error** %
Inside prediction range ($0.5 \leq c_0 \leq 6$, $0.0014 \leq u \leq 0.0042$, **and** $0.6 \leq L \leq 1.8$)									
1	0.6	0.0028	0.9	0.04	0.019	50.1	-1.39	-1.36	2.14
2	4	0.0022	1.2	0.13	0.14	6.19	-0.88	-0.84	4.16
3	2	0.00375	1.6	0.06	0.04	32.4	-1.23	-1.29	5.7
4	5	0.0017	0.6	0.44	0.47	6.2	-0.35	-0.31	-15.8
Outside prediction range ($c_0 < 0.5$, $c_0 > 6$, $u < 0.0014$, $u > 0.0042$, **and** $L < 0.6$, $L > 1.8$)									
5	0.3	0.0011	0.5	0.039	0.047	17.2	-1.39	-1.35	-3.48
6	0.3	0.0011	0.7	0.023	-0.009	62.1	-1.64	-1.52	7.46
7	0.3	0.0013	0.7	0.029	0.0016	94.7	-1.53	-1.47	3.44
8	6.5	0.0044	2	0.075	0.05	38.2	-1.13	-1.19	5.4
9	1	0.0047	0.2	0.23	0.29	27.2	-0.64	-0.9	40.3
10	3	0.003	2.5	0.03	0.24	816	-1.59	-1.5	4.26

5.5.2 Concluding remarks

The primary objective of this study in this section was the development of surrogate models for the filtration unit, which are able to accurately predict the effluent suspended solids concentration. The "logged" model provides the most accurate fit and is able to represent the mechanistic phenomena of breakthrough. Eventhough there is a slight fluctuation of over and under predicting the effluent suspended solid concentration errors are small, thus enabling the use of this model.

5.6 Disinfection surrogate model

Disinfection of clean water prior to release to customers is most commonly accomplished by the use of either chemical agents (such as chlorine and ozone) or physical agents (such as light and heat). In the literature, there are many empirical models available for a variety of disinfection models that can be utilised as simple surrogate models as described in Chapter 2. In this section, three disinfection processes: chlorine dioxide, ozonation and ultraviolet light (UV), will be explored. Chlorination is another common disinfection process but as it is ineffective in the inactivation of Cryptosporidium, and

is often used as part of a series of disinfection stages (Corona-Vasquez et al., 2002), it will not be studied here.

A number of researchers have used models to describe experimental disinfection data. The simplest disinfection model is a combined model proposed by Chick (1908) which was later extended by Watson (1908). This model is still used in current literature as the basis for disinfection models. The rate of inactivation is expressed as a first order reaction with respect to the concentration of microbes of a certain species surviving as a function of time at a constant level of disinfectant (Chick, 1908; Watson, 1908):

$$\frac{dc_m}{dt} = -kc_m \tag{5.6.1}$$

where

c_m concentration of organisms at any time after t = 0 (org/mL)
k rate constant (s^{-1})

Integrating Equation 5.6.1 gives:

$$ln\frac{c_m}{c_{m,0}} = -k\tau \tag{5.6.2}$$

where

$c_{m,0}$ concentration of organisms at time t = 0 (org/mL)
τ contact time (s^{-1})

which, in exponential form, is:

$$c_m = c_{m,0}\exp^{-k\tau} \tag{5.6.3}$$

The key assumptions for this model are shown in Table 5.15.

When the disinfectant is chlorine dioxide or ozone, then:

$$k = k_c D$$

where

k_c kinetic constant, coefficient of specific lethality for chlorine dioxide (L/mg,s)
D concentration of disinfectant (mg/L)

$$k = k_o D$$

Table 5.15: Assumptions and comments for the disinfection model development.

Assumption	**Justification**
Chick's law holds for ideal conditions.	All cells of a single species are equally susceptible to the disinfectants (Chick, 1908).
Contact tank may be modelled as a continuously stirred tank reactor.	Concentration of disinfectant and the water matrix remains constant through the contact period.
Cells and the disinfectant are uniformly dispersed in water.	The difference between the experimental lab scale predicted $D\tau$* value and the scaled up actual required $D\tau$* will only be affected by dispersion a little bit according to Crittenden et al. (2012).
3-log** (99.9% inactivation) are required for organism reduction.	Raw water sources for wastewater contains a large amount of bacteria whilse clean water treatment raw water sources contain considerably less. In practise, filtration removes majority of the organism (Crittenden et al., 2012), which is not modelled in this work as more data is needed.
No residual decay of disinfectant.	Constant disinfectant concentration is able to be maintained at lab scale.

*$D\tau$ is a parameter established by Chick (1908) and Watson (1908), where they provided a database of extensive values.

**Log inactivation is a convenient way to express the number or percentage of microorganisms inactivated (killed or unable to replicate) through the disinfection process.

where

k_o kinetic constant, coefficient of specific lethality for ozone (L/mg,s)

When the disinfectant is UV, then:

$$k = k_{UV} I$$

where

k_{UV} kinetic constant, a function of transmittance (cm^2/J,s)
I intensity of UV radiation (W/m^2)

To determine the kinetic constants, k_c, k_o, k_{UV}, for a given level of survival ($\frac{C_m}{C_{m,0}}$), where log removal/inactivation relates to the % removal/inactivation of microorganisms, such that:

- 1-log reduction = 9 out of 10 = 90% reduction

- 2-log reduction = 99 out of 100 = 99% reduction
- 3-log reduction = 999 out of 1,000 = 99.9% reduction
- 4-log reduction = 9,999 out of 10,000 = 99.99% reduction

Therefore rearranging Equation 5.6.2 and taking chlorine dioxide and a 1-log reduction as an example, then:

$$k_c = \frac{ln(0.1)}{D\tau} \tag{5.6.4}$$

when $D\tau$ is known (Chick, 1908; Watson, 1908).

Relationship between suspended solids concentration and microorganism concentration

Suspended solid particles form a great challenge for inactivating microorganisms. Suspended solids concentration is usually associated with the aesthetics of the water but there are some specific health concerns with the interaction between suspended solids concentration and microorganisms. Montgomery (1985) states that one of the specific health-related characteristics of suspended solids (turbidity) was the association of microorganisms with particulate material, with a resulting interference with disinfection. Particles affect the disinfection process in two distinct ways: 1) particles can react with the chemical disinfectant or can absorb the UV light, and 2) microorganisms can be embedded in the particles, shielding them from disinfection. Currently, there is limited information on effective methods for quantifying particle-associated microorganisms (Montgomery, 1985; Hendricks, 2006; Crittenden et al., 2012), and this brings much uncertainty into quantifying the impact of particle association on disinfection. Scheible (1987) modifies Equation 5.6.5 to account for suspended solid particles acting as an inactivation hindrance. The author proposed a sub-division of the entire microorganism load in water into two categories: microorganisms that are accessible, and can therefore be inactivated, and microorganisms associated with suspended particles and therefore not able to be inactivated easily. This subdivision of microorganisms into two groups led to the following expression of inactivation kinetics:

$$c_m = \left(c'_{m,0} + c_{m,p}\right) \exp\left(-k\tau\right) + c_{m,p} \tag{5.6.5}$$

where c'$_{m,0}$ is the initial concentration of microorganisms accessible per unit volume of water (org/mL) and $c_{m,p}$ is the concentration of microorganisms (associated with suspended solid particles) per unit volume of water to disinfection (org/mL).

