MODEL PREDICTIVE CONTROL OF WATER QUALITY IN DRINKING WATER DISTRIBUTION SYSTEMS CONSIDERING DISINFECTION BY-PRODUCTS

by

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To my wife and parents

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ABSTRACT

The shortage in water resources have been observed all over the world. However, the safety of drinking water has been given much attention by scientists because the disinfection will react with organic matters in drinking water to generate disinfectant by-products (DBPs) which are considered as the cancerigenic matters. The health-dangerous DBPs have brought potential hazards to people's daily lives. Therefore investigating the nonlinear water quality model in drinking water distribution systems (DWDS) considering DBPs and controlling both disinfection and DBPs in an appropriate way are the basis of the research of this thesis.

Although much research has been carried out on the water quality control problem in DWDS, the water quality model considered is linear with only chlorine dynamics, the existence of DBPs caused by reactions between chlorine and organic matters has not been considered in the linear model. In addition, only the disinfectant (chlorine) is considered as the objective of water quality control. Compared to the linear water quality model, the nonlinear water quality model considers the interaction between chlorine and DBPs dynamics which follow the reaction fact in the DWDS.

The thesis proposes a nonlinear model predictive controller which utilises the newly derived nonlinear water quality model as a control alternative for controlling water quality. Dealing with the optimisation problem under input and output constraints requires advanced algorithm to handle the difficulty brought by nonlinear dynamic

model. In this thesis, the model predictive control (MPC) algorithm is the main driver for solving the nonlinear, constrained and multivariable control problem. EPANET and EPANET-MSN are simulators utilised for modelling in the developed nonlinear MPC controller.

However, uncertainty is not considered in these simulators because these simulators only measure the simulation data under given control inputs. Methods of modelling the nonlinear water quality model with considering uncertainty are required for controlling water quality with DBPs properly. Hence, the method called point-parametric model (PPM) is utilised to obtain the bounded nonlinear water quality model jointly considering the uncertainty and structure error. This thesis proposes the bounded PPM in a form of multi-input multi-output (MIMO) to robustly bound parameters of chlorine and DBPs jointly and to robustly predict water quality control outputs for quality control purpose.

The methodologies and algorithms developed in this thesis are verified by applying extended case studies to the example DWDS. The simulation results are critically analysed, which demonstrate the viability of the developed controller and algorithms.

Table of Contents

List of Figures

List of Tables

List of Abbreviations

ARMA	Autoregressive moving average
CIS	Critical Infrastructure Systems
CWSs	Contamination Warning Systems
DBPR	Disinfection Byproducts Rules
DBPs	Disinfection By-products
DMC	Dynamic Matrix Control
DP	Dynamic Programming
DWDS	Drinking Water Distribution Systems
FIR	Finite Impulse Response
FSP	Fixed Speed Pumps
GA	Genetic Algorithm
GAC	Granular Activated Carbon
GPC	Generalised Predictive Control
HAA5	Haloacetic acides
HAN	Haloacetonitrile
IDCOM	Identification-Command
IO	Input-Output
IP	Interior-Point
LCL	Lower Correction Level
LLC	Lower Level Controller

LP	Linear Programming
LQR	Linear Quadratic Regulator
LTV	Linear Time Varying
MBOP	Model Based Optimisation Problem
MCL	Maximum Contaminant Level
MCLGs	Maximum Contaminant Level Goals
MIMO	Multi-Input Multi-Output
MISO	Multi-Input Single-Output
MPC	Model Predictive Control
MRDLGs	Maximum Residual Disinfectants Level Goals
MSX	Multi-Species Extension
NMPC	Nonlinear Model Predictive Control
NOM	Natural Organic Matter
NP	Nonlinear Programming
PPM	Point-Parametric Model
QP	Quadratic Programming
RCLNDNS	Reactive Carrier-Load Nonlinear Dynamic Networks Systems
RFMPC	Robustly Feasible Model Predictive Control
SQP	Sequential Quadratic Programming
SWTR	Surface Water Treatment Rule
TCR	Total Coliform Rule

TTHMs	Trihalomathanes
UCL	Upper Control Level
U.S.EPA	United States Environment Protection Agency
UV	Ultraviolet
VSP	Variable Speed Pumps
VTP	Variable Throttle Pumps

CHAPTER 1 INTRODUCTION

1.1 Background and Motivation

1.1.1 Water Supply/Distribution Systems

Water is one of the most important resources that has a significant impact on our civilisation. It circulates from nature to the physical world by three main processes: 1) supply, 2) industrial and domestic use, and 3) treatment, which are illustrated in Figure 1-1 [1].

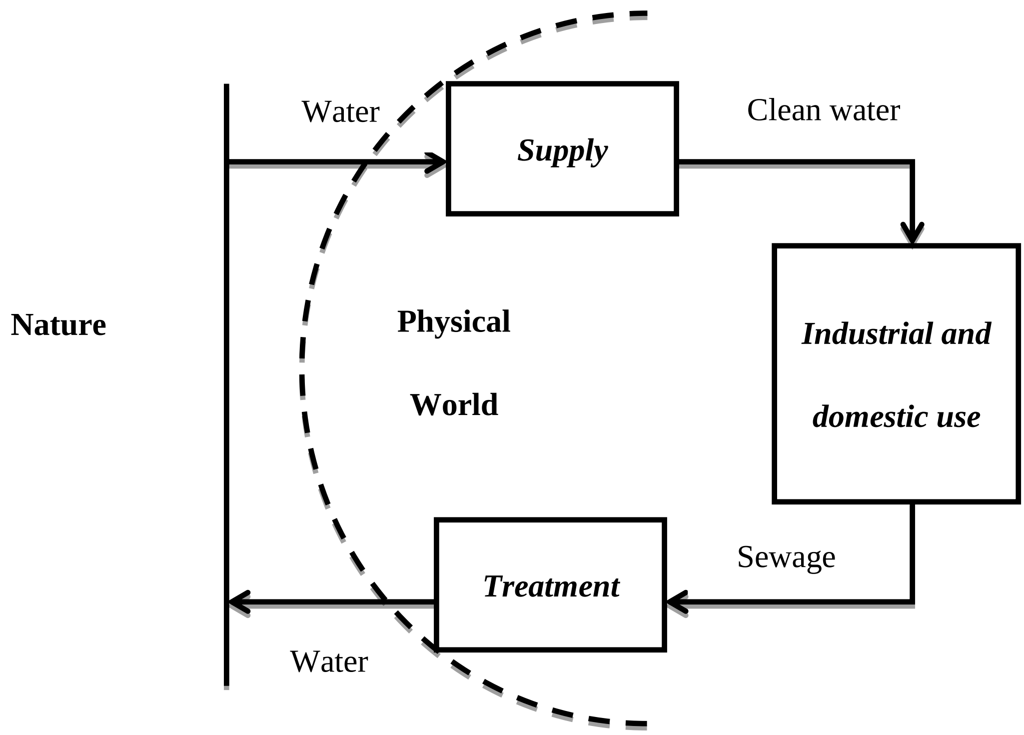

Figure 1-1 Cycle of Water Use from Nature to the Physical World

Drinking water distribution systems (DWDS) which belong to water supply/distribution systems in the supply process are the main interest of this thesis. In general, the supply process contains two types of systems which are water retention systems and water supply/distribution systems, respectively. Water retention systems contain many reservoirs built together with rivers in the environment. The basic functions of these systems are to guarantee the water supply continuity in considering seasonal fluctuations and flood prevention [1].

