Optimizing Chemical Dosage in Municipal Wastewater Disinfection with Model-based Control

by

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A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
Chemical Engineering and Applied Chemistry
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Abstract

This research thesis developed a feedforward model-based chemical dose control algorithm for municipal wastewater disinfection process and an algorithm to simulate unsteady stochastic process conditions using steady state computational fluid dynamics particle tracks. The control algorithm and simulation model utilize mechanistic models that describe disinfectant decay, CT, and disinfection levels. CT is the product of the effluent disinfectant concentration and the process average residence time. The models are integrated into the particle tracks generated from the disinfection process simulation. By utilizing the mechanistic models and the particle tracks, the control algorithm and the simulation model predict and control the process disinfection performance. The control algorithm is a feedforward control that predicts the disinfection performance, and it is not affected by the long feedback signal dead time commonly found in municipal wastewater disinfection. This thesis has shown that the mode-based dose control algorithm has reduced the disinfectant consumption up to 17%.
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# Table of Contents

Acknowledgments........................................................................................................ iii

Table of Contents ........................................................................................................ iv

List of Tables ............................................................................................................... vi

List of Figures .............................................................................................................. vii

1 Introduction ............................................................................................................... 1
  1.1 Thesis Objectives.................................................................................................. 1
  1.2 Thesis Outline...................................................................................................... 2

2 Literature Review ....................................................................................................... 3
  2.1 Process Control of Wastewater Chemical Disinfection...................................... 3
  2.2 CFD Modelling of Chemical and UV Disinfection Processes......................... 4
  2.3 Feedforward CFD Model-based Control Algorithm for Chemical Disinfection. 7

3 Methodology ............................................................................................................. 10
  3.1 Chemical Decay and Disinfection Models......................................................... 10
  3.2 Data Collection for the Chemical Decay and Disinfection Models................. 16
  3.3 Unsteady Stochastic Model (USM) ................................................................... 23
    3.3.1 Computational Fluid Dynamics (CFD) Particle Tracks................................. 24
    3.3.2 Unsteady Stochastic Model (USM) Simulation ............................................... 26
  3.4 Model-based and Other Chemical Dose Control Algorithms.......................... 32
    3.4.1 Control Setpoint .......................................................................................... 32
    3.4.2 Feedforward Model-based Control Algorithm ................................................. 33
    3.4.3 PID-type Control.......................................................................................... 37
    3.4.4 Flow Pacing Dosing Scheme ...................................................................... 37
  3.5 Methodology Summary ....................................................................................... 38

4 Results and Discussion ............................................................................................ 39
List of Tables

TABLE 3-1. PRIMARY EFFlUENT WATER SAMPLES TAKEN FROM THE POTTERSBURGH POLLUTION CONTROL PLANT (LONDON, ONTARIO). 16
TABLE 3-2. SECONDARY EFFlUENT WATER SAMPLES TAKEN FROM THE POTTERSBURGH POLLUTION CONTROL PLANT (LONDON, ONTARIO). 17
TABLE 3-3. PRIMARY EFFlUENT PAA DOSES. 18
TABLE 3-4. SECONDARY EFFlUENT PAA DOSES 18
TABLE 3-5. PRIMARY EFFlUENT PAA AND MICROBIAL SAMPLE TIME INTERVALS 20
TABLE 3-6. SECONDARY EFFlUENT PAA AND MICROBIAL SAMPLE TIME INTERVALS 21
TABLE 3-7. CFD SIMULATION BOUNDARY CONDITIONS 25
TABLE 4-1. PRIMARY EFFlUENT DISINFECTANT DECAY MODEL COEFFICIENTS. 42
TABLE 4-2. SECONDARY EFFlUENT DISINFECTANT DECAY MODEL COEFFICIENTS. 44
TABLE 4-3. PRIMARY EFFlUENT DISINFECTION MODEL COEFFICIENTS 51
TABLE 4-4. SECONDARY EFFlUENT DISINFECTION MODEL COEFFICIENTS 51
TABLE 4-5. DISINFECTANT DECAY MODEL AND CT MODEL UNSTEADY STOCHASTIC CONDITION PARAMETERS. 55
TABLE 4-6. DISINFECTION MODEL UNSTEADY STOCHASTIC CONDITION PARAMETERS. 55
TABLE 4-7. CHEMICAL DISINFECTANT CONSUMED BY THE PID CONTROL, MODEL-BASED CONTROL, AND FLOW-PACING DOSING SCHEME 61
List of Figures

FIGURE 3-1. TYPICAL DISINFECTANT DECAY CURVE IN MUNICIPAL WASTEWATER ................................................................. 11
FIGURE 3-2. CHICK-WATSON MODEL VS. TYPICAL DISINFECTION OF MUNICIPAL WASTEWATER. ............................. 14
FIGURE 3-3. CFD MODEL GEOMETRY OF THE SIMULATED CHEMICAL DISINFECTION PROCESS ...................................... 24
FIGURE 3-4. GENERAL POSITIONS OF THE SAMPLING PROBES ......................................................................................... 33
FIGURE 4-1. DISINFECTANT DECAYS OF PRIMARY EFFLUENT WITH PAA DOSES OF 2.0MG/L, 3.5MG/L, AND 5.0MG/L:
SAMPLED ON 2014-11-24. ............................................................................................................................................... 40
FIGURE 4-2. DISINFECTANT DECAYS OF SECONDARY EFFLUENT WITH PAA DOSES OF 1.0MG/L, 2.0MG/L, AND
3.0MG/L: SAMPLED ON 2014-11-24. .............................................................................................................................. 40
FIGURE 4-3. NORMALIZED DISINFECTANT DECAYS OF PRIMARY EFFLUENT (PWW) WITH PAA DOSES OF 2.0MG/L,
3.5MG/L, AND 5.0MG/L: SAMPLED ON 2014-11-24 ........................................................................................................... 41
FIGURE 4-4. NORMALIZED DISINFECTANT DECAYS OF SECONDARY EFFLUENT WITH PAA DOSES OF 1.0MG/L,
2.0MG/L, AND 3.0MG/L: SAMPLED ON 2014-11-24 ........................................................................................................... 41
FIGURE 4-5. MEASURED RESIDUAL CONCENTRATION VS. PREDICTED RESIDUAL (PRIMARY EFFLUENT) ...................... 43
FIGURE 4-6. MEASURED RESIDUAL CONCENTRATION VS. PREDICTED RESIDUAL (SECONDARY EFFLUENT) ............. 45
FIGURE 4-7. DISINFECTION EXPERIMENTAL DATA POINTS FOR PRIMARY EFFLUENTS AND THEIR CORRESPONDING
MODEL FITS ........................................................................................................................................................................... 46
FIGURE 4-8 DISINFECTION EXPERIMENTAL DATA POINTS FOR SECONDARY EFFLUENTS AND THEIR CORRESPONDING
MODEL FITS ........................................................................................................................................................................... 46
FIGURE 4-9. MODEL PREDICTED VALUES OF CT AS A FUNCTION OF TIME: PRIMARY EFFLUENT SAMPLE, NOVEMBER
24th, 2014 (DOSE = 2.0, 3.5, AND 5.0 MG/L) ..................................................................................................................... 47
FIGURE 4-10. MODEL PREDICTED VALUES OF CT AS A FUNCTION OF TIME: SECONDARY EFFLUENT SAMPLE,
NOVEMBER 24th, 2014 (DOSE = 1.0, 2.0, AND 3.0 MG/L) ..................................................................................................... 48
FIGURE 4-11. DISINFECTION OF PRIMARY EFFLUENT WITH PAA DOSES OF 4.0MG/L, 6.0MG/L, AND 8.0MG/L (2014-
11-25): MODEL-1 AND MODEL-2 REFERS TO THE FIRST AND SECOND DISINFECTION MODELS AS DISCUSSED IN
SECTION 3.1 ........................................................................................................................................................................... 49
FIGURE 4-12 DISINFECTION OF SECONDARY EFFLUENT (SWW) WITH PAA DOSES OF 1.5MG/L, 2.5MG/L, AND
3.0MG/L (2014-11-25): MODEL-1 AND MODEL-2 REFERS TO THE FIRST AND SECOND DISINFECTION MODEL
AS DISCUSSED IN SECTION 3.1 ........................................................................................................................................... 50
FIGURE 4-13. COMPARISONS OF THE PRIMARY EFFLUENT MEASURED LI AND THE PREDICTED LI FROM THE FIRST
DISINFECTION MODEL ........................................................................................................................................................... 52
FIGURE 4-14. COMPARISONS OF THE PRIMARY EFFLUENT MEASURED LI AND THE PREDICTED LI FROM THE SECOND
DISINFECTION MODEL ........................................................................................................................................................... 53
FIGURE 4-15. COMPARISONS OF THE SECONDARY EFFLUENT MEASURED LI AND THE PREDICTED LI FROM THE
SECOND DISINFECTION MODEL ........................................................................................................................................... 53
FIGURE 4-16. COMPARISONS OF THE SECONDARY EFFLUENT MEASURED LI. AND THE PREDICTED LI FROM THE SECOND DISINFECTION MODEL. ...........................................................................................................54
FIGURE 4-17. PERFORMANCE OF THE UNCONTROLLED BASE CASE: CONSTANT DOSE = 3.5MG/L ........................................56
FIGURE 4-18 DOSE APPLICATIONS OF THE PID, MODEL-BASED, AND FLOW PACING CONTROLS: THE BASE CASE IS INCLUDED FOR COMPARISONS. ...........................................................................................................57
FIGURE 4-19. DISINFECTION PERFORMANCE OF THE PID CONTROL, MODEL-BASED CONTROL, AND FLOW-PACING DOSING SCHEME...........................................................................................................58
FIGURE 4-20. DISINFECTION PERFORMANCE OF THE PID CONTROL, MODEL-BASED CONTROL, AND FLOW-PACING DOSING SCHEME: WITH INCREASED APPLIED DISINFECTANT DOSE FOR FLOW PACING. ...........................................59
FIGURE 4-21 EFFLUENT DISINFECTANT RESIDUALS OF THE PID CONTROL, MODEL-BASED CONTROL, AND FLOW-PACING DOSING SCHEME: THE BASE CASE AND SETPOINT ARE INCLUDED FOR COMPARISONS..............60
1 Introduction

Chemical disinfection is an essential component of municipal wastewater treatment, and its effectiveness has been widely accepted since the introduction of chlorine disinfection to drinking water treatment in the late 1800’s. When a suitable chemical is applied to wastewater with sufficient dose and contact time, chemical disinfection can effectively inactivate waterborne pathogens; thus protecting the environment as well as water consumers from disease outbreaks by preventing pathogenic contamination of the urban water cycle. However, high residual disinfectant concentration in the treated effluent has adverse effects on aquatic life in the environment and adds unnecessary costs to treatment plant operation for quenching the disinfectant. On the other hand, underdosing can lead to low disinfection levels, which may result in the contamination of drinking water sources within the proximity of an effluent discharge point. Hence, the optimization of chemical disinfectant dose control for municipal wastewater treatment application has been an important and ongoing research topic for water treatment engineers.

1.1 Thesis Objectives

The primary objective of this thesis is to develop a feedforward CFD model-based control algorithm that maintains the effluent disinfectant residual and CT\(^1\) setpoints of a chemical disinfection process by adjusting the applied disinfectant dose. The control algorithm will measure disinfectant concentration using multiple probes to predict the disinfectant decay kinetics. Then, the predicted disinfectant decay kinetics and the Lagrangian particle tracks generated from a CFD\(^2\) flow model will be used as inputs for a disinfectant decay model to predict the process disinfectant residual concentration and CT. Hence, the applied disinfectant dose can be adjusted to maintain the residual concentration and disinfection setpoints based on the predicted performance that is under unsteady flowrate, disinfectant decay, and

\(^1\) Disinfection level of a pathogen is a function of CT that is the product of disinfectant concentration and contact time.

\(^2\) A simulation tool for modelling the flow conditions using computational fluid dynamics.
disinfectability conditions. As a secondary objective, this thesis will also develop a process simulation model for testing the control performance of the proposed CFD model-based control algorithm. This simulation model will be capable of emulating the unsteady stochastic conditions of selected process parameters: flowrate, disinfectant decay, and disinfectability.