Scheible (1987) also states that the value of $c'_{m,0}$ is larger than the value of $c_{m,p}$, so it can be assumed that the total initial microorganism concentration, $c_{m,0}$, is equal to $c'_{m,0}$ + $c_{m,p}$. Equation 5.6.5 can now be written as an improved version of Equation 5.6.3:

$$c_m = c_{m,0} \exp(-k\tau) + c_{m,p} \tag{5.6.6}$$

It can be seen from the equation that a residual concentration of microorganisms $c_{m,p}$ persist in water, whatever the amount of disinfection applied. The persistence of Giardia and Cryptosporidium is a concern because of the difficulty in inactivating these microorganisms and they are a particularly dangerous protozoa that can cause a non-treatable form of diarrhoea (Directive, 1998; World Health Organisation, 2011). By ensuring their removal, most other organisms may also be removed. The research work of LeChevallier and Norton (1992) examines the relationship between particle count and Giardia, Cryptosporidium and suspended solids concentration (turbidity).

LeChevallier and Norton (1992) develop a "logged" polynomial regression model for the determination of the residual number of microorganisms $c_{m,p}$ due to suspended solids concentration interference:

Giardia

$$\begin{array}{cc} logc_{m,p} = & 0.664(logc_{ss}) + 0.717 \\ linear\,regression & 0.879 \end{array} \tag{5.6.7}$$

Cryptosporidium

$$\begin{array}{cc} logc_{m,p} = & 0.66(logc_{ss}) + 0.488 \\ linear\,regression & 0.83 \end{array} \tag{5.6.8}$$

where

c_{ss} concentration of suspended solids in water (mg/L)

A number of case studies for Equation 5.6.6 will be conducted to evaluate these models. Since this equation is a simple empirical equation, there is no need to develop surrogate models as there is no additional computational advantage in doing so.

5.6.1 Results and validation

For the two following case studies, Table 5.16 presents the typical ranges of operation and the justifications for the choices.

Table 5.16: Parameters ranges for disinfection units considered.

Variable	Symbol	Disinfection	Range	Justification
Concentration of disinfectant	D (mg/L)	*Chlorine dioxide*	0.2 - 1.5	Typical ranges for the dosages (Crittenden et al., 2012)
		Ozone	1 - 5	
	I (W/cm^2)	*Ultraviolet light*	20-100	
Contact time	τ (s^{-1})	*Chlorine dioxide*	600 - 1800	Typical ranges for the contact time (LeChevallier and Au, 2004)
		Ozone	300 - 600	
		Ultraviolet light	120 - 600	

Table 5.17: Values used for disinfection model development in the inactivation of Giardia for 3-log inactivation (99.9%) (Environmental Protection Agency, 2003a).

Disinfectant	Dτ		k		Conditions
Chlorine dioxide	900	(mg/L,s)	0.00768	(L/mg,s)	T =20^oC, pH = 6 - 7
Ozone	43.2	(mg/L,s)	0.159	(L/mg,s)	T =20^oC, pH = 6 - 7
Ultraviolet light	2160	(W/cm^2,s)	0.00319	(cm^2/W,s)	

Giardia

In this section, the predicted microorganism inactivation of Giardia via chlorine dioxide, ozonation and ultraviolet light using Equation 5.6.6 is tested. In this model, the rate of inactivation of a microorganism is dependent on the concentration of the disinfectant and contact time. For this case study, it is assumed that the raw water entering this unit contains 10,000 org/L of microorganism, the suspended solids concentration is 0.05 mg/L and that a 3-log inactivation is sufficient to remove the Giardia oocysts (Edzwald, 2011) in order to meet the water quality regulations of negligible (zero) microogranisms should be present prior to distribution (World Health Organisation, 2011). Table 5.17 presents the values which will be used to determine the effluent microorganism concentration.

The empirical equations for the determination of the concentration of microorganims after disinfection c_m are:

For chlorine dioxide:

$$c_m = c_{m,0} exp^{-0.00768 D\tau} + exp^{0.664(logc_{ss})+0.717} \tag{5.6.9}$$

For ozone:

$$c_m = c_{m,0} exp^{-0.159 D\tau} + exp^{0.664(logc_{ss})+0.717} \tag{5.6.10}$$

For ultraviolet light:

$$c_m = c_{m,0} exp^{-0.00319 I\tau} + exp^{0.664(logc_{ss})+0.717} \tag{5.6.11}$$

In the regression models, coded variables are used of three levels: low, centre and high which corresponds to specific numerical values from the ranges shown in Table 5.16 and graphically in Figure 5.10. Table 5.18 provides the responses when comparing all the possible combinations. Equation 5.6.6 includes the concentration of microorganisms associated with suspended solid particles, $c_{m,p}$. For clarity in the inactivation power of the different disinfectants, the responses reported in the table for concentration of microorganisms after disinfection c_m are presented without the addition of $c_{m,p}$, which is calculated to be 0.28 mg/L. Table 5.18 also shows the concentration of microorganisms after disinfection c_m for chlorine dioxide, ozone and UV disinfectants.

The values of c_m show that for the disinfection of Giardia, ozone is the most efficient at the inactivation of the microorganism and chlorine dioxide is the least efficient; this is consistent with experimental findings in the literature (Crittenden et al., 2012). Within the disinfectant concentration and contact time ranges for the three different options, it can be seen that using chlorine dioxide for the inactivation of Giardia requires the highest dose (1.5 mg/L) and contact time (1800 s^{-1}) is needed to obtain a c_m within the required purity regulation (World Health Organisation, 2011). The smallest contact time (600 s^{-1}) for chlorine dioxide has a big effect on the inactivation as it can be seen in the table, for the three doses (0.2 mg/L, 0.85 mg/L and 1.5 mg/L) with this contact time, that the microorganism concentration will never meet the required purity standards. The lowest value given for chlorine dioxide is 1×10^{-5} org/mL; even though this is a small number, it is still quite a larger amount of Giardia oocysts left meaning that chlorine dioxide might not be suitable for this inactivation. Disinfection with ozone follows a similar trend to the chlorine dioxide where the higher dose concentration and contact time result in higher inactivation thus, demonstrating that an optimal performance criteria can be determined when taking the desired ranges into account.

The predicted inactivation by ultraviolet light is more promising as, even though the largest inactivation occurred with the highest dose concentration and contact time, Runs 6 and 8 c_m predictions are same value for different doses and contact time. Taking this into account, reveals that for a dose of 60 W/cm^2 and a contact time of 600 s^{-1} or