In addition, water supply/distribution systems aim to deliver clean water from rivers, retention reservoirs or underground water sources to industrial and domestic users by applying physical or chemical processes in the treatment works. There are three main components between water sources to water users, including 1) treatment works, 2) supply networks and 3) distribution networks, which are shown in Figure 1-2:

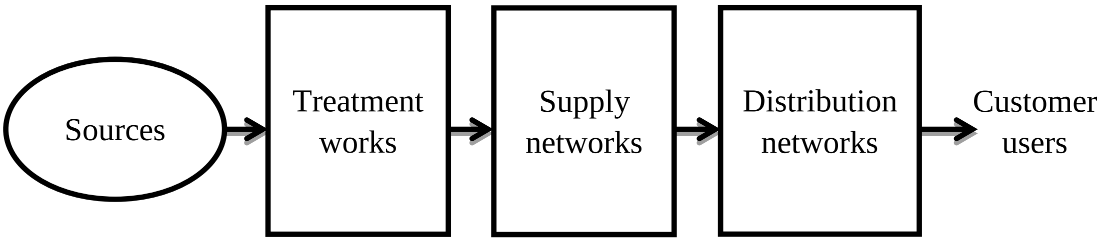

Figure 1-2 Structure of water supply/distribution systems

The 5 key elements in water supply/distribution systems are 1) treatment works, 2) underground supplies, 3) pumps, 4) pipes and valves and 5) reservoirs. The brief descriptions on treatment works and underground supplies are given as follows. The other elements are to be introduced in Chapter 3.

Water is screened to remove debris, like leaves, pieces of paper at the treatment works. And then, water is pumped to the reaction tanks, where the first stage of treatment process takes place, from the river. Processed water travels through the following stages by gravity, and then stops at the treated water reservoir. After a short period of remaining, the water in treated work reservoir is pumped down to the aqueduct by ‘high-lift’ pumps [1]. The raw water in the treatment works is sampled frequently for hardness test. And the chemical dosage for treatment process is automatically adjusted based on the prescribed limits for distributed water. The last stage in the treatment process takes place in the filtered water reservoir (treated water reservoir). The filtered water reservoir aim to remove any material in the treated water that may have been carried over from the reaction tanks by utilising a rapid gravity filter. Figure 1-3 presents a working treatment works near by a river.

Underground resource is the alternative of surface water resource. The underground water has to be pumped out from the well into a storage reservoir for further use which is one of disadvantages of underground water. However, the sub-surface water does not require much treatment and it has constant physical and chemical parameters [1].

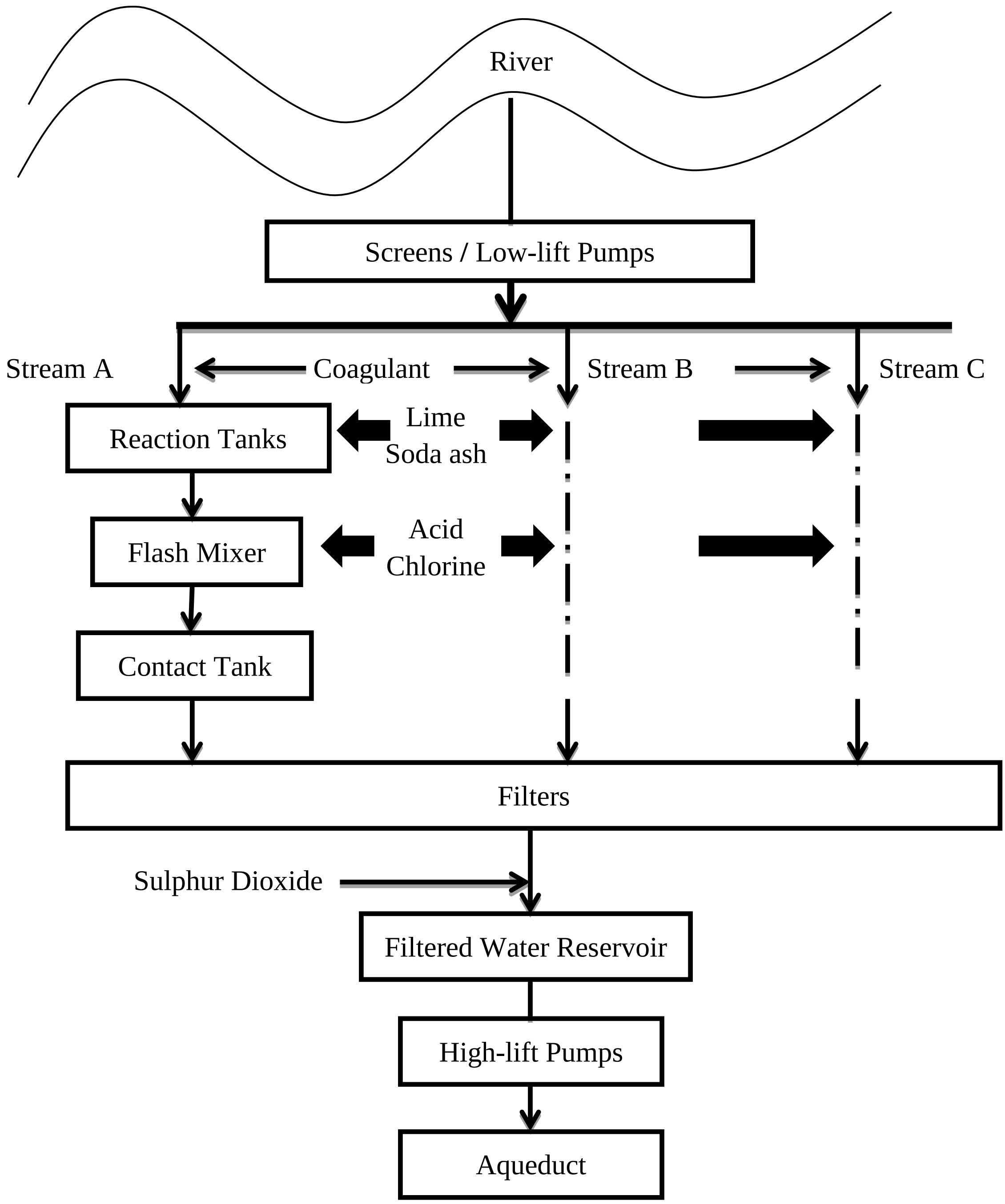

Figure 1-3 Presentation of a treatment works

Although supply systems and distribution systems have the same physical structure, the feature of these two systems is different and can be summarised as follows [1]:

Features of water supply systems:

1. Simple network structure with a limited number of connections;
2. Pipes with large diameter to transport bulk quantities of water;
3. Powerful pump stations composed of many pumps, mostly high-lifting pump;
4. Interactions with the distribution part of the system are modelled as demands which can be predicted with good accuracy;
5. System flows are insensitive based on reservoir level variations.

Features of water distribution systems:

1. Complicated network structure with hundreds of connections and many loops;
2. A typical zone contains at least one reservoir to sustain supplies and maintain pressures;
3. Reservoir level variations may have significant impact on the flows and pressures of the system.