1.2 Thesis Outline

The remainder of this thesis is organized as follows. Chapter 2 provides a review of the literature that discusses ongoing research related to disinfection process modelling and control. Chapter 3 presents the methodologies for developing the disinfection process simulation model and the CFD model-based chemical dose control algorithm. Chapter 4 provides a presentation of the simulation results of the model-based control algorithm. Chapter 5 provides a discussion of the results and related future work.
2 Literature Review

In order to develop a model-based dose control algorithm for the chemical disinfection of municipal wastewater, this thesis has reviewed a wide range of topics that include existing process control strategies for the applied chemical dose, current practices for CFD modelling of water disinfection processes, and the modelling of disinfectant decay and pathogen disinfection levels in municipal wastewater treatment. Hence, this chapter will present a comprehensive review of the literature by introducing the ideas as four main topics:

- Process control of wastewater chemical disinfection.
- CFD modelling of chemical and UV disinfection processes.
- CFD model-based control algorithm for chemical disinfection.
- Summary of the thesis research topic.

First, the topics follow a logical sequence that first present a general overview of chemical disinfection process control and chemical disinfection process CFD modelling. Then, this chapter introduces the idea of implementing CFD model-based disinfection process control by reproducing the Lagrangian CFD model commonly used in UV disinfection for chemical disinfection. Lastly, the research topic of this thesis will be clarified by summarizing the literature review of this chapter.

2.1 Process Control of Wastewater Chemical Disinfection

Municipal wastewater chemical disinfection processes, unlike most chemical engineering processes, are difficult to control using conventional PID (Proportional-Integral-Derivative) control. Demir & Woo (2014), Shen, et al. (2009), and Chien, et al. (2002), have identified long dead time as the main contributing factor to the incapability of controlling the process with conventional PID control. As described in these studies, a typical chemical disinfection contact chamber, depending on its operating flowrate, have a residence time between 15 to 40min; this forms a long dead time between the feedback signal and the control input. These studies have
also suggested that unsteady stochastic conditions such as flowrate, disinfectant decay, and disinfectability cannot be accounted for with such long dead times. Thus, the combined effects of long dead time and the unsteady stochastic process conditions have rendered the feedback signal not representative of the process response to the applied dose, which is the main cause of the PID control not being able to maintain its target set-point in wastewater treatment.

Two different approaches have been suggested in the literature to properly control municipal wastewater disinfection processes. Demir & Woo (2014) and Chien et al. (2002) have incorporated the Smith Predictor into the feedback loop of the PID control to compensate for the long dead time. Alternatively, Shen et al. (2009) and Muslim et al. (2009) have proposed the use of feedforward controls to avoid the need to account for the process dead time. Feedforward controls are predictive models utilized to meet multiple output targets by accounting for multiple input disturbances. Although both feedback and feedforward strategies have reported good control performance, they only account for the input and output parameters of a disinfection process and ignored the fluid dynamics, chemistry, and disinfection kinetics that are the fundamental mechanisms of wastewater disinfection.

2.2 CFD Modelling of Chemical and UV Disinfection Processes

Literature in the fields of CFD modelling of municipal wastewater disinfection has taken into account the fluid dynamics, chemistry, and disinfection kinetics of the UV Disinfection process. Moreover, the remainder of this literature review will mainly focus on CFD simulations of chemical and UV disinfection\(^3\) processes. Then, the aforementioned mechanistic components of water disinfection: fluid dynamics, chemistry, and disinfection kinetics will be discussed in relation to their applications in CFD modelling for the purpose of optimizing chemical water disinfection processes. In the case of UV disinfection, CFD-based control will also be discussed.

Frist, there are two main CFD frameworks: the Eulerian and Lagrangian frameworks. Rieutord (2015) has respectively explained the two frameworks as observing the parameters of a flow as functions of space and time within a process geometry; and tracking the parameters in each particle within a large population of fluid particles as they flow through the process geometry.

\(^3\) A disinfection process that uses the germicidal 254nm ultraviolet irradiance to inactivate pathogens
along their trajectories. Elyasi & Taghipour (2006) have provided explanations with respect to disinfection modelling. Disinfectant and pathogens are functions of space and time under the Eulerian framework, and their concentrations are calculated by solving their mass conservation equations throughout the process geometry. Under the Lagrangian framework, fluid particles are introduced as discrete phases that move along the process geometry. Then, disinfectant and pathogen concentrations are calculated individually in each sampled particle according to its unique residence time, chemical decay, and disinfection conditions.

Researchers have predominantly used the Eulerian CFD simulations to model chemical disinfection processes and produced accurate results that are comparable to the experimentally measured hydraulic conditions from tracer studies of disinfectant contact tanks. Amini, et al. (2011), Rauen et al. (2008), and Khan et al. (2006) have simulated the transport of an inert species in their CFD models. By comparing their CFD tracer simulation results with pilot scale experimental data, they have concluded that CFD is a suitable simulation tool to characterize the fluid dynamic conditions of their pilot disinfectant contact chambers. Their simulation results have provided information on the residence time distribution (RTD), degree of mixing, degree of short circuiting, and identified stagnant flow regions. By determining the process discrepancy from ideal plug flow conditions, CFD simulation can assist in the optimization of the contact chamber hydraulic design. An example on the industry application of Eulerian CFD simulation can be found in Zhang et al. (2011), in which a municipal drinking water service tank located in Singapore was simulated and produced accurate residence time predictions comparable to the field tracer study. However, Angeloudis et al. (2015) and Rauen et al. (2012) have pointed out that hydraulic information cannot directly predict the disinfectant residual concentration or disinfection level of a chemical disinfection process. Thus, more recent studies including Angeloudis et al. (2015), Rauen et al. (2012), and Zhang et al. (2011) have started to incorporate disinfectant decay and pathogen disinfection models into the Eulerian framework to directly assess chemical disinfection process performance, yet there have not been any works attempting to implement the Eulerian CFD models for chemical disinfection processes control. Excessively high computational demand might have been the limiting factor. Khan et al. (2006) have reported

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4 A CFD model that tracks the changes of parameters in each coordinate of the model geometry
that the hydraulic performance simulation of the pilot unit from Shiono & Teixeira (2000) using an Eulerian CFD model, with a 1.7GHz CPU and 2Gb memory computer, required simulation times ranged from 2.23hr to 1297hr depending on the cell density of the CFD mesh. Similarly, Zhang et al. (2011) have reported a simulation time of 82hr to resolve both the flow and chlorine concentration within the service tank model geometry. The long processing time associated with Eulerian CFD simulations makes it impractical for online process control.

On the other hand, researchers have predominantly implemented the Lagrangian framework to simulate UV disinfection process performance. There have been very few UV CFD studies that implement the Eulerian framework. One of the few available papers, Elyasi and Taghipour (2006) who implemented an Eulerian model for UV disinfection have referenced that Kamimura et al. (2002) was the only available study that utilized Eulerian simulation for UV disinfection design. In Munoz et al. (2007) and Wols et al. (2010), Lagrangian UV models generate particles that follow the paths of individual trajectories in pre-generated velocity fields. Each particle behaves as an individual batch reactor with a unique residence time, chemical decay, and disinfection conditions. UV-dose and disinfection level are calculated for each particle, and the overall reactor performance is calculated as the average from the distribution calculated results from the particle population. Similar to an Eulerian tracer simulation, the residence time distribution of the particles can also be used to calculate the hydraulic parameters of a disinfection process.

In addition, Lagrangian CFD modelling of UV disinfection can be utilized for online control; unlike the Eulerian models of chemical disinfection processes. Lawryshyn & Cairns (2003) proposed utilizing Lagrangian particle tracks to develop a CFD-based control algorithm, which has been patented by Trojan Technologies as the UV Dosimeter™. It stores the residence time and spatial information of pre-generated Lagrangian particle tracks and uses them as inputs for a UV intensity and a disinfection model to calculate the UV dose and disinfection level of each particle. Hence, the process performance can be controlled by predicting disinfection

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5 A method to create small control volumes, also known as cells, to solve the fluid dynamics computational method.

6 A CFD model that tracks parameter changes by following a fluid element as it moves through the model geometry.
performance using the particle track data and controlling UV-lamp output to achieve the required UV dose setpoint.

### 2.3 Feedforward CFD Model-based Control Algorithm for Chemical Disinfection.

The primary goal of this thesis is to develop a CFD model-based control algorithm that maintains the required residual disinfectant concentration and disinfection level of a chemical disinfection process using a feedforward configuration. Based on the comparison between the Eulerian and Lagrangian frameworks, the algorithm would be similar to the UV-Dosimeter described by Lawryshyn & Cairns (2003); by adopting a Lagrangian framework and generating particle track data for the disinfectant decay and disinfection models to predict the disinfectant residual concentration, CT, and disinfection level. Since the algorithm makes model prediction for process control, it has a feedforward configuration. The control algorithm will target residual concentration and disinfection level setpoints by adjusting the applied disinfectant dose to account for changes in flowrate, chemical decay kinetics, and pathogen disinfectability in the disinfection process.

In addition to the particle track data that forms the Lagrangian framework, the disinfectant decay and the disinfection models of the CFD-based control algorithm also need to be defined. They describe the mechanisms of a disinfection process that defines the disinfectant residual concentration and disinfection level. The disinfectant decay model expresses the disinfectant residual concentration as a function of time, and, in its integrated form, calculates the CT that is the independent variable of the disinfection model. Using the CT, the disinfection model calculates the disinfection level of the process. Hence, this section will review and select suitable disinfectant decay and disinfection models to be fitted using the experimental data of this research thesis.

Rauen et al. (2012) and Sohn, et al. (2004) have suggested a relatively simple first order parallel decay model to describe the initial rapid decay and subsequent gradual decay of chemical disinfectant concentration in wastewater disinfection. This model has a relatively simple form that expressed disinfectant residual concentration as a function of time. The results of the model matched the experimental results of Rauen et al. (2012) and Sohn, et al. (2004) with high accuracy, and more complicated models, such as the second order parallel form proposed by
Kohpaei & Sathasvian (2011) have not demonstrated improved accuracy. Hence, this thesis will implement the first order parallel decay model as part of the control algorithm.

Similarly, the basic Chick-Watson model is also a simple disinfection model. It predicts the log inactivation of pathogens as a linear function of CT. From Bitton (2014), the Chick-Watson model is shown to be an accurate model for drinking water disinfection, but it has failed to accurately predict the level of wastewater disinfection in other studies. Hassen et al. (2000) have found that the model cannot accurately predict the non-linear response of fecal coliform and fecal streptococci to chlorination in municipal wastewater samples and fitted the experimental results with the non-linear Collins-Selleck model. Then, Koivunen & Heinonen-Tanski (2005) and Mezzanotte, et al. (2003) have suggested, based on experimental results, that the initial lag and plateau phases of the wastewater disinfection curves have deemed the basic Chick-Watson model unsuitable for predicting the disinfection levels of wastewater. Zhang & Huang (2011) have hypothesized that the lag and plateau phases are respectively caused by scavenging species reacting at faster rates relative to the pathogen disinfection kinetics and particles shielding some of the pathogens from the disinfectant. Since scavenging species and particles are abundant in municipal wastewater, the prediction of wastewater disinfection level requires the utilization of more complicated models.

Two disinfection models are proposed in this thesis by adopting non-linear equation forms to describe the response of pathogens to disinfection in wastewater. The first model, originally proposed by Yun & Park (2003), predicts the photosynthetic activities of algae as a function of photon density. Because the shape of the photosynthetic activity curves are analogues to the wastewater disinfection curves having both lag and plateau phases, the model can be implemented for disinfection by replacing the variables with disinfection level and CT. The second model takes the form of the first order parallel equation with disinfection level and CT respectively as the dependent and independent variables. Experimental studies on UV wastewater disinfection by Bowker, et al. (2011), Li et al. (2009), and Gehr (2007) have shown that the disinfection curves of wastewater consist of an initial rapid decline of surviving pathogens, a gradual subsequent decline, and a plateau phase. Since the shape of the disinfection curves are analogues to the chemical wastewater disinfection curves found in the aforementioned studies on chemical and UV disinfection, the first order parallel equation can also be adopted for
chemical disinfection. Since both proposed models appear to be suitable for describing the shape of wastewater disinfection curves, they will both be implemented and compared in this thesis.