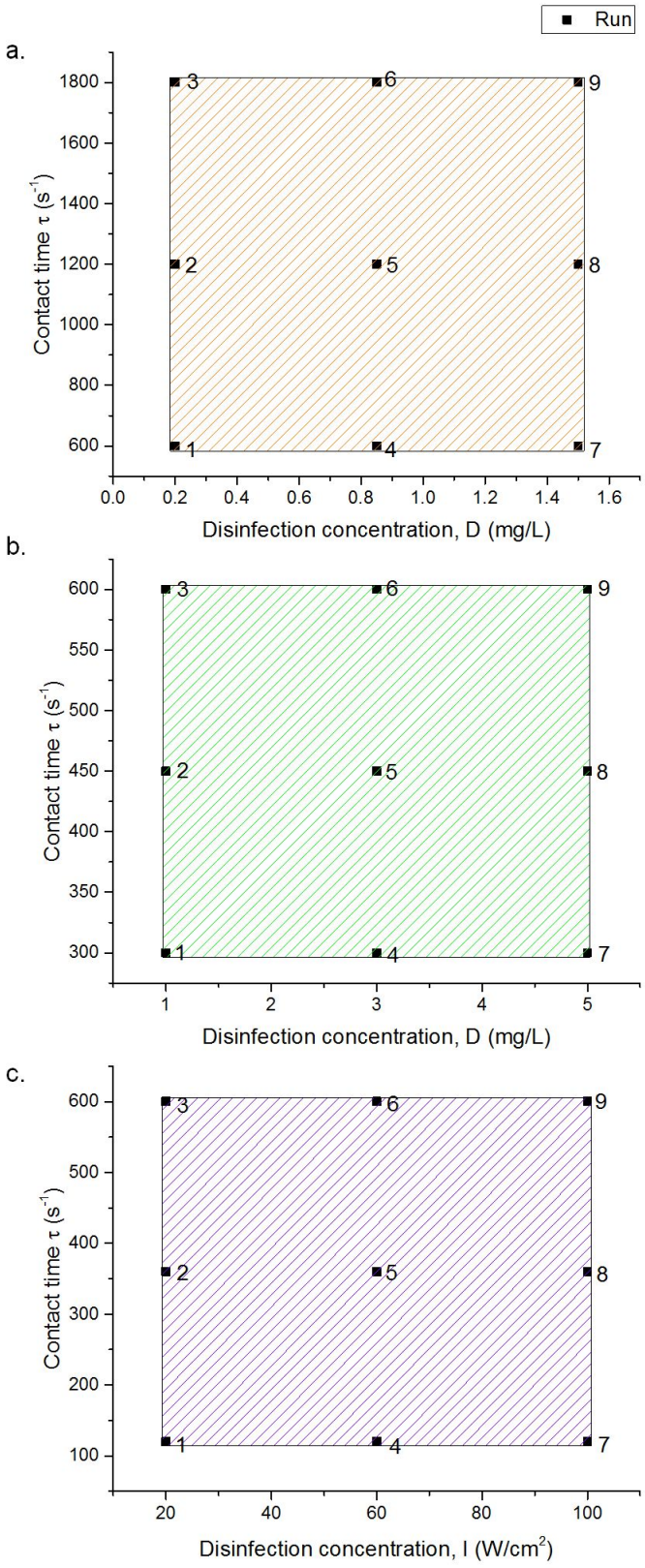


Figure 5.10: Disinfection: 2D graphical domain representation of the ranges for the runs and the data used for verification in Table 5.18 , where represented in a) chlorine dioxide range b) ozone range and c) ultraviolet light range.

Table 5.18: Model test results in the prediction of effluent microorganism concentration from Equations 5.6.9, 5.6.10, and 5.6.11 for inactivation of Giardia via disinfection using chlorine dioxide, ozone and ultraviolet light.

Chlorine Dioxide

Run	**Disinfection Concentration, D (mg/L)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	0.2	600	3981.1
2	0.2	1200	1584.9
3	0.2	1800	630.9
4	0.85	600	199.5
5	0.85	1200	3.98
6	0.85	1800	0.079
7	1.5	600	10
8	1.5	1200	0.01
9	1.5	1800	1×10^{-5}

Ozone

Run	**Disinfection Concentration, D (mg/L)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	1	300	1.47×10^{-17}
2	1	450	5.62×10^{-28}
3	1	600	2.15×10^{-38}
4	3	300	3.16×10^{-59}
5	3	450	1.78×10^{-90}
6	3	600	1×10^{-121}
7	5	300	6.81×10^{-101}
8	5	450	5.62×10^{-153}
9	5	600	4.64×10^{-205}

Ultraviolet light

Run	**Disinfection Concentration, I (W/cm^2)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	20	120	4.64
2	20	360	1×10^{-6}
3	20	600	2.15×10^{-13}
4	60	120	1×10^{-6}
5	60	360	1×10^{-26}
6	60	600	1×10^{-46}
7	100	120	2.15×10^{-13}
8	100	360	1×10^{-46}
9	100	600	4.64×10^{-80}

Please note: the small values are here for comparison purposes, in reality they are not measurable and will equal zero as the standard requires (World Health Organisation, 2011).

a dose of 100 W/cm^2 and a contact time of 360 s^{-1} will give a effluent microorganism concentration of 1×10^{-46} (negligible) so a cost trade off can be conducted to determine, which variable can be manipulated to find an optimal performance criteria.

Cryptosporidium

In this section, the predicted microorganism inactivation of Cryptosporidium via chlorine dioxide, ozonation and ultraviolet light using Equation 5.6.6 is tested. In this model, the rate of inactivation of a microorganism is dependent upon the concentration of the disinfectant and contact time. For this case study, it is assumed that the raw water entering this unit contains 10,000 org/L of microorganism, the suspended solids concentration is 0.05 mg/L and that a 2-log inactivation is sufficient enough to remove the Cryptosporidium oocysts (Edzwald, 2011) in order to meet the water quality regulations of negligible (zero) microorganisms should be present prior to distribution (World Health Organisation, 2011). Table 5.19 presents the values which will be used to determine the effluent microorganism concentration. The empirical equation for the determination of the concentration of microorganism after disinfection c_m are:

For chlorine dioxide:

$$c_m = c_{m,0} exp^{-3.29e^{-5}D\tau} + exp^{0.66(logc_{ss})+0.488} \tag{5.6.12}$$

For ozone:

$$c_m = c_{m,0} exp^{-0.00984D\tau} + exp^{0.66(logc_{ss})+0.488} \tag{5.6.13}$$

For ultraviolet light:

$$c_m = c_{m,0} exp^{-0.00794I\tau} + exp^{0.66(logc_{ss})+0.488} \tag{5.6.14}$$

In the regression models, coded variables are used of three levels: low, centre and high which corresponds to specific numerical values from the ranges shown in Table 5.16 and graphically in Figure 5.10. Table 5.20 provides the responses when comparing all the possible combinations. In line with the same reasoning as earlier, for clarity in the inactivation power of the different disinfectants, the responses reported in the table for concentration of microorganisms after disinfection c_m are presented without the addition of $c_{m,p}$, which is calculated to be 0.28 mg/L.

Table 5.19: Values used for disinfection model development in the inactivation of Cryptosporidium for 2-log inactivation (99%) (Environmental Protection Agency, 2003b).

Disinfectant	**Dτ**		**k**		**Conditions**
Chlorine dioxide	139,920	(mg/L,s)	$3.29e^{-5}$	(L/mg,s)	T =20^oC, pH = 6 - 7
Ozone	468	(mg/L,s	0.00984	(L/mg,s)	T =20^oC, pH = 6 - 7
Ultraviolet light	10	(W/cm^2,s)	0.794	(cm^2/W,s)	

Table 5.20 shows that chlorine dioxide is ineffective in the inactivation of the Cryptosporidium oocysts, and Binnie and Kimber (2009) suggest use of chlorine dioxide as a disinfectant may be considered in a series of disinfection processes as one of the steps. Disinfection with ozone shows it is able to inactivate a large portion of the Cryptosporidium with the higher dose (5 mg/L) and contact time (500 s^{-1}). However, the effluent microorganism predicted is still larger than the predicted concentration using ultraviolet light at a low dose (20 W/cm^2) and medium contact time (360 s^{-1}). UV is the most efficient at the inactivation of the microorganism and once again chlorine dioxide is the least efficient. This is consistent with experimental findings in the literature (World Health Organisation, 2011; Crittenden et al., 2012; Binnie and Kimber, 2009). The inactivation by ultraviolet light shows the same correlation with the Giardia microorganism concentration, in c_m predictions for Runs 6 and 8 have the same value for different doses (60 W/cm^2 and 100 W/cm^2) and contact time (600 s^{-1} and 360 s^{-1}, respectively). This gives some scope for optimisation around the variables in order to find an optimal performance criteria.