1.1.2 Chlorination of Drinking Water in the Chemical Process

The final stage of treatment at drinking water plant is to kill the bacteria which will cause waterborne illness is disinfection. However, disinfectant may decay during transportation in the distribution networks, and the bacteria can grow during water transportation. Although bacteria are reduced by disinfectant in the network, the re-growth of them may still cause potential problems for water users. Hence, a certain level of disinfectant concentration is required to prevent bacteria re-growth in networks. Generally, the method of maintaining disinfectant concentration at a required level in DWDS is by injecting disinfectants into the network at certain positions in the network.

There are number of chemical disinfectants that can be utilised in the DWDS, including chlorine, monochloramine, hypochlorite, chlorine dioxide, chloramines and ozone. Moreover, non-chemical methods are also considered for disinfecting water, such as irradiation, anolyte and ultraviolet (UV) [2]. Chlorine is used as a primary disinfectant in DWDS because of its low cost and effective reduction on a variety of waterborne pathogens, such as Giardia, Cryptosporidium and viruses [3].

Monochloramine is popularly used as a secondary disinfectant because of its high efficiency in killing viruses, bacteria and other harmful microorganisms. One advantage of monochloramine is its chemical stability compared to chlorine, which makes monochloramine lasting longer in DWDS than chlorine. However, it takes a much longer time to act with microorganisms than chlorine, which makes monochloramine an effective secondary disinfectant [4].

By adding the chlorine gas to water, the chemical reaction between water and chlorine can be expressed as [5]:

$$Cl_2 + H_2O \Leftrightarrow HOCl + Cl^- \tag{1-1}$$

$$HOCl + H_2O \Leftrightarrow H^+ + OCl^- \tag{1-2}$$

The combination of hypochlorous acid ($HOCl$) and hypochlorite icons (OCl^-) is called free chlorine, which is determined by the pH. Free chlorine contains approximately 95% $HOCl$ at pH 6, while it contains approximately 95% OCl^- at pH 9 [6]. From the viewpoint of water quality control, maintaining concentration of free chlorine in the DWDS at a required level is one of the objectives. In general, a minimum concentration of free chlorine is needed for controlling the hazardous microorganisms in drinking water. Moreover, a value of 0.2 mg/L is determined by the Environment Protection Agency of United States (U.S.EPA) in practice [2].

1.1.3 Disinfection by Products

In the 1970s, existence of disinfection by-products (DBPs) was observed during the water treatment process because chlorine reacts with the organic matters that exist in the bulk water or pipe walls. Health-dangerous DPBs are considered the carcinogenic matter in drinking water systems. A number of DBPs have been identified after discovering Trihalomathanes (TTHM). The reaction kinetics of producing DBPs can be found in [6-8].

Many countries have proposed several regulations for water treatment processes and the operation of DWDS for controlling the potential health hazards from DBPs. The EPA made a two-stage regulation on disinfectants and DBPs called Disinfectants and Disinfection Byproducts Rules (DBPR). The stage 1 DBPR aims to reduce drinking water exposure to DBPs. It is applied to drinking water systems that inject disinfectant into the drinking water during the treatment process. And the stage 2 DBPR emphasise on enhancing public health protection by tightening monitoring requirements on TTHM and Haloacetic acides (HAA5). The final stage 1 DBPR includes the following regulations [3]:

- Maximum residual disinfectants level goals (MRDLGs):
    1. Chlorine (4 mg/L)
    2. Chloramines (4 mg/L)
    3. Chlorine dioxide (0.8 mg/L)
- Maximum contaminant level goals (MCLGs):
    1. Three trihalomethanes:
        (a). Bromodichloromethane (zero)
        (b). Dibromochloromethane (0.06 mg/L)
        (c). Bromoform (zero)

2. Two haloacetic acids:

    (a). Dichloroacetic acid (zero)

    (b). Trichloroacetic acid (0.3 mg/L)

3. Bromate (zero)

4. Chlorite (0.8 mg/L)

- MRDLs for three disinfectants:

    1. Chlorine (4.0 mg/L)

    2. Chloramines (4.0 mg/L)

    3. Chlorine dioxide (0.8 mg/L)

- MCLs:

    1. For total trihalomethanes (0.080 mg/L): a sum of the three listed above plus chloroform,

    2. Haloacetic acids (HAA5) (0.060 mg/L): a sum of the two listed above plus monochloroacetic acid and mono- and dibromoacetic acids

    3. Two inorganic disinfection byproducts:

        (a). Chlorite (0.1 mg/L)

        (b). Bromate (0.010 mg/L)

- A treatment technique for removal of DBP precursor material.

Note that the zero MCLG for chloroform has been removed by the EPA from its National Primary Drinking Water Regulations [2].

1.1.4 Advanced Water Quality Control Algorithm-Model Predictive Control

After two quality objectives introduced in the previous two sections, an advanced control technology is required to control the two water quality objectives. The main concern of controller-designer is to meet the prescribed requirements of a given target system under different constraints. However, systems can be classified into different categories, such as linear or non-linear, small scale or large scale. In reality, the target systems are nonlinear, constrained with multi-variables. Therefore, an advanced control algorithm is needed based on the characteristics of target systems.

In this research, the designed controller needs to handle two objectives with specified constraints, which are free chlorine and DBPs, respectively. For free chlorine, the concentration of free chlorine at monitored nodes must be maintained within defined lower and upper limits. And in terms of DBPs, the concentration of DBPs at monitored nodes has to be kept as lower as possible. Let us consider the standard controller first, for example, PI controller. PI controller is utilised for tracking the defined reference for plant outputs, and it is suitable for linear systems, especially for single output single input systems. In this research, there is no output reference to track but a reference zone to maintain and a minimisation task. Therefore, the standard controllers are not suitable to handle this nonlinear system with multi-outputs when no reference provided, especially for the case that there are interactions between the outputs.

In this thesis, Model Predictive Control (MPC) is selected as the main control strategy to handle the nonlinear, constrained with multivariable problems in water quality control of DWDS. The basic principle of MPC is that MPC repetitively solves the optimisation problems on-line over the defined output prediction horizon.

The MPC algorithm repeats at every MPC control time step by updating the measured or estimated plant states into the model of the plant. This receding horizon algorithm can handle time-varying disturbance or constraints since the model is initialised at every step by taking the feedback from the plant and only the first action of optimised control sequences is utilised for the plant.

Application of MPC on DWDS has been investigated in previous research on water quality control but with a linear quality dynamic model. In this thesis, MPC is applied on a nonlinear water quality dynamic model which considers the dynamic of DBPs.

1.1.5 Motivations

Drinking water is considered a rare resource in the world, especially in developing countries. It has a significant impact on people's daily life, especially on the health of those living in a developing area. However, water systems are complex because of their nonlinearity and unknown disturbance when operating in reality.

Water quality control is one of the main topics in DWDS. Based on the discovery of scientists in recent years, people have drawn much attention to carcinogenic materials brought by DBPs. Presently, the carcinogenic mechanism brought by DBPs is still under investigation. Therefore, controlling disinfectants and DBPs in DWDS becomes a hot topic in this field. In practice, the applications of water quality control in water industries are based on the water quality concentration measurements by employing data analyser suck as colorimeter, spectrophotometers and portable equipment. The dosage of chlorine gas is determined by analysing the data collected at monitored positions and highly-qualified personnel experience [9, 10]. Besides, the previous researches on analysing water quality control are based on the linear water quality model which only considers dynamic of chlorine. The generation of DBPs in water quality dynamics makes the water quality control problem much more complicated because the dynamics become nonlinear and more objectives are involved. Hence, jointly control of DBPs and free chlorine in DWDS requires advanced control technology.