**Summary of the thesis research topic.** As mentioned above, the Lagrangian framework has been widely implemented for designing UV disinfection processes and utilized for UV dose control. On the other hand, chemical disinfection process control has relied on feedforward and feedback control strategies that ignore the process fluid dynamics and reaction mechanisms. When CFD is implemented to account for the fluid dynamics and reaction mechanisms, the Eulerian framework has been predominantly adopted and high accuracy has been reported for predicting the fluid dynamics, disinfectant decay, and disinfection, but the processing times for Eulerian simulations are too slow for online process control applications. Hence, this thesis will explore the development of a feedforward CFD model-based control algorithm utilizing the Lagrangian framework for chemical disinfection. The feedforward configuration is adopted for the algorithm to avoid the aforementioned control issues associated with long feedback signal dead times.
3 Methodology

This section is organized as follows. Section 3.1 presents the theory of chemical decay and disinfection models together with the experimental procedures utilized to obtain the disinfectant and disinfection curves that are to be fitted using the models. Section 3.3 presents the development of the simulation model to predict process performance by accounting for unsteady stochastic changes of flowrate, disinfectant decay, and disinfection conditions. Section 3.4 presents the control methodology of the CFD model-based algorithm. Section 3.5 presents the method used to evaluate the effectiveness of the CFD model-based algorithm control.

3.1 Chemical Decay and Disinfection Models

In this section, the chemical decay model and disinfection models will be developed using experimental results generated from a batch reactor to resemble the behavior of perfectly segregated fluid particles of the Lagrangian CFD model. Experimental data of disinfectant residual concentrations and disinfection levels were collected from a batch reactor to develop models that predict disinfectant residual concentration and CT as a function of time, and disinfection level as a function of the CT. The experimental results are applicable to Lagrangian CFD simulations because the method models fluid particles as perfectly segregated and the particles behave as individual batch reactors with unique residence times, chemical decay, and disinfection conditions. First, the theory of chemical disinfectant decay models and disinfection models will be explained. Then, the experimental procedures to generate the data for fitting the chemical decay and disinfection models will be provided.

Chemical Disinfectant Decay Model. The decay of disinfectant concentration is due to the disinfectant chemical being consumed by scavenger chemicals in the municipal wastewater. Rauen et al. (2012), Sohn et al. (2004), and Kohpaei & Sathasivan (2011) have observed that the decay of the disinfectant concentration follows an initial rapid decay and a subsequent gradual decay similar to the curve shown in Figure 3-1, which is plotted based on the experimental results from Chapter 4 and shown below for illustration.
As discussed in the literature review, studies (Sohn, et al., 2004 and Rauen, et al., 2012) suggest that although it is impossible to identify the numerous species and reaction mechanisms that consume the disinfectant species, $\hat{C}$, the numerous unknown species can be generalized as scavenger chemical, $\hat{S}$, which consumes the chemical disinfectant. It has been proposed that the overall reaction consists of two pseudo first order kinetic pathways that take place simultaneously. The first pathway describes the initial rapid decay of the disinfectant, as expressed by

$$\hat{C}_f + \hat{S} \rightarrow \hat{C}_f \hat{S}, \quad (3-1)$$

where $\hat{C}_f$ is the rapidly consumed disinfectant and $\hat{S}$ is the scavenger species. The second pathway describes the subsequent gradual decay of the disinfectant and given by

$$\hat{C}_s + \hat{S} \rightarrow \hat{C}_s \hat{S}, \quad (3-2)$$
where $\hat{C}_s$ is the gradually consumed disinfectant. As proposed by the aforementioned literature, the total chemical disinfectant concentration, $C$, is calculated as the sum of the concentrations of the rapidly and gradually consumed chemical disinfectants, $C_f$ and $C_s$, as expressed by

$$C = C_f + C_s.$$ (3-3)

Then, by letting $\alpha$ be the fraction of the gradually consumed concentration of $C$, $C_f$ and $C_s$ are given by,

$$C_f = (1 - \alpha) \cdot C$$ (3-4)

and

$$C_s = \alpha \cdot C.$$ (3-5)

The model assumes that the concentration of scavenger species that consumes $C_f$ and $C_s$ is abundant throughout the course of the process. Thus, the decays of $C_f$ and $C_s$ are expressed by the first order reaction equations

$$C_f(t) = C_{f,o} \cdot e^{-k_f \cdot t}$$ (3-6)

and

$$C_s(t) = C_{s,o} \cdot e^{-k_s \cdot t},$$ (3-7)

where $C_{f,o}$ and $C_{s,o}$ are respectively the initial concentrations of rapidly consumed and gradually consumed disinfectant concentrations; $k_f$ and $k_s$ are respectively their pseudo first order kinetic rate constants. By substituting equation (3-6) and (3-7) into equation (3-3), the decay of chemical disinfectant is given by

$$C(t) = C_{f,o} \cdot e^{-k_f \cdot t} + C_{s,o} \cdot e^{-k_s \cdot t}.$$ (3-8)
Based on equation (3-4) and (3-5), $C_{f,o}$ and $C_{s,o}$ can then be expressed by $C_o$ and $\alpha$. Hence, the final form of the chemical disinfectant decay model is expressed as follows

$$C(t) = (1-\alpha) \cdot C_o \cdot e^{-k_f \cdot t} + \alpha \cdot C_o \cdot e^{-k_s \cdot t}, \quad (3-9)$$

where the disinfectant concentration, $C$, is a function of time and dependent on three process condition parameters: the initial chemical dosage, $C_o$, and chemical decay rate constants, $k_f$ and $k_s$. The value of $CT$ can be calculated from a model that is the integration of equation (3-9) with time (from 0s to time, $t$) as expressed by

$$CT(t) = \frac{(1-\alpha) \cdot C_o}{k_f} \cdot \left(1 - e^{-k_f \cdot t}\right) + \frac{\alpha \cdot C_o}{k_s} \cdot \left(1 - e^{-k_s \cdot t}\right), \quad (3-10)$$

where the calculated CT accounts for both the chemical decay and residence time of the batch process. The relationship between the value of CT and the disinfection level will be explored next.

**Municipal wastewater (MWW) disinfection model.** Koivunen et al. (2005), Mezzanotte et al. (2003), and Hassen et. Al (1999) have found that the conventional Chick-Watson model does not accurately predict the disinfection levels of chemical wastewater disinfections. The model equation is expressed by

$$\log\left(\frac{N}{N_0}\right) = \Lambda \cdot CT, \quad (3-11)$$

where $\Lambda$ is the organism sensitivity, called the Chick-Watson coefficient and CT that is the product of disinfectant residual concentration and the reaction time, $N$ and $N_0$ are respectively the number of surviving organisms and initial number of organisms, and $\log(N/N_0)$ is the log inactivation, and can be expressed by

$$LI = -\log\left(\frac{N}{N_0}\right), \quad (3-12)$$
and in this thesis LI\(^7\) (log inactivation) is used interchangeably with disinfection level. Previous work (Hassen, et al. (2000)) has shown that the linear Chick-Watson model cannot accurately describe the typical non-linear response of pathogens in wastewater to chemical disinfection; similar to the curve shown in Figure 3-2, which is plotted based on the experimental results from Chapter 4 and shown below for illustration. Zhang and Huang (2011) have stated that a typical municipal wastewater chemical disinfection curve has the lag and plateau phases, which the disinfection behavior is deviated from the Chick-Watson model.

![Figure 3-2. Chick-Watson Model vs. typical disinfection of municipal wastewater.](image_url)

In order to accurately predict the disinfection levels by chemical disinfection in wastewater, two models are proposed in this thesis. Both models are non-linear and designed to describe the lag and plateau phases observed in the data, and they are hereby referred to as the first and second model respectively.

The First Disinfection Model was originally presented by Yun and Park (2003) to predict the photosynthetic activities of algae as a function of photon density. It describes the lag and plateau

---

\(^7\) One log inactivation (e.g. LI = 1) is equivalent to inactivation 90% of the microbial population.
phases of photosynthetic activities. When the form of the equation is adopted to model chemical wastewater disinfection, the relationship between $LI$ and $CT$ is expressed by

$$LI = \frac{LI_{\text{plateau}}}{1 + e^{-k_1(CT-P_1)}} + \frac{LI_{\text{plateau}}}{1 + e^{-k_2(CT-P_2)}},$$  \hspace{1cm} (3-13)

where $LI_{\text{plateau}}$ is the plateau disinfection level; $k_1$ and $k_2$ are the rate constants of approaching the plateau value; and $P_1$ and $P_2$ are the critical values of $CT$ that the slope rate of change switches direction in the model.

The Second Disinfection Model used in the thesis is the \textit{first order parallel equation}, which has been commonly used to describe disinfection kinetics of municipal wastewater UV disinfection, as shown in previous works (i.e. Bowker et al. (2010), Li et. Al (2008), and Gehr (2007)) discussed in the literature review. The mathematical form of the model resembles Equation (3-9) as,

$$\frac{N}{N_o} = (1 - \beta) \cdot e^{-k_a CT} + \beta \cdot e^{-k_p CT},$$  \hspace{1cm} (3-14)

where $\beta$ is the fraction of pathogen population shielded by the particles; and $k_a$ and $k_p$ are respectively the disinfection kinetic rate constants of pathogens accessible to the chemical disinfectant and pathogens that are shielded by particles. For comparison with the first model, $\frac{N}{N_o}$ can be converted to log inactivation, $LI$, using equation (3-12).

Thus, two wastewater chemical disinfection models that use the value of $CT$ to predict disinfection level are proposed here. The first model has greater degrees of freedom and can account for the curvature in the disinfection data. The second disinfection model is capable of describing the plateau, but its mathematical form cannot account for the curvatures at the lag phase. Both models are fitted to experimental data and the results are presented in Chapter 4.
3.2 Data Collection for the Chemical Decay and Disinfection Models

From November 18th to December 5th, 2014, primary and secondary wastewater effluent samples were taken almost daily from the Pottersburgh Pollution Control Plant located in London, ON. Peracetic acid (PAA) was selected as the disinfectant to develop datasets for the disinfectant decay and disinfection models. In addition, wastewater quality parameters: chlorine level, %UVT\(^8\), and turbidity were monitored as shown in Table 3-1 and Table 3-2. It was important to ensure that there was no chlorine residual in the samples as the chlorine would interfere with the disinfection experiments. Other water quality parameters were measured to see if relationships could be drawn from these parameters and disinfectant decay parameters and disinfection parameters.

Table 3-1. Primary effluent water samples taken from the Pottersburgh Pollution Control Plant (London, Ontario).

<table>
<thead>
<tr>
<th>Date</th>
<th>Chlorine level (ppm)</th>
<th>%UVT (%/cm)</th>
<th>Turbidity (NTU)</th>
<th>TSS (mg/L)</th>
<th>N(_o) (cfu/100mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>0.0</td>
<td>19.0</td>
<td>89.5</td>
<td>72.0</td>
<td>4.3×10^6</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>0.0</td>
<td>17.1</td>
<td>56.5</td>
<td>56.8</td>
<td>6.6×10^6</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>0.0</td>
<td>39.3</td>
<td>32.6</td>
<td>63.0</td>
<td>-</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>0.0</td>
<td>29.5</td>
<td>46.5</td>
<td>62.6</td>
<td>2.9×10^6</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>0.0</td>
<td>21.7</td>
<td>67.1</td>
<td>54.5</td>
<td>2.0×10^7</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>0.0</td>
<td>18.5</td>
<td>76.2</td>
<td>78.5</td>
<td>1.1×10^7</td>
</tr>
</tbody>
</table>

\(^8\) The water transmittance of 254nm UV irradiance measured from a 1cm path length.
Table 3-2. Secondary effluent water samples taken from the Pottersburgh Pollution Control Plant (London, Ontario).