5.6.2 Concluding remarks

The primary objective of this study was the utilisation of an improved Chick-Watson empirical model (Equation 5.6.6) that can predict the effluent microorganism concentration after disinfection. This equation takes into account the concentration of microorganisms that will be affected by the presence of suspended solids concentration that remain in water. Testing the three different disinfection empirical models within the desired ranges for the inactivation of Giardia revealed that both ozone and ultraviolet disinfection can be utilised to successfully disinfect the Giardia oocysts. Ozone is the best form of disinfection whilst chlorine dioxide is not adequate to be used for this microorganism but could possibly be used as a primary disinfection treatment followed by a secondary disinfection treatment. For the testing of Cryptosporidium, the

Table 5.20: Model test results in the prediction of effluent microorganism concentration from Equations 5.6.12, 5.6.13 and 5.6.14 for inactivation of Cryptosporidium via disinfection using chlorine dioxide, ozone and ultraviolet light.

Chlorine Dioxide

run	**Disinfection Concentration, D (mg/L)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	0.2	600	9960.6
2	0.2	1200	9921.3
3	0.2	1800	9882.2
4	0.85	600	9833.5
5	0.85	1200	9669.9
6	0.85	1800	9508.9
7	1.5	600	9708.1
8	1.5	1200	9424.8
9	1.5	1800	9149.7

Ozone

run	**Disinfection Concentration, D (mg/L)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	1	300	522.3
2	1	450	119.4
3	1	600	27.3
4	3	300	1.42
5	3	450	0.017
6	3	600	2.03×10^{-4}
7	5	300	3.89×10^{-3}
8	5	450	2.42×10^{-6}
9	5	600	1.5×10^{-9}

Ultraviolet light

run	**Disinfection Concentration, I (W/cm^2)**	**Contact time, τ (s^{-1})**	**c_m (org/L)**
1	20	120	1×10^{-4}
2	20	360	1×10^{-20}
3	20	600	1×10^{-36}
4	60	120	1×10^{-20}
5	60	360	1×10^{-68}
6	60	600	1×10^{-116}
7	100	120	1×10^{-36}
8	100	360	1×10^{-116}
9	100	600	1×10^{-196}

Please note: the small values are here for comparison purposes, in reality they are not measurable and will equal zero as the standard requires (World Health Organisation, 2011)),

same trend was shown where both ozone and ultraviolet disinfection can be utilised for successful inactivation. Ultraviolet light is the best form of disinfection whilst chlorine dioxide will not be able to work alone and if used, and again will have to be in a series of disinfection treatment.

5.7 Conclusion

Due to the complex nature of drinking water treatment unit processes, the process models, where they exist, are often site specific. The use of detailed dynamic models can be computationally expensive and provide more information than necessary for industrial purposes, such as for overall plant design. Simple surrogate models that encapsulate the physical phenomena occurring, and which can provide a similarly accurate response, are of great benefit to the water industry. In this chapter, surrogate models have been developed for all the alternative processing units of operation discussed in Chapter 3.

The use of polynomial regression to determine multi-variable polynomial regression equations used in this study proved to be an extremely valuable tool to analyse data obtained from detailed mathematical models for the clean water treatment processes where the characteristics of the water are constantly changing. Following the methodology described in Section 5.2.2 for the detailed models, surrogate models for two coagulation/flocculation units (rapid mixing and flocculation in compartments), a clarification (sedimentation) and filtration (rapid gravity filtration) units were successfully developed. The results showed that the surrogate models, used in their logarithmic transformation form enabled visualisation of the data and the percentage errors, when comparing with the detailed models. The log transformation is a widely used method to address skewed data.

Three disinfection units, chlorine dioxide, ozonation and ultraviolet light, were considered for the inactivation of Giardia and Cryptosporidium. These two protozoa are particularly difficult to inactive in water (World Health Organisation, 2011), and thus, ensuring their removal means most other organisms are removed. Simple empirical equations exist in literature (Chick, 1908; Watson, 1908) and these have been improved to include a correlation incorporating suspended solids concentration interference (LeChevallier and Norton, 1992) as this has a minor affect on the microorganism inactivation but should not be ignored when designing the disinfection section. The closeness of the data points to the x=y lines on the parity plot reinforces the accuracy of the developed surrogate models and the utilisation of the three level factorial design.

Chapter 6

Conclusions and recommendations

The primary aim of this thesis is to draw upon previous work in the literature to develop a first principles mathematical model of an entire conventional clean water treatment work. The thesis contains four distinct contributions. The key outcome of the work is that there are significant advantages to be gained by the used of detailed and surrogate mathematical models of the complete conventional clean water treatment works in industry. The recommendations for future work is to incorporate enterprise wide modelling, which would bring together the various modelling tools and expert guidance to enable industrial users to quickly and efficiently implement the available models within industrial constraints in order to shift from a reactive industry to a more proactive one. The key areas discussed that need addressing are related to the use of simulation tools in clean water treatment, model calibration and broader recommendations.

6.1 Review of project deliverables

The overall aim of this thesis was to derive fundamental process understanding of conventional clean water treatment works, when evaluated as an entire process. The goal was to add to the development of detailed modelling and analysis of the dynamics of clean water treatment works as a whole, whilst providing a detailed review of the current state-of-art and utilising processing systems engineering tools.

6.1.1 Critical assessment of the current state-of art

Traditionally, the water industry has been sitting within the civil engineering domain rather than the chemical engineering domain as the civil engineers took the lead role in the design of the plants, e.g. creating the layout of the entire system based on traditional processing units. Due to the increasing pressure for companies to remain competitive in the national or global marketplace, the search for efficient methodologies for operational management and mitigation of risk has led some to consider the use of Process Systems Engineering (PSE) methods found in the chemical engineering domain, in particular, detailed modelling from first principles and optimisation based on rigorous optimisation algorithms, which have been highly successful within the chemical industries.

In Chapter 2, the current state-of-art of mathematical modelling in the clean water treatment industry is assessed, by focusing on detailed mathematical models and optimisation techniques. The review shows that process engineering plays a major role, in not only modelling of the system processes; but also increasing the fundamental understanding of the phenomena occurring. An integrated approach to modelling and optimisation has been found in literature to provide a competitive advantage (Larsson and Skogestad, 2000; Shah, 2005; Charpentier, 2005; Grossmann, 2005; Varma et al., 2007). An integrated approach can also be a driving force for operational level optimisation based on explicit objectives in the development of novel designs. The developed models can incorporate water quality data to predict the changes in process parameters by preceding processing steps or how this change influences subsequent processing steps. Chapter 2 provides a critical analysis of current work, which shows that an understanding of the phenomena of process units will lead to developed understanding for better process design.

6.1.2 Dynamic modelling of conventional clean water treatment work

Simulation is a useful tool and Chapter 3 focused on the use of numerical simulation for the dynamic modelling of unit processes in clean water treatment works. Chapter 3 examined mathematical models of the most common physical water treatment processes, namely coagulation/flocculation, clarification, and filtration units, available in the current literature. The models considered the key factors that affected the effluent suspended solids concentration for each unit. Via a sensitivity analysis, each individual

unit was examined and limitations were tested. The results implied that the models derived were in good agreement with the literature and could predict successfully predict propagation of change.

There are a few limitations with the implementation of the models developed. Firstly, ideal conditions are often assumed which will have an effect on the predicted concentration once the units have been combined to make a complete water treatment model. The individual unit will behaviour in an ideal manner when a change is proposed meaning the propagation will have limitations. Secondly, due to the nature of the process models, empirical parameters are needed for accurate simulation of a process on a specific site, which requires experiments or historical data to find empirical relationships. Thirdly, since the existing work on dynamic modelling of water treatment processes considers these as separate units, there is therefore a lack of a complete understanding as to how these models fit together into a model of a complete water treatment plant. The knowledge and understanding from considering the models of the individual units was used to direct the efforts in the formulation of a robust complete water treatment plant model.