Although much work has been done to address the water quality control problem, research work on the consideration of DBPs still needs to be enhanced. For example, the water quality dynamic model is not linear anymore which means a new control mechanism is needed. Therefore, it is worthwhile to carry out studies on such nonlinear water quality models from the aspect of its characteristic of nonlinear dynamics, modelling in parameters with uncertainty, monitoring the disinfectants and DBPs in the DWDS.

The motivations of conducting this research can be summarised as follows:

1. Safety of limited drinking water resource has been draw people's great attention on daily use, especially after discovery of health-dangerous DBPs.
2. The measurement equipment employed in practice is expensive, and the high-qualified personnel experience is also difficult to achieve. Therefore, it is necessary to investigate intelligent control methods to meet water quality control objectives.
3. As explained in the previous section, when compare to the standard controller, such as PI controller, MPC control algorithm is suitable to handle the nonlinear multivariable system with input-output constraints.

1.2 Aims and Objectives

This thesis aim to control the dynamic of both chlorine and DBPs in a proper way based on the newly derived nonlinear water quality model [7] that 1) free chlorine can be maintained within the prescribed limits so that the bacteria re-growth is halted in the whole DWDS, and 2) the potential hazards brought by cancerigenic matter DBPs can be dramatically reduced.

In reality, chlorine should not be the only objective considered in the water quality control problem. The cancerigenic objective DBPs is also required to be taken into consideration for decreasing the potential hazards in drinking water systems. In this thesis, the objective and sub-objectives of controlling water quality with considering DBPs can be summarised as follows.

1. The nonlinear MPC controller is to be designed.

(a). The model of the plant is modelling based on a simulator at this stage, which is EPANET simulator that is widely used in generating hydraulic and quality data. However, EPANET is only used for simulating linear water quality models which means only disinfectant data is to be generated. Therefore, the Multi-Species Extension of EPANET (EPANET-MSX) is required for adding DBPs into the simulator.

(b). In general, the modelling horizon for DWDS is set to 24 hours. The size of control horizon and output prediction horizon for the MPC controller are needed. Determination of these two time horizons is based on the quality control performance. In order to observe the influence caused by inputs, the control horizon must not be longer than the prediction horizon since detention time generated by water transportation. Setting a shorter controller horizon could reduce the computation time at each MPC time step, but efficiency of MPC controller will decrease as well because more MPC control steps are needed. Increasing controller horizon could observe more quality outputs and reducing the impact brought by transfer delay, however, the computation increases dramatically. Therefore, determining control horizon and output prediction horizon properly is a challenge in water quality control.

(c). A further problem in designing the MPC controller is to select a proper optimisation solver and define the objective function for the MPC controller. The selection is based on the characteristics of the defined objective function and behaviour of DWDS. Performance of such optimization solver requires analysis. Can DBPs be controlled by a defined optimisation problem? What difference can be observed between the linear water quality model and the nonlinear water quality model? Whether these questions can be solved theoretically has to be answered by analysing the simulation results.

(d). Tuning parameters of reaction kinetics in quality dynamics for obtaining a better performance.

2. Taking the uncertainty into consideration when the nonlinear water quality model is used.

(a). Linearization is commonly used in dealing with nonlinear problems but creates another problem which is structure error caused by linearization. Select a proper way to implement linearization of nonlinear water quality model is an important part of modelling.

(b). Bounding approach is a general way to handle unknown parameters of model. Once the model considering uncertainty is accomplished, bounding chlorine and DBPs separately or jointly is the other problem need to be solved.

(c). Validation on the completed model is needed for verifying its accuracy.

(d). Robustly predicting outputs of obtained model is one of main challenges in this research.

(e). Simulating the accomplished model and analysing the simulation results are essential to describe the performance of obtained model with considering uncertainty.

1.3 Contributions

The main contributions of this thesis can be summarised as follows:

- In the previous research on optimising water quality control, only the dynamic of disinfection is considered in the linear water quality model. The thesis has developed the nonlinear MPC controller for controlling water quality in DWDS based on the advanced nonlinear water quality dynamic model which jointly considers disinfection and DBPs objectives.
- The quantity in DWDS operates at a slow dynamic time scale measured in hours while quality operates in a fast dynamic time scale measured in minutes. The two different time-scale operation makes optimsing control on water quality much more complicated. The developed nonlinear MPC controller has been demonstrated its capability on handling highly nonlinear, constrained with multivariable and multi time-scale systems.
- In the previous research, the chlorine and DBPs were controlled independently and the interaction between chlorine and DBPs is ignored. In this thesis, the interaction between chlorine (disinfection) and DBPs are considered and jointly controlled under their dependent constraints within the developed nonlinear MPC controller.
- In the previous research, the PPM is applied to handle the uncertainty and structure error in water quality model. However, only the multi-input

single-output (MISO) PPM framework is obtained and only the parameters of chlorine (disinfection) are bounded and estimated. In this thesis, the multi-input multi-output (MIMO) model structure on nonlinear dynamic water quality model considering DBPs has been derived and presented. The parameters explaining dynamics of chlorine and DBPs are jointly bounded and estimated. And the outputs, including both chlorine and DBPs, are predicted robustly.

- The output prediction algorithm has been modified to incorporate the MIMO model in order to robustly estimate the parameters of the nonlinear quality model within the augmented objective-DBPs.
- In previous research, the PPM is applied to linear water quality model. In this thesis, an advanced nonlinear water quality model is applied to derive the MIMO PPM. The capability of the PPM in appropriately processing nonlinear systems optimisation problems has been proved by simulation results.

1.4 Thesis Outlines

Based on the above research focuses, the content of each chapter is summarised as follows:

Chapter 2: A literature review concerning existing research on operational control of DWDS is presented. The corresponding reviews on water quality control and MPC control mechanisms are presented in detail. The literature on introducing GA is also presented.

Chapter 3: The fundamentals of operational control in DWDS are presented. The physical elements in DWDS are introduced and their operational laws are presented in detail. Fundamentals, physical components and the related operation laws are to be employed in the simulated DWDS network utilised in Chapter 4 and Chapter 5. The path analysis algorithm is explained. And the application of path analysis algorithm is presented in Chapter 5.

Chapter 4: This chapter introduces the two time-scale hierarchical structure in DWDS which integrates quantity and quality. A newly derived nonlinear water quality model is presented. The MPC controller for jointly controlling chlorine and DBPs under input and output constraints is designed and presented. Application of such MPC controller to a case study DWDS network is presented in detail.

Chapter 5: Because the uncertainty is not considered in EPANET and EAPENT-MSX simulators, an advanced nonlinear water quality model with uncertainty is required. Therefore, PPM is introduced in this chapter. The MIMO structure for jointly bounding chlorine and DBPs is presented for the first time. The experiment design on obtaining the PPM is explained in detail. The algorithm for obtaining piece-wise constant parameters is presented. The modified robust output prediction algorithm is also presented in this chapter.