<table>
<thead>
<tr>
<th>Date</th>
<th>Chlorine level (ppm)</th>
<th>% UVT (%/cm)</th>
<th>Turbidity (NTU)</th>
<th>TSS (mg/L)</th>
<th>No. (cfu/100mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>0.0</td>
<td>67.8</td>
<td>1.7</td>
<td>6.0</td>
<td>1.8×10^4</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>0.0</td>
<td>65.5</td>
<td>2.2</td>
<td>7.3</td>
<td>2.7×10^4</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>0.0</td>
<td>69.4</td>
<td>4.77</td>
<td>12.7</td>
<td>-</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>0.0</td>
<td>72.9</td>
<td>2.0</td>
<td>6.0</td>
<td>1.3×10^4</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>0.0</td>
<td>69.9</td>
<td>1.8</td>
<td>4.7</td>
<td>3.8×10^4</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>0.0</td>
<td>69.1</td>
<td>2.0</td>
<td>5.0</td>
<td>1.8×10^4</td>
</tr>
</tbody>
</table>

Experiments were designed to develop three sets of chemical decay and disinfection curves by applying high, middle, and low PAA doses to each water sample, as shown below in Table 3-3 and Table 3-4. The applied disinfectant doses were selected based on experience with wastewater sample water quality, and it was assumed that water with lower %UVT had higher concentrations of scavenger species and thus required a higher dose of PAA to be applied.
Table 3-3. Primary effluent PAA doses.

<table>
<thead>
<tr>
<th>Date</th>
<th>Low dose (mg/L)</th>
<th>Middle dose (mg/L)</th>
<th>High dose (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>6.0</td>
<td>8.0</td>
<td>-</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>4.0</td>
<td>6.0</td>
<td>8.0</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>2.0</td>
<td>3.5</td>
<td>5.0</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>2.5</td>
<td>4.0</td>
<td>5.5</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>3.0</td>
<td>4.5</td>
<td>5.5</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>4.0</td>
<td>6.0</td>
<td>8.0</td>
</tr>
</tbody>
</table>

Table 3-4. Secondary effluent PAA doses

<table>
<thead>
<tr>
<th>Date</th>
<th>Low dose (mg/L)</th>
<th>Middle dose (mg/L)</th>
<th>High dose (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>1.5</td>
<td>3.0</td>
<td>4.5</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>1.5</td>
<td>3.0</td>
<td>4.5</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>1.0</td>
<td>2.0</td>
<td>3.0</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>1.5</td>
<td>2.5</td>
<td>3.0</td>
</tr>
</tbody>
</table>
A batch reactor with a maximum capacity of 10-L was used in the experiment. In order to ensure an ideal well-mixed condition, test sample volume was limited to 1-L to reduce the depth of the batch system, and a magnetic stir bar was installed to provide continuous mixing. The chemical disinfectant, PAA, was dosed at the beginning \( t = 0 \) of each test for developing the disinfectant decay curves, and the applied doses used in the experiments are shown above in

<table>
<thead>
<tr>
<th>Date</th>
<th>Dose 1</th>
<th>Dose 2</th>
<th>Dose 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-12-02</td>
<td>1.5</td>
<td>3.0</td>
<td>5.0</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>1.5</td>
<td>3.0</td>
<td>4.5</td>
</tr>
</tbody>
</table>

Table 3-3 and Table 3-4. The applied PAA concentration, \( C_o \), at \( t = 0 \) was calculated based on the dilution of the concentrated PAA solution that was added into the reactor volume, and is calculated by

\[
C_o = \frac{C_{dose} \times V_{dose}}{V_{reactor}},
\]

where \( C_{dose} \) is the concentration of the concentrated PAA solution, \( V_{dose} \) is the volume of the concentrated PAA solution, and \( V_{reactor} \) is the total volume of the batch reactor. The first PAA measurement and the microbial sample of each experiment were taken from the reactor at \( t = 30s \) to capture the initial rapid disinfectant decay. Then, four subsequent samples were taken at different sample times, where the sample times were determined based on the following conditions:
- sufficient change in residual concentration compared with the previous sample,
- measurable number of surviving fecal coliforms, and
- measurable disinfectant residual concentration.

Similar to selecting the applied disinfectant dose, the sample times of each experiment as shown in Table 3-5 and Table 3-6. were also determined based on previous experience with the wastewater source and the measured water quality. The objectives were to apply appropriate values of \( CT \) to observe measurable reduction of the microbial population without reducing it to zero count; and to maintain measurable disinfectant residual concentration throughout the experiment. Water with high turbidity was assumed to have higher counts of particle\(^9\) associated microbial that are more difficult to disinfect, and as previously mentioned, water with lower \%UVT was assumed to have a slower rate of chemical disinfectant decay. Hence, samples with higher turbidity were given longer residence times, and low-%UVT samples were given longer interval between each sample time.

### Table 3-5. Primary effluent PAA and microbial sample time intervals

<table>
<thead>
<tr>
<th>Date</th>
<th>PAA dose (ppm)</th>
<th>( t_1 (s) )</th>
<th>( t_2 (s) )</th>
<th>( t_3 (s) )</th>
<th>( t_4 (s) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>6.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>8.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>4.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>6.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
</tbody>
</table>

---

\(^9\) Particles in wastewater can shield microbial populations from the disinfectant.
<table>
<thead>
<tr>
<th>Date</th>
<th>PAA dose (mg/L)</th>
<th>t₁(s)</th>
<th>t₂(s)</th>
<th>t₃(s)</th>
<th>t₄(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>1.5</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>3.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>4.5</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>2.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>3.5</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>2.5</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>4.0</td>
<td>330</td>
<td>930</td>
<td>2100</td>
<td>3726</td>
</tr>
<tr>
<td></td>
<td>5.5</td>
<td>330</td>
<td>1110</td>
<td>2700</td>
<td>4500</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>3.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>1500</td>
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<td>4.5</td>
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<td>930</td>
<td>1500</td>
<td>2100</td>
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<td>5.5</td>
<td>330</td>
<td>960</td>
<td>1800</td>
<td>2400</td>
</tr>
<tr>
<td>2014-12-04</td>
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<td>600</td>
<td>1500</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>6.0</td>
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<tr>
<td></td>
<td>8.0</td>
<td>300</td>
<td>600</td>
<td>1500</td>
<td>2700</td>
</tr>
</tbody>
</table>

Table 3-6. Secondary effluent PAA and microbial sample time intervals
<table>
<thead>
<tr>
<th>Date</th>
<th>1.0</th>
<th>2.0</th>
<th>3.0</th>
<th>4.5</th>
<th>5.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-20</td>
<td>3.0</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>4.5</td>
<td>180</td>
<td>450</td>
<td>900</td>
<td>2700</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>1.0</td>
<td>330</td>
<td>900</td>
<td>1800</td>
<td>3600</td>
</tr>
<tr>
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<td>900</td>
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<td>3000</td>
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<td>2014-12-02</td>
<td>1.5</td>
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<td>450</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>3.0</td>
<td>193</td>
<td>450</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>600</td>
<td>900</td>
<td>1500</td>
<td>2700</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>1.5</td>
<td>600</td>
<td>1200</td>
<td>1800</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>3.0</td>
<td>600</td>
<td>1200</td>
<td>1800</td>
<td>2700</td>
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<tr>
<td></td>
<td>4.5</td>
<td>600</td>
<td>1200</td>
<td>1800</td>
<td>2700</td>
</tr>
</tbody>
</table>

At each sample time of each experiment, the disinfectant residual concentration was measured using the *peracetic DPD test method*\(^\text{10}\), and a microbial sample was collected. The residual disinfectant in the microbial sample was then quenched immediately using sodium sulphite.

solution and analyzed using the *standard fecal coliform filter procedure*\(^{11}\) to obtain the surviving microorganism count.

Finally, the experimental results were fitted to the disinfectant decay and disinfection models by utilizing non-linear regression to determine the model parameters. From the chemical decay model, Equation (3-9), the fraction of slow decay, \(\alpha\), the fast reaction rate constant, \(k_f\), and the slow reaction rate constant, \(k_s\), were determined. These disinfection model coefficients were then used in equation (3-10) to calculate the value of \(CT\). Then, the disinfection results of how \(LI\) responds to the applied \(CT\) were fitted to the disinfection models in equation (3-13) and equation (3-14) to estimate the respective disinfection parameters. The disinfectant decay and disinfection model parameters were utilized as inputs to the simulation model and control algorithm, to be discussed in the next two sections. These parameters also provide a better understanding of the underlying mechanisms of disinfectant decay and chemical disinfection in wastewater treatment.

### 3.3 Unsteady Stochastic Model (USM)

This section will provide details of the Unsteady Stochastic Model (USM), which, as mentioned previously, is a simulation algorithm based on the Lagrangian framework. The USM is capable of predicting the disinfectant residual concentration and disinfection level of a wastewater chemical disinfection process operating under unsteady and stochastic conditions using pre-generated steady state particle tracks. Dynamic conditions accounted for by the model are changing flowrate, and varying disinfectant decay and disinfection parameters. Unlike unsteady CFD simulations, the USM does not require CFD simulations to be repeated at each time step. Hence, this method requires significantly less computational time.

The remainder of this section introduces the main components that enable unsteady simulation in the USM. Initially, the steady state particle track data generated from a Lagrangian CFD simulation is required to provide the particle residence time distribution (RTD) as an input for the USM to determine the residence times, disinfectant decay conditions, and disinfection

---

\(^{11}\) USEPA Standard Methods 9222D. Fecal Coliform Membrane Filter Procedure
conditions of the sampled particles. The particle residence times generated from the CFD simulation is based on a constant flowrate defined by the user, so the residence time of a particle obtained from the RTD must be scaled according the ratio of the user defined flowrate to the process operating flowrate. The USM accounts for this by utilizing a function, herein referred to as the *dynamic flow function*, which will be introduced later in this section. Then the USM utilizes the *time referencing function*, introduced below, to identify, at each sample occasion, the entry time and the corresponding disinfectant decay and disinfection conditions of the sampled particles. The entry time and the associated particle conditions (i.e. the process flow rate at the entry time, as well as the stochastic disinfectant decay and disinfection parameters) are stored in a matrix in the USM, herein referred to as the *unsteady stochastic inlet condition timeframe matrix* (UITM). The number of rows in the matrix is equal to the number of time steps for the duration of the entire simulation.

### 3.3.1 Computational Fluid Dynamics (CFD) Particle Tracks.

The steady state particle tracks data were generated from the CFD simulation of a 2D chemical disinfectant contact tank. The tank is 0.94m wide and 2m long with seven identical rectangular baffles that are 0.72m long and 0.05m wide, as shown in Figure 3-3. The default depth for the 2D CFD simulation is 1m, and thus the system has a total volume of 1.88m³.

![CFD Model Geometry of the Simulated Chemical Disinfection Process.](image)
The CFD simulation was completed using ANSYS Fluent by discretizing the domain into \(1.67 \times 10^4\) quadrilateral cells. Mesh independence was demonstrated by comparing the velocity gradients at each compartment with two densely meshed cases using \(2.94 \times 10^4\) and \(6.60 \times 10^4\) quadrilateral cells respectively. Boundary conditions of the CFD simulation are provided in Table 3-7.

Table 3-7. CFD simulation boundary conditions

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Magnitude</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Constant velocity</td>
<td>(8.72 \times 10^{-3}) m/s</td>
<td>• Perpendicular to inlet boundary.</td>
</tr>
<tr>
<td>Outlet</td>
<td>Constant pressure</td>
<td>1 atm</td>
<td></td>
</tr>
<tr>
<td>Surface</td>
<td>Symmetry</td>
<td>-</td>
<td>• Wave or air-water interaction is not accounted for.</td>
</tr>
<tr>
<td>Wall</td>
<td>No-slip</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

The CFD simulation case was solved with the SIMPLE scheme and applied second order upwind discretization for the momentum, turbulent kinetic energy, and turbulent dissipation rate equations. The turbulent flow of the CFD simulation was solved with the realizable k-\(\varepsilon\) model with enhanced wall treatment; both of which are standard models in ANSYS FLEUNT and commonly used in CFD simulations (Rauen, et al., 2012). The steady state velocity field was generated by solving the fluid dynamics as shown in Figure 3-3. After a stable solution for the velocity components were found, Largangian particles were generated using the discrete phase and random walk models from ANSYS. The particle track data consists of the residence time of each particle, \(i\), as a function of its location in the model geometry. Thus, particle RTD can be generated from user defined sample locations (e.g. the outlet boundary) of the model by obtaining the unique CFD generated residence time, \(t_{\text{res},i,\text{CFD}}\) of each particle, \(i\). The particle RTD is used as an input for the USM.