In Chapter 4, the individual water treatment models were combined and it was demonstrated that the models are able to predict the expected response to propagating changes. Three different scenarios were presented with three alternative clean water treatment configurations. When a change was imposed, there was successful suspended solids concentration propagation through the clean water treatment simulation. The modelling approach based on first principles was found to be useful for: (1) increasing the understanding of the process by providing a more informative method for exploring how different processing units are affected by sequential event, and (2) allowing for a variety of scenarios to be tested out, which can enhance process management such as the process design stage, depending on the raw water source available. For a model like this to be fully utilised it needs to be operator friendly and currently the detailed mathematical models require knowledge on process systems engineering. By using detailed modelling (especially gPROMS utilised in this work), an advantage gained is that operation and variations in time can be evaluated in the design; however, the calculation times will be longer than with simpler surrogate models.

6.1.3 Surrogate model development of clean water treatment work

Without knowledge of advanced simulation tools or having a background in process modelling, the detailed models developed in this work would not be fully utilised if implemented in the water industry, if utilised at all. These complex models use fundamental knowledge and are only concerned with the phenomena occurring within the individual units. Linking these dynamic models together increases the complexity, which results in detailed integrated models which may be difficult to calibrate on a water treatment plant and also potentially difficult to solve. The idea of simpler surrogate models, that can be used to predict the effluent suspended solids concentration given a number of independent variables, would therefore be of greater value. In Chapter 5, response surface modelling of the effluent suspended solids concentration is implemented via regression analysis using least squares methods. The developed models are second order polynomials as it has been demonstrated that this order is sufficient to reflect the data as the phenomena occurring within the units are represented by the surrogate models. The models have been developed using the same methodology, where both the "logged[1] " and "unlogged" data are validated against the detailed dynamic models. The values are provided as both "unlogged" and "logged" due to a log scale making it easy to compare values that cover a large range. The results imply that the log form of the models is the most accurate and provide the best fit with the R^2 coefficient being close to 1. The transformation of the polynomial surface response for the product purity (in this case the suspended solids concentration) results in simpler surrogate models which are easier to use for optimisation purposes.

6.1.4 Concluding remarks

From the work presented in this thesis, the mathematical modelling and programming techniques employed can be widely applied in the advancement of the water industry. The mathematical modelling approaches have successfully dealt with the integration of complete water treatment models and provided a proof of concept in the application of superstructure optimisation techniques.

The surrogate model approach to plant wide superstructure optimisation used in this work involves four major steps. The preliminary steps (conducted in Chapter 3)

[1]For ease of interpretation, the logarithmic transformation of models in the text are referred to as *"logged"* and the regular model notation is referred to as *"unlogged"*.

involved development of the detailed mathematical models for the clean water treatment units. The detailed models once combined needed to be tested for robustness and sensitivity towards plant wide modelling, in Chapter 4. Finally, once these models were constructed, the next step involved choosing the surrogate modelling methodology and the form of the approximate models (conducted in Chapter 5).

The work in this thesis, which not only has developed some novel approaches to literature problems but also, considered some problems that have not been investigated before, is a complement to the literature research work on modelling in the clean water industry.

6.2 Direction for future research

This thesis shows that there are valuable advantages to be gained from the use of detailed mathematical models of the conventional clean water treatment works in industry. However, there are still areas of weakness that need to be addressed before models can be fully integrated in industrial practise. There are still several research directions that could be considered for future work as the extension of the current study and in the following section, potential directions for future work related to use of detailed and surrogate models in industry are discussed.

6.2.1 Use of numerical simulation tools in drinking water treatment

Model enhancement

As mentioned in Chapter 1, the overall aim of this work is to model a complete conventional clean water treatment work in order to predict situational changes that may propagate through the system. Since the focus of this project has been the main physical water treatment processes, a clear direction would be to include chemical processing steps, such as the chemical coagulant dosing stage before the flocculation unit.

The current complete water treatment model presented in this work is simplified by assumptions and does not take into pH parameters important to maintaining a high

water quality that may vary depending on each process unit. The level of assumptions will need to be adjusted through the development of the individual plant units. Parameters, such as temperature and pH, have a significant effect on the treatment process and final water quality; however, more research is needed on how these parameters can affect a deterministic model as current literature focusses on empirical models which are site specific.

In Chapter 2, it was highlighted that, in the absence of satisfactory means for determining the number concentration, particle mass concentration is often substituted for number concentration. In some studies (Edzwald and Van Benschoten, 1990; Hannouche et al., 2011), a linear relation between suspended solids concentration and turbidity is assumed and suspended solids concentration is replaced by the easy-to-measure turbidity; however, with the development of a direct correlation based on fundamental knowledge then the validity of the suspended solids concentration will be strengthened. The models developed are in terms of concentration and data given is in terms of turbidity, so for validation purposes either verified correlations presented in literature will be used to validate this assumption or experiments calculating the mass of the settled particles and the turbidity measured to generate a correlation will be used.

Plant-wide surrogate modelling

Although the models created in this study are fairly detailed, they do not approach the full scale of industrial models. The applicability of the surrogate model approach to industrial-scale models can only be predicted in this study. To better determine the benefits of the surrogate model approach for an industrial-scale clean water treatment model, more detail must be added to the detailed plant model. Presented in this work, is the development of individual surrogate models connected to make an overall plant model for optimisation purposes. An interesting direction for this work would be the development of a complete plant wide surrogate model in order to compare against a detailed model. If data is provided, this can also be compared with plant data.

Another direction would be to extend the surrogate model. The approximate models used in this work were formulated using detailed models. Several other modelling methodologies and approximate model types could be used in the surrogate model approach. In this study, no attempt is made to compare these options. Although some other modelling methodologies and approximate model types were discussed in this study, a detailed comparison was not performed. More studies on the application of these different modelling methodologies and approximate model types could give an indication of which options provide the best results for large-scale optimisation.

6.2.2 Plant optimisation

For many years, process optimisation has been used extensively in traditional chemical engineering sectors such as oil and gas, and is a proven approach for gaining maximum value out of a process (Grossmann and Biegler, 2004). With the increase in alternative processes readily available for water treatment plants, the selection of the treatment processes, which is a combination of unit operations, is a task that has not only increased the importance of early stage decision making, but also increased the complexity in a company's ability to remain competitive with increasingly stringent water quality regulations. With the increase in alternative processing steps readily available for clean water treatment plants, the selection of the individual treatment processes for each processing step is a task that has not only increased the importance of early stage decision making, but will also increase the plant's ability to remain competitive with the increasingly stringent water quality regulations.

Superstructure optimisation of clean water treatment work

A plant-wide approach, using surrogate models, for performance optimisation will be of significant benefit to the water industry as a means to increase the overall process efficiency and thus decrease plant costs. Many criteria have to be met for cost effectiveness, while always meeting stringent purity specifications. Particularly challenging in this context is the optimum selection of a process sequence from available clean water treatment steps.

By considering the plant as a whole, the interactions between individual processing units can be taken into account and properly balanced. A design and operating procedure that simultaneously considers series of several unit operations, including units which may run in parallel, and aims to reduce the number of processing steps required to achieve a given product quality, will therefore improve the overall plant efficiency. Recently, there have been some contributions in plant-wide water and desalination (as drinking water) treatment superstructures (Dharmappa et al., 1994; Khezri et al., 2011; Khor et al., 2014; Koleva et al., 2016) where non-linear programming (NLP) or mixed integer non-linear programming (MINLP) were studied to find a cost objective function. Presented in Figure 6.1 is a general superstructure for the synthesis of of treatment processes for clean water treatment works; it consists of four main stages, with some containing different alternative treatment techniques: coagulation/flocculation, clarification, filtration and disinfection.