Chapter 6: The research work of this thesis is concluded in this chapter, together with a presentation of the further research topics.

CHAPTER 2 LITERATURE REVIEW

Model predictive control for water quality in drinking water distribution system that considers the impact of disinfectant by-products is a new topic in the water quality control field. Lots of literature has contributed to this research topic.

The review conducted in this chapter is carried out under the following aspects: 1) operation control on drinking water distribution systems including chlorine residual control, overview of disinfection by-products, placement of booster stations and monitoring sensors; 2) overview of model predictive control, including linear and nonlinear MPC, robust MPC, and optimisation improvement in MPC.

2.1 Overview of Operational Control on Drinking Water Distribution Systems

Drinking water distribution systems (DWDS) have been the subject of research for many years in order to guarantee the safe delivery of drinking water [11]. DWDS are groups of large scale complex networks containing water reservoirs (part of a water resource), storage tanks, pumps, valves and pipes which distributed across the whole network and connected with each network component to deliver safe water to the user's taps [2]. In order to supply high quality water to customers and satisfy consumers' demand in terms of both quantity and quality, implementation of the operational control of DWDS is necessary [2].

Quantity and quality are the two major aspects in the operational control of DWDS. The main objective of quantity control is handling the flow of pipes and pressures at the network junction nodes by producing optimal control schedules on valves and pumps, so that the customer water demand is satisfied and the electrical energy cost cause by pumping is minimised [1, 12].

In the other hand, maintaining the free disinfectant concentration at the monitored nodes (selected based on the characteristic of target DWDS) within the prescribed limits, including upper and lower limits, in such a way that the bacterial re-growth over a whole DWDS is halted is the main objective of water quality control [13].

However, as the free disinfectant reacts with the organic matter during the transportation over the DWDS producing so called disinfectant by-products (DBPs), which are dangerous to health, the DBPs concentration level over the DWDS are required to be as low as possible [14]. Minimising DBPs concentration at monitored nodes is considered as another objective of the water quality control in DWDS [13]. This augmented objective has enriched the objective in water quality control, and made the water quality control more complicated.

There is interaction between quality and quantity although it is a one way interaction from quantity to quality [13]. "Water quality is significantly determined by water quantity" this implies that in order to obtain a desirable water quality, controlling water quantity is a necessary step [15]. This feature makes it impossible to control quality or quantity without support from the other aspect. Therefore, an integrated manner for controlling both quantity and quality is needed.

However, due to different time scales in the internal dynamics of the hydraulic and quality, which can be described as slow and fast, respectively, a dimension complexity of the integrated control task becomes large. This makes the direct application of integrated control on water quality and quantity impossible, even for a small size DWDS [16].

To solve such problem, a hierarchical two time-scale control structure was proposed in[17, 18]. The basis of the control structure consists of two levels: Upper Control Level (UCL) and Lower Correction Level (LCL). Each level has its own optimising controller. The controller at the UCL operates on a slow hydraulic time (e.g. our hour) scale based on the accurate hydraulic model and simplified water quality model with the same time step (e.g. one hour). The models in UCL are used to predict the quantity and quality controlled outputs over the hydraulic prediction horizon (e.g. 24 hours). At the beginning of a control period, states of water quantity and quality, including 1) water flows, 2) pressures and 3) disinfectant concentrations at junction nodes or distributed in pipes are measured or estimated, and then sent to the integrated quantity and quality optimiser. Moreover, the prediction of water demand is also provided to the optimiser.

Due to the one-way interaction between quantity and quality, the hydraulic controls resulting from solving the optimisation task in UCL are truly optimal. The quality dynamics model in this optimisation problem has the same time step to the quantity dynamic model. Although the dimension of the optimisation problem is decreased, the modelling error of water quality dynamic is increased.

Therefore, improvement on the quality model is needed and this can be done at the LCL by applying the fast quality feedback controller which operates at a faster quality time scale (e.g. 5 minutes). The flows, considered as one of the quality controlled inputs and required at the LCL by the fast quality controller, are determined at the UCL.

There are several essential problems contained in the operational control of DWDS, which include 1) water quantity control, 2) water quality control, and 3) integrated control on both quantity and quality, 4) placement of hard sensors and booster stations and 5) soft monitors design. Literature related to these topics will be critically reviewed in the following sections.

2.1.1 Review on Quantity Control in Drinking Water Distribution Systems

The optimisation problem on quantity control considered by UCL includes 1) optimising the operation schedule of pumps and storage facilities, 2) minimising the energy cost and 3) optimising the valve and flow schedules.

According to the least cost design problem of DWDS proposed in [19-21], optimising pump operation becomes a hot topic in the field of managing DWDS [22]. Various methods have been developed to solve this problem since 1970 when dynamic programming (DP) was employed in [23] and [24] for energy saving optimisation. The results analysed in [24] has been shown that a conventional dynamic programming method can be applied to a simple DWDS. The total pumping costs can be evaluated accurately by taking account of factors including reservoir constraints, pumping efficiency, maximum demand tariffs and so on. Generally, DP can be used to solve some complex optimisation problems by breaking these problems into several simpler sub-problems, and solving each of the sub-problems and storing their solutions by utilising a memory which is data based structure. DP examines the previously solved sub-problems and combines their solutions to generate the best solution for the succeeding problems. However, DP is limited on solving those optimisation problems composed of unsolvable sub-problems or parametrised independently sub-problems. Different from DP, the linear programming (LP) procedure was utilised as the core of the developed planning model to deal with the pump operation problem in large-scale DWDS with a directed graph algorithm [25]. The results have been shown that the combination of LP and directed graph algorithm provides an extremely versatile tool to assist in the planning and management of a large-scale DWDS. Although LP is widely used, the linear assumption is a key weakness which limits its application.

Model predictive control (MPC) with genetic optimisation solver and adaptive multi-objective MPC were implemented in [26] and [27], respectively, for providing the optimal solution of quantity control in DWDS. Both of them are based on MPC driver but with different type of objective functions. Quantity optimisation problems were combined with quality optimisation in [26], while [27] solved the quantity optimisation problems independently as form of multi-objectives. However, the computation in [26] is more time-demanding compared to that in [27]. Other methods, such as nonlinear programming (NP) [28, 29], mixed-integer [30, 31] and metamodeling [32, 33] also performed well in providing proper solutions for quantity operation optimisation. Different methods applied are based on the characteristic of defined objective function or the purpose of solving described problems. For example, mixed-integer can be utilised in [30] because the gradients of objective function were known so that sequential quadratic programming (SQP) was applied for solving the optimisation task. And metamodeling was employed in [32] due to the purpose of reducing the computation time in solving the control optimisation problem in DWDS which means developing on modelling is significant. The further developed robustly feasible model predictive control (RFMPC) approach has been applied to quantity control in DWDS in [34] for solving the online optimising control problem in nonlinear plants with output constraints under uncertainty. Compared to normal MPC approach, RFMPC is more reliable and feasible in handling the uncertainty of control optimisation problems in DWDS.

2.1.2 Review on Chlorine Residual Control in Drinking Water Distribution Systems

Water is an important resource for both industrial and domestic usage [2]. However, due to climate change, a rising population and environment pollution, an increasing shortage of natural water resources around the world has been observed [35, 36]. This makes the protection of drinking water more important.