---

\(^{12}\) The commercial software used in the development of the CFD particle tracks.
3.3.2 Unsteady Stochastic Model (USM) Simulation

In addition to the particle RTD generated from the Lagrangian CFD particle tracks, the USM requires as inputs the conditions stored in the UITM and the simulated sample times to simulate the unsteady stochastic process. Both the UITM and simulated sample times are defined by the user and stored in respective matrices. The simulation is discretized into \( n \) steps as calculated by,

\[
n = \frac{T}{\Delta t},
\]

where \( T \) is the duration time of the unsteady simulation and \( \Delta t \) is the simulation time step size. Each row of the UITM matrix contains the unsteady stochastic inlet conditions associated with the conditions as of simulation time, \( t_j \), where \( t_j \) is calculated for the \( j^{th} \) (\( j = 1...n \)) time step as,

\[
t_j = \Delta t \times j.
\]

The UITM is expressed as follows

\[
[UITM] = \begin{bmatrix}
\bar{t} & \bar{Q} & \bar{\alpha} & \bar{k}_f & \bar{k}_s & \bar{N}_o & LI_{plateau} & \bar{P}_1 & \bar{P}_2 & \bar{\beta} & \bar{k}_a & \bar{k}_p
\end{bmatrix},
\]

where the discretized time \( \bar{t} \), the process flowrate \( \bar{Q} \), the disinfectant decay model parameters \( \bar{\alpha}, \bar{k}_f, \) and \( \bar{k}_s \), the initial microbial counts in the process inlet \( \bar{N}_o \), and the model parameters of the first disinfection model \( LII_{plateau} \), \( \bar{P}_1, \bar{P}_2 \), \( \bar{\beta} \), \( \bar{k}_a \), and \( \bar{k}_p \) are stored as vectors of equal length. The discrete time steps, \( t_j \), are stored in the vector column \( \bar{t} \) as expressed by

\[
\bar{t} = \begin{bmatrix}
t_1 \\
\vdots \\
t_j \\
\vdots \\
t_n
\end{bmatrix}.
\]
and the calculation of the unsteady stochastic inlet conditions associated with each discrete time step, \( t_j \), are presented next using the process flowrate, \( Q \), as an example. The unsteady stochastic process flowrate consists of the time dependent average flowrate, \( Q_{avg}(t) \), that can be actual flow data or calculated using a time dependent function defined by the user, and the stochastic component, \( S_Q \). Hence, the process flowrates contained in \( \bar{Q} \) are given by

\[
\bar{Q}_j = Q_{avg}(t_j) + S_Q, \tag{3-20}
\]

The user defined time dependent function utilized in this thesis was a sinusoidal function, as expressed by

\[
Q_{avg}(t_j) = A_Q \sin(\omega_Q t_j - \phi_Q) + B_Q, \tag{3-21}
\]

where \( A_Q \), \( \omega_Q \), \( \phi_Q \), and \( B_Q \) are the sine function scaling parameters that are defined by the user to emulate the unsteady stochastic process flow conditions. The stochastic component of the process flow was calculated as

\[
S_Q = \sigma_Q \cdot X_j, \tag{3-22}
\]

where \( \sigma_Q \) is the user defined stochastic noise amplitude and \( X_j \) is a random number generated at every \( j^{th} \) time step. As mentioned previously, the other parameters that are stored in the \( UITM \), \( \bar{\alpha}_j, \bar{k}_f, \bar{k}_s, \bar{N}_o, \bar{L}_I\), \( \bar{k}_1, \bar{P}_1, \bar{k}_2, \bar{P}_2, \bar{\beta}_j, \bar{k}_a, \) and \( \bar{k}_p \), are generated in the same manner as \( \bar{Q} \). Next, the simulated sample times, \( t_{sam} \), as previously mentioned, was stored in a vector. It is a subset of the discrete time vector, \( \bar{t} \), as expressed by

\[
X_j \text{ is a random number generated by the randn function from Matlab at every timestep.}
\]
where \( t_{\text{sam}, j_{\text{sam}}} \) is the sample user defined sample time for the \( j_{\text{sam}}^{\text{th}} \) sample time step, where \( j_{\text{sam}}^{\text{th}} = 1 \ldots n_{\text{sam}} \), and \( n_{\text{sam}} \) is the total number of sampling occasions in the simulation.

The USM simulation output parameters are disinfectant residual concentration, \( C \) and the disinfection level. They are simulated by the USM, which utilizes the unsteady process conditions stored in the UITM and the sample times stored in \( \bar{t}_{\text{sam}} \). Initially, the output parameters measured from a user defined sample location, denoted as \( K \) in this thesis, are calculated for each particle, \( i \), at the sample time, \( t_{\text{sam}, j_{\text{sam}}} \). For example, the outlet was selected by the USM in order to capture the overall process performance of the contact tank geometry. Then, the USM calculated the residence time of the particle, \( i \), sampled in the model geometry location, \( K \); and the entry time that the particle entered the process. The particle residence time and the particle entry time are calculated in the USM using the *dynamic flow function* and the *time referencing function* respectively.

The *dynamic flow function* calculates the particle residence time, \( t_{\text{res}, j} \), as a function of the operating process flowrate that is dependent on the simulation sample times, \( t_{\text{sam}} \). The particle residence time is calculated by scaling the CFD-generated particle residence time, \( t_{\text{res}, j, CFD} \), using the ratio of the flowrate used in the CFD simulation and the operating process flowrate. It is assumed that the CFD particle track trajectories remain identical at different flowrates, and hence the particle residence time is scalable using the ratio of the flowrate used in the CFD simulation, \( Q_{\text{CFD}} \), and process operating flowrate, \( Q \), as expressed by

\[
t_{\text{res}, j} (t_j) = t_{\text{res}, j, CFD} \times \left( \frac{Q_{\text{CFD}}}{Q(t_j)} \right),
\]

(3-24)
and the assumption remains valid provided that the changes with flowrate are moderate. The CFD-generated residence time of a particle, $t_{res,i,CFD}$, is discretized into $m$ number of steps by dividing with the simulation time step size, $\Delta t$, and the number of time steps, $m$, of a CFD-generated particle residence time is calculated by,

$$m_i = \frac{t_{res,i,CFD}}{\Delta t}.$$  \hfill (3-25)

Then, the residence time of a particle can also be expressed by the sum of $m$ number of $\Delta t$, as expressed by,

$$t_{res,i,CFD} = \Delta t_1 + \Delta t_2 + \ldots + \Delta t_m. \hfill (3-26)$$

In order to calculate $t_{res,i}$, each of the $\Delta t$ term in equation (3-26) is scaled with a process flowrate, $Q_j$, that is simultaneous with the $\Delta t$ term of the $j^{th}$ time step. Each $Q_j$ is simultaneous with its corresponding $\Delta t$ term that is associated with a discrete time step. When a particle is sampled at $t_j = t_{sam}$, its $\Delta t_m$ is therefore associated with $t_{sam}$. The previous term, $\Delta t_{m-1}$ is associated with $t_{sam} - \Delta t$ and so on, until the final term, $\Delta t_{m_m}$ that is associated with $t_{sam} - m_i \cdot \Delta t$. Hence, the process flowrates assigned to the $\Delta t$ terms for scaling are obtained from the vector $\vec{Q}_j$ at time steps that are between $t_j = t_{sam} - m_i \cdot \Delta t$ and $t_j = t_{sam}$. Hence, the dynamic flow function, which determines the residence time of a sampled particle as a function of $t_j$ is expressed by,

$$t_{res,i}(t_{sam}) = t_{sim} \cdot \left( \frac{Q_{CFD}}{Q(t_{sam})} \right) + t_{sim} \cdot \left( \frac{Q_{CFD}}{Q(t_{sam} - 1 \times \Delta t)} \right) + \ldots + t_{sim} \cdot \left( \frac{Q_{CFD}}{Q(t_{sam} - m_i \times \Delta t)} \right). \hfill (3-27)$$

The time referencing function tracks the particle entry time, $t_{ent,i}$, of a sampled particle, $i$, which is calculated as the difference of the sample time and particle residence times, $t_{res,i}$:

$$t_{entry,i} = t_{sample} - t_{res,i}, \hfill (3-28)$$
where \( t_{res,i} \) is calculated as shown in equation (3-37). Then, the function identifies the disinfectant decay model and disinfection parameters of the particle from the UTIM by searching for the parameters from the row in the UTIM associated with \( t_f = t_{ent,i} \).

Then, the particle residence time as calculated from equation (3-37) and the particle disinfectant decay model and disinfection parameters identified using the particle entry time are substituted into the disinfectant decay model, equation (3-9); the CT model, equation (3-10); and the two disinfection models, equation (3-13) and (3-14). Since \( t_{res,i} \) and \( t_{ent} \) are dependent on \( t_{sam} \), the models are expressed for each sampled particle as functions of the simulation sample time:

\[
C^K_i(t_{sam}) = \left[ 1 - \alpha(t_{ent,i}) \right] C_o(t_{ent,i}) e^{-k_i(t_{res,i})t_{res,i}} + \alpha(t_{ent,i}) C_o(t_{ent,i}) e^{-k_i(t_{res,i})t_{res,i}}, \tag{3-29}
\]

where \( C^K_i(t_{sam}) \) is the residual disinfectant concentration of a fluid particle, \( i \), sampled from the location \( K \) at \( t_{sam} \);

\[
CT^K_i(t_{sam}) = \left[ 1 - \alpha(t_{ent,i}) \right] C_o(t_{ent,i}) \left[ 1 - e^{-k_i(t_{res,i})t_{res,i}} \right] + \alpha(t_{ent,i}) C_o(t_{ent,i}) \left[ 1 - e^{-k_i(t_{res,i})t_{res,i}} \right], \tag{3-30}
\]

where \( CT^K_i(t_{sam}) \) is the value of the applied CT of the fluid particle, \( i \), sampled from the location \( K \) at \( t_{sam} \);

\[
LI^K_i(t_{sam}) = \frac{LI_{plateau}(t_{ent,i})}{1 + e^{-k_i(t_{res,i})[CT^K_i(t_{sam}) - P(t_{ent,i})]}}, \tag{3-31}
\]

where \( LI^K_i \) is the disinfection level calculated from using the first disinfection model, where the disinfection level is expressed in terms of log inactivation achieved by the fluid particle applied CT calculated from equation (3-30); and

\[
\frac{N^K_i(t_{sam})}{N_o(t_{ent,i})} = \left[ 1 - \beta(t_{ent,i}) \right] e^{-k_i(t_{res,i})CT^K_i(t_{sam})} + \beta(t_{ent,i}) e^{-k_i(t_{res,i})CT^K_i(t_{sam})}, \tag{3-32}
\]

where \( N^K_i \) is the survived microbial counts resulted from the fluid particle applied CT, using the second disinfection model. Disinfection level is expressed in terms of the fraction of
surviving microbes. Survived microbial counts from the two disinfection models proposed by this thesis are calculated respectively using equation (3-31) as and rearranging equation (3-32) to get

\[ N_{i}^{K}(t_{sam}) = N_{i}(t_{out,i}) \cdot \log\left(\frac{1}{LI_{i}^{K}(t_{sam})}\right). \]  

(3-33)

Finally, the performance outputs of the USM are the average disinfectant residual concentration, \( C_{\text{avg}} \), and the average survived microbial counts, \( N_{\text{avg}} \). They are calculated as averages from their corresponding particle distribution.

\[ C_{\text{avg}}(t_{sam}) = \frac{\sum_{i=1}^{n_{\text{part}}} C_{i}(t_{sam})}{n_{\text{part}}}, \]  

(3-34)

\[ N_{\text{avg}}(t_{sam}) = \frac{\sum_{i=1}^{n_{\text{part}}} N_{i}^{K}(t_{sam})}{n_{\text{part}}}. \]  

(3-35)

where \( n_{\text{part}} \) is the total number of Lagrangian fluid particles utilized by the CFD simulation; and

Equation (3-34) and (3-35) predict the performance of the chemical disinfection process by calculating the outlet residual concentration that is the performance factor of evaluating whether a dosing strategy can meet the target residual setpoint; and by calculating the surviving microbial counts, the capability of the process to meet regulatory limits of target pathogens or required log inactivation can be estimated.