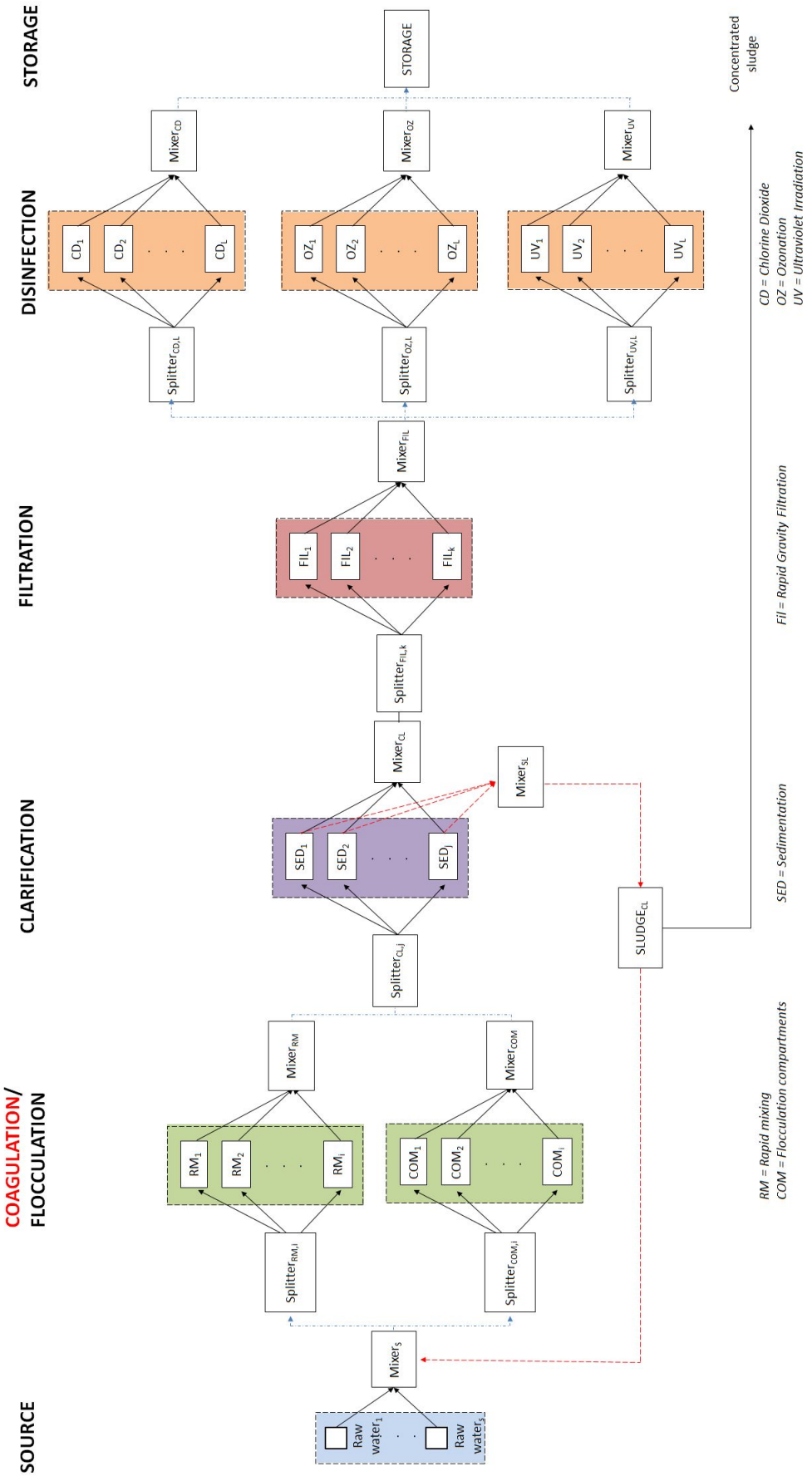


Figure 6.1: Example of a clean water treatment superstructure.

As shown in Figure 6.1, the superstructure begins with a choice of raw water (Raw water$_s$); this can be a mixture of pipelines sourced directly from groundwater, surface water or from a reservoir. These pipelines are mixed (mixer$_s$) before the first technology selection needs to be made. There are two alternative coagulation/flocculation technologies available for selection, which are the rapid mixing unit (RM$_i$) and a series of flocculation compartments occurring in parallel (COM$_i$). As only one of these units can be selected, the splitters prior to these units (splitter$_{RM,i}$ and splitter$_{COM,i}$) are a binary selection where i denotes the number of parallel processing units for a chosen path. The mixer (mixer$_{RM}$ or mixer$_{COM}$) is selected based on if the corresponding splitter has been chosen, indicating that the path is active.

The mixer (mixer$_{RM}$ or mixer$_{COM}$) connects to a splitter (splitter$_{CL,j}$) which splits the pipeline effluent into the number of determined clarification units. The clarification processing step only incorporates one technology - sedimentation - which (as mentioned in Chapter 3) is solely considered due to the current limitations in predictive mathematical models for dissolved air flotation units. There are two outlets from the sedimentation unit: the clarified effluent water goes to the mixer$_{CL}$ and the underflow sludge pipeline goes to mixer$_{SL}$. The red dotted line shows a sludge recycle stream that leaves from the sedimentation unit (Sed$_j$), enters a sludge settling unit (sludge$_{CL}$) before the effluent is recycled to mix with the raw water (mixer$_s$).

The mixer (mixer$_{CL}$) connects with (splitter$_{FIL,k}$) and the number of filtration units are denoted by k. Rapid gravity filtration is the most commonly used filtration unit for clean water treatment (Hendricks, 2006; Crittenden et al., 2012) and is used as the only technological option for the processing step. The total effluent from the filtration units (Fil$_k$) are mixed before the final technology selection is made. The disinfection processing step has three alternative technologies: chlorine dioxide, ozone and ultraviolet radiation. A binary variable is used for the selection of pre-splitter (splitter$_{CD}$ or splitter$_{OZ}$ or splitter$_{UV}$) and post mixing units (mixer$_{CD}$ or mixer$_{OZ}$ or mixer$_{UV}$). Once the optimal path has been selected, the water will be collected in the storage unit before distribution.

The splitters and mixers present in the figure represent pipelines that would actually be present on the industrial plant, but for modelling purposes, they are presented as splitters and mixers. The selection of all these technologies are the most commonly used alternative processing steps in the UK (Crittenden et al., 2012) and the processing step is often selected due to varying factors, such as raw water available in the location and the intended use of the treated water.

To utilise this proposed superstructure, the clean water treatment work optimisation problem can be formulated as a mixed integer non-linear programming (MINLP) problem, where the selection of separation techniques and their configuration is made through discrete decisions, expressed by binary variables, and the selection of process variables, e.g. flowrates and suspended solids concentrations, by continuous decisions.

6.2.3 Model calibration

Experimental validation

In this thesis, data from literature was used to validate the mathematical models developed. The ideal methodology would be to actually run experiments for the examples being used, by running them though the specific water treatment site in order to calibrate the models. Although there are different approaches for model calibration that have been published (Environmental Protection Agency, 2003a; Jarvis et al., 2005), there is a lack of guidance or comparisons on which approach to take in specific scenarios. This work showed how it is possible to integrate a detailed model based approached for individual clean water treatment processes into a complete conventional clean water treatment work model based on fundamental knowledge. There are some processes that have been derived using empirical models and are site specific, meaning that experiments would be needed for calibration of the model. The next step for the detailed modelling is to extend the empirical models, such as the dissolved air flotation models, in order to be generally applicable to multiple water treatment sites.