Drinking water is transported by DWDS from the water plant to consumer taps. As a result, meeting the demand for drinking water within the prescribed quality limits requires advanced control technology to operate DWDS. The advanced control technologies are discussed in this thesis. As mentioned above, quality control is divided into two parts: maintaining chlorine residual concentration throughout the whole water network within the prescribed limits, and keeping the concentration of disinfectant by-products as low as possible since disinfectant by-products are dangerous to health [13].

Modelling the quality model in a proper way is essential for achieving the quality control purpose. The previous research on water quality control mainly focused on a linear quality model. It means that chlorine residual is the only target to be maintained within the limits or minimised based on specified objectives.

A mass-transfer-based model was proposed in [37] for predicting chlorine decay in DWDS. The first-order reactions of chlorine occurring in the bulk flow and at the pipe wall are considered in this model. It is capable to explain the observed phenomena during the process of chlorine decay. However, all pipes in a network use the single wall decay would not be suitable for DWDS. In [6], a second-order kinetics model has been developed for better describing the chlorine decay and explaining the relationship between chlorine decay and the impact caused by bulk flow and the pipe wall.

In terms of controlling water quality at the monitored nodes in DWDS, a robust model predictive controller has been developed in [38] to maintain chlorine residuals within the prescribed upper and lower limits based on a state-space water quality model. The comparison between input-output modelling and state-space modelling regarding chlorine residuals control in DWDS has been presented in [2]. Compared to the result obtained from input-output modelling, that obtained from state-space modelling has been shown a more smooth performance. However, the computation time in state-space modelling is much more than that in input-output modelling.

Control of an uncertain time-varying linear dynamical system with deferred inputs has been achieved in [39]. The disturbance inputs, model parameters and the model structure errors of these systems are totally unknown. However, the inputs, parameters and structure errors can be bounded in an appropriate way. The output constraints are regulated by employing a model based predictive controller which uses a set of bounded uncertainties and appropriate safety zone design. This regulating method simplified the calculation on searching unknown parameters with limited information. And the designed safety zone guaranteed satisfaction on output constraints. However, feasible solutions may not be existed with obtained safety zone which requires a further investigation on the safety zone design approach.

The further developed intelligent model predictive controller is proposed in [40] for maintaining the bounding limits of chlorine residuals under uncertainty caused by modelling and demand prediction, and also under control input constraints. The quality feedback controller has been designed to implement the linear quality control, and the model parameter estimation and model output prediction have been achieved by utilising the set-bounded modelling of an uncertainty. The further developed robust MPC controller is more feasible than previous one as the constraints of input are considered in this controller.

Apart from applying model predictive control technology, the decentralised model reference adaptive control is implemented to control water quality in water distribution networks in [41], and the further developed adaptive control formulation to maintain chlorine residuals in DWDS is proposed in [42]. The adaptive control approach and related formulation are based on approximation of the input or output dynamic behaviour of chlorine in DWDS. The approximated dynamic behaviour is considered as the discrete linear time-varying model with unknown parameters. The foundation of adaptive control is parameter estimation which makes adaptive control popular especially in solving the optimisation problem with known varying parameters, or initially unknown parameters. However, MPC algorithm is not adept at solving problems unknown parameters independently. Combination of adaptive control and MPC may able to provide a reliable and feasible solution for these highly-nonlinear, multi-constrained with unknown parameters control optimisation problems.

2.1.3 Review on Disinfectant by-Products: History, Formation, Regulation and Control

Trihalomethanes (TTHMs) were the first class of halogenated DBPs identified in chlorinated drinking water [43, 44]. And the coincided related findings highlighted the link between the cancer and consumption on chlorinated water [45]. The National Organics Reconnaissance Survey conducted in 1975 by the U.S. Environmental Protection Agency (EPA) found that chloroform caused by chlorination was ubiquitous in all chlorinated water [46].

The National Cancer Institute identified chloroform as a carcinogen in 1976 [47]. Therefore, the EPA defined the limits of TTHMs [48] in drinking water. The maximum contaminant level (MCL) of total TTHMs was 0.1 mg/L. After identifying the existence of TTHMs in chlorinated finished drinking water, it was then discovered that only TTHMs were produced in the chlorination process.

Dichloroacetic acid and trichloroacetic acid were identified and known as the second class of DBPs in chlorinated drinking water [49-53]. Asides the halogenated DBPs mentioned above, there were other identified halogenated DBPs, such as 1) chloral hydrate, 2) haloacetonitriles, 3) chloropicrin, 4) haloketones, and 5) cyanogen chloride. These DBPs are of a lower concentration (compared to TTHMs) however still have effects on human health[54]. In order to investigate the adverse health effects associated with these specified halogenated DBPs, so many epidemiological researches have been developed since 1974. A feeble link between chlorinated water and cancers, such as bladder, colon and rectal cancer, has been gradually found in these researches [54, 55].

To achieve the required 0.1 mg/L MCL of TTHMs, water supply industries have adopted various strategies to comply with the new regulation. The most common treatments include: 1) moving chlorination downstream point into the treatment train, 2) reducing the chlorine doses and 3) employing an alternative disinfectant like chloramines to replace free chlorine [56]. The second treatment is the safest way to achieve the required MCL of TTHMs but with the worst performance, because reducing the chlorine doses may also reduce the chlorine concentration at remote junction nodes lower than minimum requirement. The third treatment is not recommended in normal case as chloramine is danger to use than chlorine.

Although new modifications mentioned above have shown that the target MCL for TTHMs could be achieved at an acceptable cost, problems about the impact of these modifications were raised, such as whether the microbial quality of finished drinking water was compromised as a result of these modifications [45]. The Surface Water Treatment Rule (SWTR) and the Total Coliform Rule (TCR) was published by the U.S.EPA in 1989. The rules above aim to 1) guarantee the microbial quality of treated water was not compromised, and 2) address the concerns on waterborne diseases/viral diseases [57, 58].

The EPA has tried a number of methods to balance the risk brought by DBPs and microbial disease [59]. However, the uncertainty on health effects and other promiscuous factors have made the EPA continue a negotiated rule-making method for appropriately regulating DBPs in drinking water [60].

According to the recent research on water quality control, chlorine residue is not the only objective any more. The prediction of chlorine residuals in DWDS is now taking the effect of disinfectant by-products into consideration [13]. This makes the linear water quality model become nonlinear. The augmented DBPs objective makes the water quality control problem more complicated.

Since the 1970s, the research on drinking water has mainly focused on understanding the occurrence of DBPs in chlorinated drinking water [61]. The interest on the developed models which applied to estimate the formation and the impact of DBPs has grown during recent years. This is because of the potential association of DBPs with cancer, particularly bladder and rectal cancer [54, 55].

The disinfection process starts at the beginning of the 20th century to inactivate and eliminate the pathogens in DWDS [61, 62]. The disinfection process in DWDS reduces the microbial risks, but simultaneously results in a chemical risk caused by

DBPs. DBPs are by-products of the disinfection process. They are produced by the reaction of disinfectant and the natural organic matter (NOM) and/or inorganic matters existed in DWDS.