Applications of the USM. The first application of the USM is to provide a platform to simulate the performance of different dosing strategies for chemical wastewater disinfection processes by accounting for the unsteady stochastic process conditions; without the needs to utilize unsteady CFD simulations. For example, the different control methods that are discussed next were all simulated by the USM. The second application is that the dynamic flow function, time referencing function, and the calculation of overall process performance are utilized as the modelling components of the mode-based chemical dose control algorithm to be introduced next.
3.4 Model-based and Other Chemical Dose Control Algorithms

The model-based control algorithm is developed from a feedforward predictive model that is based on in-situ probe measurements of the disinfectant residual concentration and the particle tracks generated from the CFD simulation of the process flow geometry. In this thesis, the probe measurements are disinfectant residual concentration simulated by the USM, but actual in-situ probe measurements can be used when the algorithm is implemented in an actual process. Using the probe measurements and particle track data, the algorithm can predict the unsteady stochastic chemical disinfectant decay model parameters at the inlet. Then, using the USM; the algorithm can predict the process effluent disinfectant residual concentration and adjust the applied disinfectant dose, $C_o$, to meet the required disinfectant residual setpoint. The remainder of this section presents the model-based control algorithm, and briefly explains a PID-type control algorithm dose and a flow pacing algorithm. The control performance of all three control strategies are presented in Section 4.2 to evaluate the model-based control in comparison to PID control and flow pacing.

3.4.1 Control Setpoint

First, the control setpoint is defined for the control algorithm. The user defines a disinfection level setpoint (i.e. microbial counts or number of log inactivation), and then a corresponding $CT$ setpoint is identified using a suitable disinfection model, such as equation (3-13) or equation (3-14). Then, the disinfectant residual concentration set point is calculated from the $CT$ setpoint by dividing it with the averaged residence time of the flowrate dependent process RTD. Hence, the process control algorithm is designed to meet the unsteady disinfectant residual setpoint, $C_{sp}$, that is a function of the discrete time, $t_j$. Thus, the setpoint function is given by

$$ C_{sp} (t_j) = \frac{CT_{sp}}{t_{res,avg} (t_j)} , $$

where $CT_{sp}$ is the $CT$ setpoint and $t_{res,avg}$ is the average of the particle RTD.
3.4.2 Feedforward Model-based Control Algorithm.

From equation (3-9), the chemical decay model coefficients are the fraction of slow decaying disinfectant, \( \alpha \), the rapid decay kinetic coefficient \( k_f \), and the gradual decay kinetic coefficient, \( k_s \). Since there are three coefficients to be predicted, three equations are required to solve for the three unknowns. Thus, the system of equations will be developed based on measured disinfectant residual concentration at three sample locations using three concentration measurement probes; and the particle residence times of the sampled fluid particles from each probe and the process outlet as obtained from Lagrangian CFD particle track data. Hence, the model-based control algorithm has a feedforward configuration.

The control algorithm utilizes the applied dose, the measured concentration, flowrate, and the particle residence time information for the probe locations and process outlet to develop a system of three equations to solve for \( \alpha \), \( k_f \), and \( k_s \). The general positions of the probes in the proposed model-based control algorithm should be located near the inlet of the process model as shown in Error! Reference source not found.. This is because the particle RTD near the inlet is closer to the plug flow condition and allows the algorithm to estimate the disinfectant decay model parameters based on the average residence time of a particle RTD.

![Inlet zone](image)

Figure 3-4. General positions of the sampling probes

The plug flow assumption is crucial to tracking the measured average residual disinfectant concentration decay under a unified time frame of averaged residence time, because residual
concentration in each individual particle cannot be measured. Then, the disinfectant residual concentrations are measured by the measurement probes, namely Probe-1, Probe-2, and Probe-3. Hence, equation (3-9) can be expressed for the measured concentration as

\[
[1 - \alpha(t_o)] \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,1}(t)} + \alpha(t_o) \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,1}(t)} = C_k(t_k),
\]

where \( t_o \) is the time of disinfectant dose application, \( C_o \) is the applied disinfectant dose, \( t_{\text{res},k} \) is the plug flow residence time of Probe-\( K \) (i.e., \( K=1,2,3, \ldots \)), \( t_k \) is the time that the concentration measurement is made by Probe-\( K \), and \( C_k \) is the disinfectant residual concentration measured by Probe-\( K \). The known variables are the applied dose \( C_o \), the measured residual concentrations \( C_1, C_2, \) and \( C_3 \), and the residence time of each probe. The average residence time of the probes, \( t_{\text{res},P1}, t_{\text{res},P2}, \) and \( t_{\text{res},P3} \), are obtained from the average of their respective residence time distribution.

Hence, \( \alpha \), \( k_f \), and \( k_o \) can be solved using the system of equations that is expressed by

\[
[1 - \alpha(t_o)] \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,1}(t)} + \alpha(t_o) \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,1}(t)} = C_1(t_1)
\]

for Probe-1,

\[
[1 - \alpha(t_o)] \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,2}(t)} + \alpha(t_o) \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,2}(t)} = C_2(t_2)
\]

for Probe-2, and

\[
[1 - \alpha(t_o)] \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,3}(t)} + \alpha(t_o) \cdot C_o(t_o) \cdot e^{-k_f(t_o)\tau_{res,3}(t)} = C_3(t_3)
\]

for Probe-3.

The model-based control algorithm assumes that the concentrations measured by each probe belong to the same sampled particles. Therefore, when concentration measurements are made with Probe-3 at each sample time, the sample times of the Probe-2, and Probe-1 measurements, \( t_2 \) and \( t_1 \), must be related \( t_3 \) using the respective residence times and time intervals of each probes. At the time of sampling, Probe-3 measurement time is equivalent to the sample time, as written by
\[ t_3 = t_{sam}. \quad (3-41) \]

In order to find the concentration measurement from Probe-2 for the same particles, the Probe-2 concentration measurement time, \( t_2 \), is calculated from \( t_3 \) and the residence time interval between Probe-3 and Probe-2, \( \Delta t_{3-2} \), as expressed by

\[ t_2 = t_{sam} - \Delta t_{3-2} \left( t_{sam} \right), \quad (3-42) \]

where the time intervals, \( \Delta t_{3-2}, \Delta t_{2-1}, \) and \( t_{res,3} \), are scaled with changing flowrate, and will be explained in further detail later. Similarly, the Probe-1 concentration measurement time, \( t_1 \), is calculated in the similar way as \( t_3 \) and the residence time interval between Probe-3 and Probe-2, \( \Delta t_{3-2} \), and Probe-2 and Probe-1, \( \Delta t_{2-1} \), as expressed by

\[ t_1 = t_{sam} - \Delta t_{3-2} \left( t_{sam} \right) - \Delta t_{2-1} \left( t_{sam} \right). \quad (3-43) \]

Lastly, the time of the applied dose, \( t_o \), is calculated as the difference between the sample time, \( t_{sam} \), and the Probe-3 residence time as

\[ t_o = t_{sam} - t_{res,3} \left( t_{sam} \right). \quad (3-44) \]

Based on the relationships shown in equation (3-41) to (3-44), the measured concentrations \( C_o \left( t_o \right), C_1 \left( t_1 \right), C_2 \left( t_2 \right), \) and \( C_3 \left( t_3 \right) \) are correspond to the same particles that are sampled by Probe-3 at the sample time, \( t_3 = t_{sam} \).

Lastly, in order to account for the unsteady flowrate during the disinfection process, the CFD-generated residence times and time interval between the probes are modified using the dynamic flow function. The terms \( \Delta t_{3-2, CFD}, \Delta t_{2-1, CFD}, \) and \( t_{res,3, CFD} \) are the time intervals between probes based on the CFD residence times, and they are discretized into \( m \) time steps as calculated by

\[ m_{3-2, CFD} = \frac{\Delta t_{3-2, CFD}}{t_{sim}}, \quad (3-45) \]
where \( m_{3-2, CFD} \) is the number of discretized steps for \( \Delta t_{3-2, CFD} \):

\[
m_{res,2-1} = \frac{\Delta t_{2-1, CFD}}{t_{sim}},
\]

(3-46)

where \( m_{2-1, CFD} \) is the number of discretized steps for \( \Delta t_{2-1, CFD} \); and

\[
m_{res,3, CFD} = \frac{t_{res,3, CFD}}{t_{sim}},
\]

(3-47)

where \( m_{res,3, CFD} \) is the number of discretized steps for \( t_{res,3, CFD} \). Then \( \Delta t_{3-2} \), \( \Delta t_{2-1} \) and \( t_{res,3} \) are calculated by applying the dynamic flow functions, as expressed by

\[
\Delta t_{3-2}(t_{sam}) = t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam})} + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - 1 \times t_{sim})} + ... + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - m_{3-2, CFD} \times t_{sim})} \right) \right) \right),
\]

(3-48)

\[
\Delta t_{2-1}(t_{sam}) = t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam})} + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - 1 \times t_{sim})} + ... + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - m_{2-1, CFD} \times t_{sim})} \right) \right) \right),
\]

(3-49)

and

\[
t_{res,3}(t_{sam}) = t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam})} + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - 1 \times t_{sim})} + ... + t_{sim} \left( \frac{Q_{CFD}}{Q_{op}(t_{sam} - m_{res,3, CFD} \times t_{sim})} \right) \right) \right).
\]

(3-50)

By relating \( t_3, t_2, t_1 \), and \( t_0 \) to \( t_{sam} \) with the terms \( \Delta t_{3-2} \), \( \Delta t_{2-1} \), and \( t_{res,3} \) expressed by equation (3-48), equation (3-49), and equation (3-50) as a function of the operating flowrate, the three equations can be continuously applied to solve for the chemical decay model parameters, \( \alpha \), \( k_f \), and \( k_s \), at every sample time, \( t_{sam} \). Then, the applied dose, \( C_o \), at every \( t_{sam} \) is calculated by replacing \( C \) with \( C_{sp} \) in equation (3-9) and then solving for \( C_o \), as expressed by

\[
C_o(t_{sam}) = \frac{C_{sp}(t_{sam})}{(1-\alpha) \cdot e^{-k_f \cdot t_{res,eff}(t_{sam})} + \alpha \cdot e^{-k_s \cdot t_{res,eff}(t_{sam})}},
\]

(3-51)
where $\alpha$, $k_f$, and $k_s$ are estimated by the model-based control algorithm and $t_{res,eff}$ is the averaged particle residence time of the process effluent.

### 3.4.3 PID-type Control.

PID controllers are commonly found in chemical engineering applications for process control. The disinfectant dose is adjusted according to the error term, $e$, that is calculated from the feedback measurement of the output parameter and the setpoint value. For a chemical disinfection process, the setpoint is the effluent residual concentration, $C$. The error term is written by:

$$e = C_{sp} - C$$  \hspace{1cm} (3-52)$$

that is the difference between the disinfectant residual concentration setpoint and the actual measured concentration. The error term is modified by proportional, integral, and derivative gains in the PID control equation to adjust the applied disinfectant dose until the actual residual concentration reaches the setpoint. The equation is expressed by

$$C_o(t) = K_p \cdot e(t) + K_i \cdot \int_0^t e(\tau) d\tau + K_d \frac{d}{dt} e(t),$$  \hspace{1cm} (3-53)$$

where $t$ is the continuous time, $C_o$ is the disinfectant dose determined by the control, $K_p$ is the proportional gain, $K_i$ is the integral gain, $K_d$ is the derivative gain. Then, in order to be implemented in the USM for comparison to the model-based control and flow pacing control; the equation is modified as

$$C_o(t_{sam}) = K_p \cdot e(t_{sam}) + K_i \sum_{t_{sam}=1}^{n_{sam}} e(t_{sam}) + K_d \cdot \frac{e(t_{sam}) - e(t_{sam-1})}{t_{sam} - t_{sam-1}}$$  \hspace{1cm} (3-54)$$

that is the discrete form of equation (3-53), where time is discretized by the sample time steps.

### 3.4.4 Flow Pacing Dosing Scheme

The flow pacing dosing scheme is commonly used to scale the applied disinfectant dose according to the operating process flowrate. Field tests are conducted to identify a baseline
applied dose, $C_{o,\text{base}}$, under certain flowrate, $Q_{\text{base}}$. Then, the operating applied dose is calculated by scaling the baseline dose with the operating flowrate $Q$, as expressed by

$$C_o(t_j) = C_{o,\text{base}} \cdot \frac{Q_{\text{base}}}{Q(t_j)},$$

(3-55)

where $C_o$ is the applied dose determined by the dosing scheme at sample time $t_j$.