Economic evaluation

Economic evaluation can be incorporated either in the objective function by adding flow rate correlations in order to find an approximate cost of each processing unit. This can also be done in great detail using factors such as plant size, source and quality of water, plant location, energy and chemical costs. This can have a significant improvement in the optimisation by improving the accuracy of the results. There is also a real need for examples of optimisation where the objective function is more relevant, such as maximising process robustness.

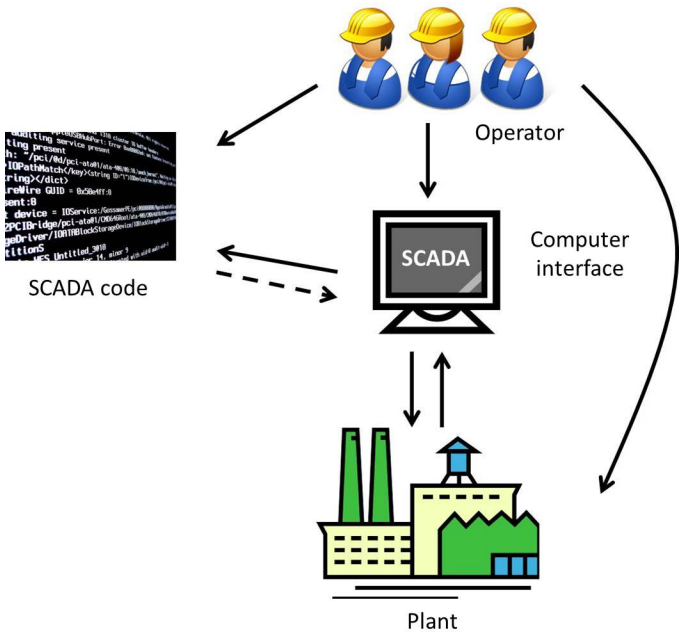


Figure 6.2: Integrated framework for process systems engineering in a clean water treatment work.

6.2.4 Broader recommendations

An integrated approach to modelling and optimisation can provide a competitive advantage (Yeomans and Grossmann, 1999; Heckl et al., 2007; Oluleye et al., 2016). An integrated approach can also be a driving force for operational level optimisation based on explicit objectives in the development of novel designs and discovering changes in the traditional concept of drinking water treatment. These models can receive water quality data that can predict the development of process parameters by upstream processes or influence downstream processes, and as can be seen Chapter 2, current work shows an understanding of the phenomena will lead to developed understanding for better process design. To ensure the successful implementations of mathematical models in the clean water industry, regulators, water companies and modelling experts need to come together to develop formal guidance on good modelling practices which describe how models must be used in industry. Figure 6.2 represents an integrated framework for the application of a process systems engineering method into the water treatment industry.

The collection of data in the water industry is by Supervisory Control and Data Acquisition (SCADA) which can be used to monitor and control plant or equipment. The control may be automatic, or initiated by operator commands. Ideally, a developed

full plant model should be able to receive data from the SCADA screen to be able to predict how an imminent change in one unit will affect the quality of the water at a later stage to be able to mitigate the risk. The benefits of having a system like this in place will allow for process feedback, whether it is fully automated or user controlled. This would lead to enhanced management of the water treatment plant.

6.3 Summary and main contributions

This thesis has developed and presented a full mathematical model based on first principles and an optimisation-based model for the synthesis and operation of an entire conventional clean water treatment work. Several illustrative case studies and sensitivity analysis have been presented. The main contributions from this thesis are:

1. A critical assessment of the current state-of-art in mathematical modelling in the clean water treatment industry, focussing on detailed mathematical models and optimisation techniques.

2. Development and validation of mathematical models for each of the main unit operation in a conventional clean water treatment works.

3. A detailed mathematical model for a complete conventional clean water treatment work demonstrating how a change would propagate a change through the work.

4. A modelling framework based on surrogate models for the individual processes in clean water treatment works, thus reducing the complexity of the models needed.

List of Communications

1. Folashade Akinmolayan, Afshin Anssari-Benham, Nina Thornhill, Eva Sørensen, 2012, Real-time operational risk management through advanced multi-scale modelling, **CPSE Consortium**, London, UK.

2. Visalinie Thivyathasan, Folashade Akinmolayan, Lazaros Papageorgiou, Eva Sørensen, 2013, Optimisation techniques: Application to conventional clean water treatment plants, **European Congress on Chemical Engineering**, The Hague, Netherlands.

3. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2013, Real-time operational risk management of water treatment processes, **IChemE Fluid Separations Special Interest Group Research Event: What's New in Fluid Separations**, London, UK.

4. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2013, Predictive modelling of a conventional clean water treatment work, **2013 AIChE Annual meeting**, San Francisco, USA.

5. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2014, A superstructure optimisation approach for a clean water treatment process case study, **ChemEngDayUK**, Manchester, UK.

6. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2014, Superstructure optimisation of clean water treatment processes, **International Water Association (IWA) UK 15th National Young Water Professionals Conference**, Manchester, UK.

7. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2014, Optimal performance management of clean water treatment processes, **2014 AIChE Annual Meeting**, Atlanta, USA.

8. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2014, Predictive modelling of a conventional clean water treatment work, **CPSE Consortium**, London, UK.

9. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2015, A detailed mathematical representation of Clean Water Treatment Plants, 12th International Symposium on Process Systems Engineering and 25th on Computer Aided Chemical Engineering, **ESCAPE25**, Volume 37, 2537 - 2542.

10. Folashade Akinmolayan, Nina Thornhill, Eva Sørensen, 2015, Surrogate based design and optimisation of clean water treatment works, **European Congress on Chemical Engineering**, Nice, France.

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Appendix A

A.1 General introduction

A.1.1 Water quality regulations

Directive (1998) distinguishes between different contaminants by dividing them into two types: mandatory (these cannot exceed a specific parameter value) and non-mandatory (the specific parameter value can be used as an indicator) Binnie and Kimber (2009). The mandatory standards covers 28 microbiological and chemical parameters that are essential to be removed, whilst the non-mandatory standards covers 20 further microbiological, chemical and physical parameters that are prescribed for monitoring purposes

Table A.1: Microbiological parameters (Directive, 1998)

Parameter	**Parametric value**	**Unit**
Escherichia coli (E. coli)	0	number/100 ml
Enterococci	0	number/100 ml

Table A.2: Chemical parameters (Drinking Water Inspectorate, 2010)

Parameter	**Parametric value**	**Unit**
Acrylamide	0.10	$\mu g l^{-1}$
Antimony	5.0	$\mu g l^{-1}$
Arsenic	10	$\mu g l^{-1}$
Benzene	1.0	$\mu g l^{-1}$
Benzo(a)pyrene	0.010	$\mu g l^{-1}$
Boron	1000	$\mu g l^{-1}$
Bromate	10	$\mu g l^{-1}$
Cadmium	5.0	$\mu g l^{-1}$
Chromium	50	$\mu g l^{-1}$
Copper	2000	$\mu g l^{-1}$
Cyanide	50	$\mu g l^{-1}$
1, 2-Dichloroethane	3.0	$\mu g l^{-1}$
Epichlorohydrin	0.10	$\mu g l^{-1}$
Fluoride	1500	$\mu g l^{-1}$
Lead	10	$\mu g l^{-1}$
Mercury	1.0	$\mu g l^{-1}$
Nickel	20	$\mu g l^{-1}$
Nitrate	50 000	$\mu g l^{-1}$
Nitrite	500	$\mu g l^{-1}$
Pesticides	0.10	$\mu g l^{-1}$
Pesticides - Total	0.50	$\mu g l^{-1}$
Polycyclic aromatic hydrocarbons	0.10	$\mu g l^{-1}$
Selenium	10	$\mu g l^{-1}$
Tetrachloroethene and Trichloroethene	10	$\mu g l^{-1}$
Trihalomethanes - Total	100	$\mu g l^{-1}$
Vinyl chloride	0.50	$\mu g l^{-1}$