Currently, there are no less than 600 different DBPs have been identified [63]. The major classes of DBPs generated from different disinfectants have been listed in Table 2-1. Several of them have not been identified in field-scale studies, but observed in laboratory based studies [64]. Chlorination has been used as the main-stream disinfectant process for domestic use in DWDS for a long period. Details on chlorination have been introduced in Chapter 1. Minimising the chlorinated DBPs by employing advanced control technology is one of the main objectives in water quality control, which will be discussed later in the thesis. However, existence of the chlorinated DBPs in DWDS like TTHMs emphasises the significance of discovering alternate disinfectants and new approaches in treatment process.

Table 2-1 Major groups of DBPs

Class of DBPs	Common Examples
Trihalomethanes (TTHMs)	Chloroform
Haloacetic acids (HAA5)	Chloroacetic acid

Haloacetonitrile (HAN)	Chloroacetonitrile
Inorganic compounds	Bromate, Hypobromite, Chlorite and Chlorate etc.

Several strategies for controlling halogenated DBPs formation have been proposed in [45] and listed below in Table 2-2:

Table 2-2 Strategies for Controlling halogenated DBPs formation

Main Strategies	Examples
Source Control	
Precursor Control	1. Enhance coagulation 2. Granular activated carbon (GAC) adsorption 3. Membrane filtration
Alternative oxidants and disinfectants	1. Combined chlorine (monochloramine) 2. Ozone 3. Chlorine dioxide 4. Permanganate 5. UV light
Air Stripping	

Source control emphasises the water sources management to reduce the NOM concentrations and bromide. Similar to source control, precursor control also aims to decrease the NOM concentration. The alternative oxidants and disinfectants focus on supplementing or replacing the chlorination process. Air stripping moves air through contaminated groundwater or surface water into an above-ground treatment system. However, the removed chemicals called 'Volatile Organic Compounds' are easily evaporated. This danger characteristic makes air stripping not recommended as a desirable treatment strategy.

2.1.4 Integrated Control of Both Quality and Quantity in DWDS

As described in previous section, quantity and quality are the two major aspects in control of DWDS with observed interactions. For the purpose of satisfying the quantity-quality interaction, [65-68] developed several proposals for considering both quantity and quality into one integrated control scheme. [65, 66] have implemented optimal operation control of a multi-quality supply/distribution system under different hydraulic conditions, steady-state flow and unsteady conditions, respectively. Results analysed in these two literatures have demonstrated that optimal operation of integrated quantity and quality control can be formulated and solved. But, they are limited to small-size networks because large-size networks make the formulation of optimisation problem much more difficult, even impossible to be formulated. In order to transfer the real-measured data into the integrated online-solved optimisation problems, receding horizon control technology was proposed in [67]. This control scheme provided a possible strategy to solve the integrated control problem on-line. [68] has employed the NP to solve the optimal pumping schedule problem considering water quality. However, the optimal solution obtained from the proposed methodology cannot be applied in practise because the optimal solution is local optimal, not global optimal.

Minimising the operational cost, satisfying the water demand with required quality and maintaining multi-constraints on quantity and quality are the main objectives in the optimising integrated control of water quality and quantity in DWDS [17, 69]. The constrained optimisation problems are complex because of following reasons: 1) nonlinearities, 2) large dimension, 3) output constraints, 4) mixed-integer structure of the involved variables, and 5) two time-scale dynamics in the system [16, 18].

An integrated approach named as the hierarchical control has been proposed in [17, 18, 69], where a hierarchical two-level structure was applied for incorporating the defined controller objective functions and making the synthesis of them possible. A feedback optimisation control in DWDS has been proposed in [70] with the optimising model predictive controller to overcome the integrated quantity and quality control problem. The proposed hierarchical structure uses two independent optimisation solvers for each control level because two time-scales of dynamics existed in quantity and quality. However, the feedback optimisation control built a link between two independent optimisation solvers and made interaction between two independent optimisation solvers possible.

2.1.5 Placement of Booster Stations and Hard Sensors in Drinking Water Distribution Systems

The treatment plant controls chlorine residuals directly to ensure the water entering into the entire DWDS compiles with the related standards. However, during the water transportation throughout the whole network, the free chlorine consumes bacteria and reacts with NOM. This will result in major decay and generation of DBPs, respectively. Thus the water safety may not be guaranteed especially at those remote junction nodes for domestic users. It is necessary to inject free chlorine by employing booster stations located at appropriate junction nodes of DWDS.

Booster disinfection is the additional disinfectant located at certain specified point distributed throughout a DWDS. It is used to ensure that the disinfectant residuals in DWDS are greater than the minimum amount [71]. Booster disinfection reduces the disinfectant dose amount compared to the conventional methods that use disinfectant only at the water source [71]. Such booster disinfections can reduce the mass of disinfectant and maintain a detectable residue at consumption junctions around the distributed network, which could lead to decreased formation of disinfectant by-products[72].

The problem of allocating disinfectant booster stations so that the amount of dosage required can be minimised and residuals concentration throughout the DWDS can be maintained at a required level is presented in [73]. The booster disinfectant location model involved is formulated by mixed integer linear programming. Although the results have been shown that the booster disinfectant location model can be applied to real-scale network, the solution efficiency is lack of validation. Furthermore, the booster station locations and related injection scheduling problem are discussed in [71] where a formulated multi-objective optimisation model was proposed. The objectives of the proposed optimisation model are: 1) minimisation of the total disinfection dosage, and 2) maximisation of the volumetric demand within prescribed limits. Multi-objective genetic algorithms were utilised for solving the optimisation problems. Moreover, a parallel multi-objective genetic algorithm was applied in [74] for optimising the allocations of booster disinfection in DWDS. Compare the three methods descried above, the problem considered in [74] is more comprehensive which makes the approach of parallel multi-objective genetic algorithm more reliable and realistic.

However, the quality model utilised above is linear and only takes chlorine residue into consideration. With further development on water quality model, a nonlinear water quality dynamic model which takes DBPs into consideration is proposed in [7]. The optimisation problem of locating disinfectant booster stations requires a new approach for dealing with the new water quality model.

The optimised allocation of disinfectant booster stations has been addressed in [75] based on linear and nonlinear water quality models for determining the impact of different model structures. The allocation task was also formulated as multi-objective but with both nonlinear and linear mixed-integer optimisation problems. Determining the allocation of disinfectant booster stations is one of the key issues in implementing quality control, and the placement of sensors on monitoring water quality is also important in this field.

The Safe Drinking Water Act requires that the water quality of drinking water in DWDS is to be sampled at certain locations where can represent the quality status of the whole distribution networks [76], however, the act does not explain how to select these sampling locations. Moreover, residual concentration is not the only objective that requires sampling and monitoring, contamination in drinking water distribution systems require hard sensors for monitoring as well.

Therefore, Contamination Warning Systems (CWSs) are introduced as a promising technology for reducing contamination risks in DWDS [77]. The critical problem in designing a working CWS is to develop the strategies on placing online sensors that can rapidly detect contaminations [77]. Approaches of locating monitoring stations in a DWDS are first presented in [76] by solving formulated integer programming problems. The synthesis of coverage matrices, integer programming and pathway analysis provides a first step towards appropriate algorithms for locating monitors in DWDS.