### 3.5 Methodology Summary

This chapter has recommended various functions and algorithms for the prediction and control of the operating performance of municipal wastewater chemical disinfection process. In Section 3.1, the disinfectant concentration decay models, CT model, and disinfection models for waterborne pathogens in wastewater equation were developed using experimental data. In Section 3.3, the Unsteady State Stochastic Model (USM) was developed to simulate unsteady steady state stochastic disinfectant decay and disinfection conditions using the steady state particle tracks. This provides a simulation platform for predicting the disinfection process behavior under unsteady conditions and for testing dosing strategies to control the disinfection process. In Section 3.4, the feedforward CFD model-based control algorithm, the PID-type control, and the flow pacing dosing scheme were presented to adjust the applied disinfectant dose.
4 Results and Discussion

This chapter summarizes the experimental and modelling component of this thesis. Section 4.1 presents the results of the experiments that were conducted to develop the proposed models to predict chemical disinfectant decay, CT, and disinfection level of wastewater disinfection process. Section 4.2 presents the results of the process performance from implementing the model-based control algorithm, the PID-type controller, and the flow pacing dosing scheme using the USM as a simulation platform. Then, potential disinfectant savings and improved performance of the model-based control compared to the PID controller and flow pacing scheme are presented.

4.1 Disinfectant Decay and Disinfection Models

The decay of the chemical disinfectant (PAA) residual concentration and the disinfection levels were measured according to the methodologies given in Section 3.2. The disinfectant decay data were fitted to the disinfectant decay model, equation (3-9), and estimated the model parameters: $\alpha$, $k_f$, and $k_r$. Based on the experimental data, it was verified that disinfectant decay data of the same water sample can be pooled into a single dataset for regression analysis. Using the primary effluent samples from the Pottersburgh Wastewater Treatment Plant on November 24th, 2014 as an example, the decay data of the disinfectant concentration disinfectant decay curves, with applied dose of 2.0, 3.0, and 4.5 mg/L, were not lined up with each other as shown below in Figure 4-1.
Figure 4-1. Disinfectant decays of primary effluent with PAA doses of 2.0mg/L, 3.5mg/L, and 5.0mg/L: sampled on 2014-11-24.

Similar observation was also found in the secondary effluent samples, as shown in Figure 4-2.

Figure 4-2. Disinfectant decays of secondary effluent with PAA doses of 1.0mg/L, 2.0mg/L, and 3.0mg/L: sampled on 2014-11-24.
However, when disinfectant residual is normalized as \( C/Co \), where \( C \) is the measured residual concentration and \( Co \) is the applied dose, the data were in line with each other as shown below in Figure 4-3 and Figure 4-4.

![Figure 4-3](image1.png)

Figure 4-3. Normalized disinfectant decays of primary effluent (PWW) with PAA doses of 2.0mg/L, 3.5mg/L, and 5.0mg/L: sampled on 2014-11-24

![Figure 4-4](image2.png)

Figure 4-4. Normalized disinfectant decays of secondary effluent with PAA doses of 1.0mg/L, 2.0mg/L, and 3.0mg/L: sampled on 2014-11-24
Hence, the normalized disinfectant decay data generated from different initial applied doses can be pooled as a single dataset. Good prediction accuracy was observed in Figure 4-3 and Figure 4-4 when the pooled dataset was fitted to the model, and regression analysis found that the fits have R-square values of 0.99 and 0.97 respectively.

4.1.1 Estimation of the Disinfectant Decay Model Parameters.

The normalized disinfectant decay data were pooled according to their sample date and effluent type and fitted to the disinfectant decay model, and differences in their applied doses were disregarded. As shown below in Table 4-1, the disinfectant decay model parameters ($\alpha$, $k_f$, and $k_s$) for primary effluent samples are listed.

Table 4-1. Primary effluent disinfectant decay model coefficients.

<table>
<thead>
<tr>
<th>Sample Date</th>
<th>$\alpha$</th>
<th>$k_f$</th>
<th>$k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>2.8×10^{-1}</td>
<td>2.9</td>
<td>6.7×10^{-3}</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>2.9×10^{-1}</td>
<td>4.4</td>
<td>1.4×10^{-2}</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>7.7×10^{-1}</td>
<td>30</td>
<td>1.7×10^{-2}</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>8.0×10^{-1}</td>
<td>31</td>
<td>2.6×10^{-2}</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>4.8×10^{-1}</td>
<td>2.4</td>
<td>2.2×10^{-2}</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>4.9×10^{-1}</td>
<td>2.3</td>
<td>2.2×10^{-2}</td>
</tr>
</tbody>
</table>

An overall comparison for the predicted disinfectant residual concentrations and the corresponding measured concentrations of all the collected data of this study demonstrated high accuracy as shown below in Figure 4-5.
Figure 4-5. Measured residual concentration vs. predicted residual (primary effluent)

Regression analysis calculated a R-square value of 0.98 and demonstrated almost an 1:1 ratio between the sampled and predicted residual concentration. Similarly, the disinfectant decay model parameters from the regression analysis of the secondary effluent data are shown below in Table 4-2.
Table 4-2. Secondary effluent disinfectant decay model coefficients.

<table>
<thead>
<tr>
<th>Sample Date</th>
<th>$\alpha$</th>
<th>$k_f$</th>
<th>$k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-11-18</td>
<td>$7.4 \times 10^{-1}$</td>
<td>42</td>
<td>$9.9 \times 10^{-3}$</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>$8.7 \times 10^{-1}$</td>
<td>42</td>
<td>$9.8 \times 10^{-3}$</td>
</tr>
<tr>
<td>2014-11-24</td>
<td>$8.6 \times 10^{-1}$</td>
<td>28</td>
<td>$9.6 \times 10^{-3}$</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>$9.9 \times 10^{-1}$</td>
<td>40</td>
<td>$1.4 \times 10^{-2}$</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>$8.3 \times 10^{-3}$</td>
<td>44</td>
<td>$9.7 \times 10^{-3}$</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>$9.5 \times 10^{-1}$</td>
<td>34</td>
<td>$1.5 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Then, the comparisons of the actual and predicted residual concentrations are shown below in Figure 4-6.
Regression analysis of the secondary effluent data also demonstrated an almost 1:1 ratio between the model prediction and measured residuals and a high R-square value of 0.96. Finally, all of the data points from the disinfection experiments and their model fits are shown below in Figure 4-7 and Figure 4-8.
Figure 4-7. Disinfection experimental data points for primary effluents and their corresponding model fits.

Figure 4-8 Disinfection experimental data points for secondary effluents and their corresponding model fits.
The results presented above have demonstrated that equation (3-9) is a suitable disinfectant decay model for predicting the chemical disinfectant decay of the water samples tested in this study. Since the dataset with different applied doses can be pooled and fitted to the model, the disinfectant decay model parameters $\alpha$, $k_f$, and $k_s$ were shown to be independent from the applied disinfectant dose and dependent only on the wastewater quality. This implies the disinfectant decay model parameters can be estimated without accounting for the initial applied doses, provided that subsequent residual concentrations are measured. This is crucial for the model-based control algorithm, which estimate the decay model parameters by measuring the disinfectant concentration decay of applied doses that are adjusted continuously according to the process conditions.

**Development of the CT model.** The disinfectant decay model is a function of time. Hence, an applied CT model can be derived by integrating the decay model from $t = 0$ to time, $t$. The calculated CT is a function of both the disinfectant residual concentration and the reaction time. It is a monotonic function such that CT increases with time from $t = 0$ to time, $t$ while the disinfectant concentration decreases. Using the primary effluent data sampled from the Pottersburgh Treatment Plant on November 24th, 2014 as an example, the functions of CT using the applied initial doses of 5, 3.5, and 2.5mg/L are plotted with time in Figure 4-9.

![Figure 4-9. Model predicted values of CT as a function of time: Primary effluent sample, November 24th, 2014 (Dose = 2.0, 3.5, and 5.0 mg/L)](image-url)
Similarly, the CT can also be applied to secondary effluent as shown below in Figure 4-10.

![Graph showing model predicted values of CT as a function of time.](image)

Figure 4-10. Model predicted values of CT as a function of time: *Secondary effluent sample, November 24th, 2014 (Dose = 1.0, 2.0, and 3.0 mg/L)*

The model predicted CT presented here accounts for the chemical disinfectant decay and contact time. The model predicted CT is also independent to the applied dose. This is opposed to the conventional CT obtained from regulatory disinfection tables, which the value of CT is dependent on the initial applied dose and calculated from the product of the effluent residual concentration and the flow residence time.

4.1.2 Estimation of Disinfection Model Parameters and Selection of Disinfection Models.

When log inactivation was plotted against CT, it was observed that the disinfection data lined up to form a single disinfection curve despite differences in the applied doses, $C_o$. This shows that disinfection level is independent from the applied initial dose but dependent on the value of CT and the water quality that is related to the disinfection model parameters. The observation is

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14 For example: Guidance Manual for Compliance with the Filtration and Disinfection Requirements for Public Water Sources (AWWA, 1991) calculates CT as the effluent residual concentration and $t_{10}$ of the process effluent residence time distribution.
shown using the disinfection experiment data obtained from the Pottersburgh Wastewater Treatment Plant on December 4\textsuperscript{th}, 2014 as an example below in Figure 4-11 and Figure 4-12.

Figure 4-11. Disinfection of primary effluent with PAA doses of 4.0mg/L, 6.0mg/L, and 8.0mg/L (2014-11-25): \textit{model-1 and model-2 refers to the First and Second Disinfection Models as discussed in Section 3.1.}
Figure 4-12 Disinfection of secondary effluent (SWW) with PAA doses of 1.5mg/L, 2.5mg/L, and 3.0mg/L (2014-11-25): model-1 and model-2 refers to the First and Second Disinfection Model as discussed in Section 3.1.

The two disinfection models are proposed by this thesis to account for the non-linear response of disinfection level to CT shown in Figure 4-11 and Figure 4-12, and they both predicted the experimental results with good accuracy. Regression analysis calculated R-values of 0.96 and 0.95 respectively by fitting the example data shown in Figure 4-11 and Figure 4-12 to the First and Second Model. Next, the model parameters of the disinfection models are compared in Table 4-3 and Table 4-4 below.
### Table 4-3. Primary effluent disinfection model coefficients

<table>
<thead>
<tr>
<th></th>
<th>First Disinfection Model [Equation (3-13)]</th>
<th>Second Disinfection Model [Equation (3-14)]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$LI_{plateau}$</td>
<td>$k_1$</td>
</tr>
<tr>
<td>2014-11-18</td>
<td>3.3</td>
<td>1.8</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>3.3</td>
<td>5.6</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>4.2</td>
<td>40</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>9.6</td>
<td>4.4×10^{-1}</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>4.4</td>
<td>6.6</td>
</tr>
</tbody>
</table>

### Table 4-4. Secondary effluent disinfection model coefficients

<table>
<thead>
<tr>
<th></th>
<th>First Disinfection Model [Equation (3-13)]</th>
<th>Second Disinfection Model [Equation (3-14)]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$LI_{plateau}$</td>
<td>$k_1$</td>
</tr>
<tr>
<td>2014-11-18</td>
<td>3.2</td>
<td>13</td>
</tr>
<tr>
<td>2014-11-20</td>
<td>2.9</td>
<td>2.5×10^{-1}</td>
</tr>
<tr>
<td>2014-11-25</td>
<td>3.4</td>
<td>5.8</td>
</tr>
<tr>
<td>2014-12-02</td>
<td>2.9</td>
<td>14</td>
</tr>
<tr>
<td>2014-12-04</td>
<td>2.9</td>
<td>31</td>
</tr>
</tbody>
</table>

The model parameters of the two disinfection models as shown in Table 4-3 and Table 4-4 estimated the mechanistic model parameters of the chemical disinfection process by identifying
the values of the disinfection plateau, $LI_{\text{plateau}}$, the critical CT values for the disinfection lag and plateau, $P_1$ and $P_2$, the fraction of pathogens shielded by wastewater particles, $\beta$, and the disinfection kinetic rate constants for the pathogens shield by particles and ones that are readily accessible by the disinfectant, $k_p$ and $k_a$. The aforementioned model parameters can provide important understanding of the disinfection mechanism.

**Disinfection Model Comparisons.** The second disinfection model was selected based on the comparisons of the two models according to the accuracy of their predicted disinfection level and their ease of use in numerical simulation. Both models have predicted the experimental disinfection levels with high accuracy. The goodness of fit for the primary effluent data is shown below in Figure 4-13 and Figure 4-14 for primary effluent data and Figure 4-15 and Figure 4-16 for secondary effluent data.