Table A.3: Indicator parameters (Directive, 1998)

Parameter	Parametric value	Unit
Aluminium	200	μgl^{-1}
Ammonium	500	μgl^{-1}
Chloride	250	mgl^{-1}
Clostridium perfingens (including spores)	0	number/100 ml
Colour	Acceptable to consumers and no abnormal change	
Conductivity	2500	$\mu Scm^{-1}\, at\, 20^oC$
Hydrogen ion concentration	$\geq$ 6.5 and $\leq$9.5	pH unit
Iron	200	μgl^{-1}
Manganese	50	μgl^{-1}
Odour	Acceptable to consumers and no abnormal change	
Oxidisability	5.0	$mgl^{-1}\, O_2$
Sulphate	250	mgl^{-1}
Sodium	200	mgl^{-1}
Taste	Acceptable to consumers and no abnormal change	
Colony count	No abnormal change	
Coliform bacteria	0	number/100 ml
Total organic carbin (TOC)	No abnormal change	
Turbidity	Acceptable to consumers and no abnormal change	

Appendix B

B.1 Modelling the conventional clean water treatment process units

B.1.1 Modelling coagulation and flocculation unit

Results of pilot-plant experiments Pilot plant performance was determined by measuring the concentration of primary particles in each one of a series of four equal volume compartments. Argaman (1971) conducted several experiments employing G between 15 and 120 s^{-1}, Figure B.1 shows the experimental and theoretical curves plotted. This curve was used to determine the constants K_A and K_B, which are used in Chapter 2, section 1.2.3.

The aggregation constant K_A and the break up constant K_B can be determined empirically in laboratory or pilot scale tests (Argaman, 1971; Bratby and Miller, 1977; Odegaard, 1979). The ranges of reported values for the aggregation and break up constants are shown in Table B.1.

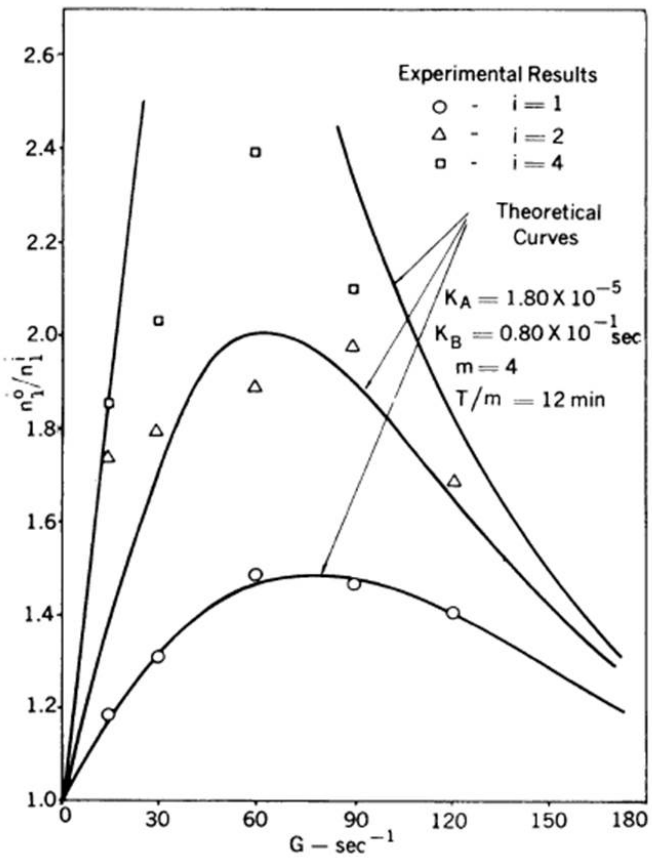

Figure B.1: Results of pilot plant experiments (Argaman, 1971)

System	*Kinetic Parameters*		Reference
	collision constant, K_A (-)Appendix C	**break-up constant, K_B (s)**	
Kaolin-alum	4.5 x 10^{-5}	1 x 10^{-7}	(Argaman and Kaufman, 1970)
	2.5 x 10^{-4}	4.5 x 10^{-7}	(Bratby and Miller, 1977)
Natural particulates-alum	1.8 x 10^{-5}	0.8 x 10^{-7}	(Argaman, 1971)
Alum-phosphate precipitate	2.8 x 10^{-4}	3.4 x 10^{-7}	
Alum-phosphate plus polymer	2.7 x 10^{-4}	1 x 10^{-7}	(Odegaard, 1979)
Lime-phosphate, pH 11	5.6 x 10^{-4}	2.4 x 10^{-7}	

Table B.1: Reported kinetic parameters for flocculation kinetics Crittenden et al. (2012)

Appendix C

C.1 Implementation of SST model

C.1.1 Approximation of convective flux

The Godunov numerical algorithm is a widely used numerical technique in one-dimensional SST modelling Jeppsson and Diehl 1996; Plosz et al. 2012; Li and Stenstrom 2014. The numerical method is based on the division of the z-axis by n grid points equally distributed, such that z = Top and z = Bottom are located half-way between the first two and the last two grid points, respectively, as shown in Figure C.1.

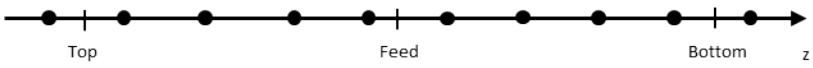

Figure C.1: Locations of grid points in case n=10

Let the index j stand for the space grid point, where the convective flux $F(C, z, t)$ in Equation 3.3.1 at the boundary between layers j and $j+1$ should be replaced by a numerical convective flux F_j^{num} associated with position z_j. Since the model will eventually be included into a complete water treatment model, simulation speed is a factor and from the works of Burger et al. (2011), it can be seen that the Godunov numerical algorithm can be used to approximate kynch batch function, $f_{bk}(C(z_j,t))$:

$$G_j = G_j\left(C_j, C_{j+1}\right) = \begin{cases} \min\limits_{C_j \le C \le C_{j+1}} f_{bk} & if\ C_j \le C_{j+1} \\ \max\limits_{C_j \le C \le C_{j+1}} f_{bk} & if\ C_j > C_{j+1} \end{cases}$$

Hence, we obtain the numerical flux

$$F_j^{num} = F_j^{num}(C_j,\, C_{j+1},\, t) = \begin{cases} & -Q_e(z_j)C_{j+1}/A\ for\ j = Top-1, ..., Top-N \\ G_j & -Q_e(z_j)C_{j+1}/A\ for\ j = Feed-1, ..., top \\ G_j & -Q_e(z_j)C_{j+1}/A + Q_u(z_j)C_j/A\ for\ j = Feed \\ G_j & +Q_u(z_j)C_j/A\ for\ j = Feed+1, ...Bottom \\ & +Q_u(z_j)C_j/A\ for\ j = Bottom+1, ...Bottom+N \end{cases}$$

Where N is an arbitrary number of layers above and below the SST boundary to account for flow into exiting pipes. The steady state solution has a discontinuity, the sludge blanket, in the thickening zone so this presented numerical method is stable and non-oscillatory near discontinuities and it is mass preserving. This implies that even if a discontinuity is smeared out by numerical diffusion (due to the discretisation), it is located at the right position, that is, it will have the same speed as the discontinuity of the analytical solution of 3.3.1.