![Figure 4-13](image_url)

**Figure 4-13.** Comparisons of the primary effluent measured LI and the predicted LI from the First Disinfection Model.
Figure 4-14. Comparisons of the primary effluent measured LI and the predicted LI from the Second Disinfection Model.

Then, the similar comparison was made for the secondary effluent measurements and the predict LI using the First and Second Disinfection Models, as shown below.

Figure 4-15. Comparisons of the secondary effluent measured LI. and the predicted LI from the Second Disinfection Model.
As shown above, both disinfection models predicted the experimental disinfection levels with high accuracy, and the regression analysis of their comparisons have shown R-square values between 0.99 and 1.0. However, the first model has estimated values between different samples to be up to 100 – 1000 times different in magnitude. Whereas the second model does not have this issue. One explanation was that the first model has five degrees of freedom and each experiment only had up to fifteen data points. This could imply that the model parameters of the first model could have been impacted by small variable in the measured results.

4.2 Disinfectant Dose Control Performance Evaluation

A chemical disinfectant process was simulated using the USM under unsteady conditions for a total simulated process operation time of $1.2 \times 10^3$ min. The unsteady and stochastic parameters utilized by the simulation to create the inlet conditions are given by Table 4-5 and Table 4-6.
Table 4-5. Disinfectant decay model and CT model unsteady stochastic condition parameters.

<table>
<thead>
<tr>
<th></th>
<th>$\bar{X}$</th>
<th>$\sigma_X$</th>
<th>$A_X$</th>
<th>$f_X$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>$5.0 \times 10^{-1}$</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$5.0 \times 10^{-1}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_f$</td>
<td>2.0</td>
<td>$5.0 \times 10^{-2}$</td>
<td>1.5</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_s$</td>
<td>$2.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-4}$</td>
<td>$1.5 \times 10^{-2}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 4-6. Disinfection model unsteady stochastic condition parameters.

<table>
<thead>
<tr>
<th></th>
<th>$\bar{X}$</th>
<th>$\sigma_X$</th>
<th>$A_X$</th>
<th>$f_X$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_o$</td>
<td>$1.0 \times 10^5$</td>
<td>3.3</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$5.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$H_{plateau}$</td>
<td>3.3</td>
<td>1.8</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$k_1$</td>
<td>1.8</td>
<td>2.7</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$P_1$</td>
<td>2.7</td>
<td>$4.0 \times 10^{-1}$</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$5.0 \times 10^{-2}$</td>
</tr>
<tr>
<td>$k_2$</td>
<td>$4.0 \times 10^{-1}$</td>
<td>7.5</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$P_2$</td>
<td>7.5</td>
<td>3.3</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$5.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$9.0 \times 10^{-4}$</td>
<td>$5.0 \times 10^{-8}$</td>
<td>$5.0 \times 10^{-5}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_a$</td>
<td>$5.0 \times 10^{-1}$</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$5.0 \times 10^{-2}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_p$</td>
<td>$1.0 \times 10^{-2}$</td>
<td>$5.0 \times 10^{-4}$</td>
<td>$5.0 \times 10^{-3}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

The simulation objective was to evaluate the performances of the feedforward model-based control algorithm as compared to the PID control and the flow pacing dosing scheme, and the basis for the evaluation is savings on disinfectant consumption to maintain effluent microbial count lower than a user defined limit. In addition, a based case that applied a constant dose
throughout the simulation was included to demonstrate worst case scenario where there is no process control. The process effluent microbial counts and the residual concentration resulted from the base case using a dose of 3.5mg/L is shown in Figure 4-17.

**Figure 4-17. Performance of the uncontrolled base case: constant dose = 3.5mg/L.**

The simulation has shown that under the unsteady stochastic operating conditions; the base case could not provide reliable disinfection performance and was not capable of maintaining the residual concentration setpoint. The model-based control, PID control, and the flow pacing dosing scheme adjust their applied dose according to their specific functions, which has already been described in Section 3.4. The model-based control and PID target to meet residual concentration setpoint to achieve a user defined CT that would provide an expected disinfection level. On the other hand, the flow pacing scheme scale a baseline dose by using a flowrate ratio of the operating flowrate and the flowrate used for CFD simulation. The dose applications of the different dosing models throughout the simulation are shown in Figure 4-18.
Figure 4-18 Dose applications of the PID, model-based, and flow pacing controls: the base case is included for comparisons.

Then, the disinfection performance of the PID control, model-based control, and the flow pacing dosing scheme were compared by their simulated effluent microbial counts. An arbitrary microbial limit of 1000 cfu/100mL was introduced to evaluate the disinfection performance of the proposed dosing methods, as shown in Figure 4-19.
Figure 4-19. Disinfection performance of the PID control, model-based control, and flow-pacing dosing scheme.

The model-based control was able to maintain effluent counts below the regulatory limit during the course of the simulation. The PID control was able to comply with the microbial limit during the majority of the simulated operation but it was not able to do so during its starting up stage by gradually adjusting from a dose of zero to an applied dose capable of meeting the disinfectant residual setpoint as described in Section 3.4.3. The flow pacing scheme did not comply to the limit for a period of approximately 200min as shown in the figure above, but it was identified that by increasing the baseline dose of the flow pacing scheme from 3.5mg/L to 4.5mg/L, the scheme would meet the microbial limit as shown in Figure 4-20 below.
Figure 4-20. Disinfection performance of the PID control, model-based control, and flow-pacing dosing scheme: *with increased applied disinfectant dose for flow pacing.*

As previously mentioned in Section 3.4.4, the flow pacing dose application is calculated by scaling the baseline dose with the ratio of the operating flow and the flowrate used to generate the CFD simulation. Increasing the baseline dose from 3.5mg/L to 4.5mg/L is equivalent to consuming 29% more disinfectant, and increase the magnitude of overdosing during when the process experience conditions that do not require the baseline applied dose to be increased. Next, the models were evaluate based on meeting the disinfectant residual setpoint.
Figure 4-21 Effluent disinfectant residuals of the PID control, model-based control, and flow-pacing dosing scheme: the base case and setpoint are included for comparisons.

As presented in Section 3.4.1, the residual setpoint is a function of the CT setpoint and the process operating flowrate, thus it is not a constant value but varies with time. The residual setpoint in this sense is actually a setpoint curve. Hence, the control methods were targeting to meet the curve that is a function of time as opposed to a meeting a fixed target. By inspecting Figure 4-21, it was found that the effluent residual maintained by the model-based control was the closest to the residual setpoint curve. The shape of the residual concentration curve from the PID control was similar to the setpoint curve but consistently demonstrated a time delay, as its peaks were translated to the right relative to the residual setpoint curve. Whereas the flow pacing dosing scheme does not utilize the residual setpoint for adjusting the applied dose, and its disinfectant residuals did not appear to be matching up with the residual setpoint curve.

Last, the chemical consumptions of the disinfectant dose controls are compared. The calculations were based on the dosing curves shown in Figure 4-18 and the operating flowrates obtained from the CFD simulation. The modelled geometry is a pilot scale disinfectant contact tank with a system volume of 1.88m³ as presented by Section 3.3.1. From 333.0 to 1200min of the
simulation, the chemical consumed by the model-based control, the PID control, and the flow pacing dosing scheme are shown below in Table 4-7.

Table 4-7. Chemical disinfectant consumed by the PID control, model-based control, and flow-pacing dosing scheme

<table>
<thead>
<tr>
<th></th>
<th>PID control</th>
<th>Model-based control</th>
<th>Flow pacing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Disinfectant consumption (g)</td>
<td>345</td>
<td>338</td>
<td>395</td>
</tr>
<tr>
<td>% of disinfectant if replaced by the Model-base control</td>
<td>2.0</td>
<td>-</td>
<td>17.0</td>
</tr>
</tbody>
</table>

The total disinfectant consumption by the model-based control was lower comparing with the PID control and flow pacing, and potential disinfectant savings of 2% and 17% were found if a model-based control is utilized in instead of the flow pacing scheme for maintaining the same disinfection level.
5 Conclusions

Based on the results of the disinfectant decay and the disinfection experiments in the municipal wastewater disinfection study, this thesis proposed the disinfectant decay model, the CT model, and disinfection models that were utilized by the USM, a CFD-based simulation model, to predict and control the process performance of a chemical disinfectant contact chamber. The USM has reduced computation time by simulating the unsteady process with steady state CFD particle tracks. Then, the USM was utilized to validate the process control performance of the feedforward model-based control algorithm that uses in-situ disinfectant measurements from within the disinfection flow to predict disinfectant decay model parameters. Using the predicted results, the algorithm calculates an applied disinfectant dose to meet the effluent residual concentration setpoint. When compared to the PID-type controller and the flow pacing dosing scheme, the model-based control demonstrated savings of 2% and 17% respectively to maintain a microbial limit of lower than 1000 cfu/100mL. The simulated system was the CFD geometry shown in Section 3.3.1 operating under unsteady stochastic conditions.

5.1 Disinfectant Decay and Disinfection Modelling of Municipal Wastewater Chemical Disinfections

This thesis has developed mechanistic models that are capable of predicting disinfectant residual and disinfection level with high accuracy as presented in Section 4.1. The models are not dependent on the initial applied disinfectant dose but dependent only on the water quality. The water quality parameters accounted are for by the model parameters, presented in Section 4.1. Because the models are capable accounting for water quality that are corresponded to the disinfection mechanisms, they are applicable to different disinfection process with different source water quality. Their parameters can provide a quantitative understanding on the disinfectant decay and disinfection mechanisms of the water. Additionally, it is important that the decay model is independent from the applied dose from a model-based process control prospective. It is because the decay model parameters are predicted by the in-situ probe concentration measurements of residuals concentrations that resulted from different initial doses.
5.2 Potential Benefits of the Model-based Control Algorithm

This thesis has proposed a methodology to develop a model-based control algorithm that utilizes the residual concentration measurements of three probes to predict the chemical disinfectant decay in the process. Using the predicted coefficients for a disinfectant decay model and the particles residence time distribution generated from a Lagrangian CFD simulation, the algorithm was able to control a simulated chemical disinfection process using the USM. The simulation results have demonstrated that the model-based control algorithm has better performance compared to the conventional PID control and flow pacing dosing scheme. From Section 4.2, it was found that the model-based control algorithm achieve 2% and 17% disinfectant savings to achieve the same level of disinfection in a simulated 20hr operation when compared to the PID control and flow pacing scheme.

5.3 Future Work

There are three areas that can be explored in addition to this thesis. The first area is to validate the modelling results of this research: the disinfectant decay parameter predicted by the USM, and the performance of the model-based control algorithm. The experiment is recommended to be set up as a pilot scale chemical contact chamber with continuous test water supply, which the disinfectant decay and disinfection conditions together with other water quality parameters are characterized. Identical operating conditions should then be tested in the pilot unit and by the simulation procedures presented in this thesis. This allows the modelling results to be compared to reliable experimental data for validation. The validation results could then be used to fine tune the models.

The second area is to develop additional functions for the model-based control algorithm to predict the disinfection parameters. At this stage, the model-based control algorithm cannot predict disinfection model parameters because surviving waterborne pathogen counts cannot be measured online for the model to estimate the disinfection model parameters. However, it may be possible to correlate the disinfection model parameters to surrogate parameters that can be measured online. Hence, the objective here is to develop additional functions to predict disinfection model parameters using surrogate parameters that are correlated to the disinfection model parameters through statistical analysis. The research would involve identifying potential surrogate parameters and developing the statistical correlation.
The third area is to investigate possible ways to reduce the error associated with the model-based control algorithm. Despite of the potential benefits and advantages shown in this thesis, the feedforward configuration of the control is prone to prediction error. The three parameter non-linear disinfectant decay model expressed by equation (3-9) might be sensitive to the probe locations. It is because the probes must be placed in optimal positions to predict the curvature of the non-linear disinfectant decay curve. Since the initial drop is much faster than the gradual decay, it might be possible to research on two parameter decay models that assumes an instantaneous drop in disinfectant concentration. Also, the prediction error could be further reduced by incorporating the model-based algorithm with a suitable feedback controller, which could be incorporated in future research.
References