With further investigation into the sensor placement problem, several sensor placement strategies were explored. 1) Expert opinion is the strategies that guided by human judgment, its reliability is based on people's experience and expertise accumulated during solving related tasks in the past. For example, [78] and [79] evaluated sensor placements by experts who did not use computational models to determine the best sensor locations. 2) The ranking method is a similar further approach that aims to use expert information to rank potential locations for monitoring sensors [80-82]. 3) Formulating the task of sensor placement as an optimisation problem is the most popular strategy to use so that the performance of a possible sensor placement can be estimated computationally. Formulating a optimisation problem is more reliable than the other two strategies especially in some complicated networks, because calculation on optimisation problem is always stable and reliable when the formulation is correct while mistakes could be made from people's previous experience.

There has been a lot of research on sensor placement for DWDS in the past several years, it is impossible to review all of them, but their valuable research contributes to the development on controlling water quality in DWDS.

2.1.6 Monitoring by Soft Sensors on Water Quality in DWDS

For implementing MPC control on water quality in DWDS, the quality state feedback is essential to update at each control time step which means the proper on-line monitoring system for water quality is required.

Only few DWDS states which include concentrations of chemical and biological components can be measured on-line by hard sensors located at specified positions in DWDS due to the sensor access problems, the limit on costs and maintenance [7, 83]. Therefore, the missing information has to be collected by soft sensors which gather the variable measurements and mathematical models of quality states into water quality state estimators [7].

Several approaches were developed for achieving the robustness of estimates, including a set-member ship approach [84, 85], optimisation based set-membership algorithms [86, 87], cooperative dynamics [88] and interval observers and the interval state estimation [89-92]. Compared to the follow two methods, the first two methods are limited to on-line estimation because of the large demand on computation.

In the previous research [18, 69, 93, 94], a free chlorine concentration was utilised for the assessment of water quality state. The recent research work from [13] takes the additional quality state DBPs into consideration by applying a nonlinear dynamic water quality model derived based on the work presented in [6, 8, 95]. And monitoring water quality in DWDS by applying the derived nonlinear water quality model is addressed in [7].

2.2 Model Predictive Control Overview

Model Predictive Control (MPC), also known as Receding Horizon Control and Moving Horizon Optimal Control, has been utilised as a high-efficiency strategy to solve those constrained multivariable control problems for more than 30 years in the industry [96, 97]. The ideas of these control strategies can be traced back to the 1960s [98].

And, after several papers which mainly focused on presenting 1) Identification-Command (IDCOM) [99], 2) dynamic matrix control (DMC) [100] and 3) generalised predictive control (GPC) [101, 102] published in the 1980s, researchers have taken a keen interest in investigating this field.

DMC was developed to handle the constrained multivariable control problems especially in the chemical industries, while GPC was utilised to provide an alternative adaptive control. Therefore, industries preferred DMC more than other approaches because DMC brought a striking impact on industry. The original purpose of research on MPC was developed by trying to understand the operation of DMC [96].

2.2.1 Linear Model Predictive Control

Research on MPC nowadays is normally implemented on the controlled system described by a discrete time-varying linear model [96]:

$$x(k+1) = Ax(k) + Bu(k), \quad x(0) = x_0 \tag{2-1}$$

where $x(k) \in R^n$ and $u(k) \in R^m$ denote the state and control input, respectively. The receding horizon control is formulated as an open-loop optimisation problem [98]:

$$J_{(p,m)}(x_0) = \min_{u(\cdot)} \left[x^T(p)P_0x(p) + \sum_{t=0}^{p-1} x^T(i)Qx(i) + \sum_{t=1}^{m-1} u^T(i)Ru(i) \right] \tag{2-2}$$

subject to

$$Ex + Fu \leq \psi \tag{2-3}$$

where p denotes the prediction horizon, m denotes the control horizon or input horizon.

If the prediction horizon and control horizon both approach infinity without any constraints, the standard linear quadratic regulator (LQR) problem would be obtained, which was studied around the 1960s and 1970s [103]. However, by choosing the finite control and prediction horizons, the dimension of quadratic program can be finite and solved based on the process of implementing linear MPC algorithms. The constraints described in equation (2-3) may make the optimisation problem infeasible. Algorithms for pre-calculating the feasible region within non-zero initial conditions under certain possibility of stabilisation were proposed by [104, 105]. The proposed algorithms are based on several assumptions which limited the application of these algorithms.

It is not clear that what kind of conditions make the closed-loop system stable in either the finite or the infinite horizon constrained problem. The problem of stability was targeted in the 1990s [96], and there were two approaches proposed to solve the stability problem: one is based on the original problem described by equation (2-1) to equation (2-3), and the other approach has an extra contraction constraint [106, 107].

Stability of constrained MPC, which based on the monotonicity property of the value function have been verified in [108]. However, the most compact and comprehensive analysis was described in [109] and [110]. It simplified the problem by taking the assumption that $p = m = N$, and defining $J_{(p,m)} = J_N$ which is defined in equation

(2-2). Furthermore, use of the value cost function *J*, also the optimal finite horizon cost, as a Lyapunov function. It is required to prove that [96]:

$$J_N(x(k)) - J_N(x(k+1)) > 0 \qquad for \quad x \neq 0 \tag{2-4}$$

By rewriting $J_N(x(k)) - J_N(x(k+1))$ the function can be extended as follows [96]:

$$\begin{aligned} & J_N(x(k)) - J_N(x(k+1)) = \\ & [x^T(k)Qx(k) + u_N^{*T}(x(k))Ru_N^*(x(k))] \\ & +[J_{N-1}(x(k+1)) - J_N(x(k+1))] \end{aligned} \tag{2-5}$$

The stability can be proven if the right hand side of equation (2-5) is proven to be positive. Several approaches presented to verify that the right hand side of equation (2-5) is positive have been introduced in [96].

2.2.2 Nonlinear Model Predictive Control

When employ MPC algorithm to implement nonlinear system control, the nonlinear MPC is then required. Nonlinear MPC deals with the problem where the involved target system is based on nonlinear dynamic. Applications on different types of model, which have been described in discrete time algebraic descriptions, differential equations, Wiener models, differential-algebraic equations and neural nets, have been tested. The theoretical simulation results for several applications are described in [111-119].

However, different to the linear MPC, the possible mismatch between the performance of open-loop and closed-loop is unresolved in nonlinear MPC [96]. Furthermore, the feasibility of the nonlinear MPC is still a difficult topic. The additional difficulty in nonlinear MPC is the described optimisation task required to be on-line solved. It is difficult because those tasks are nonlinear programs, and have no redeeming feature that implies the indeterminacy of a global optimum [96].

From the control point of view, the global optimum must be calculated at each control time step to ensure the system stability. Within the infinite horizon, feasibility of a certain period can be considered as fixed once the feasibility at the first time step of this period can be found [96]. Applications on utilising infinite prediction horizon and control horizon was analysed in [108] for a discrete time case and in [120] for a continuous time case, respectively.

It is unfortunate that the problem within infinite horizon cannot be solved numerically in nonlinear MPC. Moreover, optimisation problem with equality constraints in nonlinear MPC can be solved but it is more computational and can only be met asymptotically [96].

A new idea in solving the optimisation and feasibility problems globally in nonlinear MPC has been proposed in [121] by introducing Variable horizon MPC. With the defined variable horizon time, a feasible control on solving the current on-line optimisation problem could be constructed from that employed at the previous iteration, and then the feasible control can be improved gradually. In addition, the Quasi-infinite MPC, which was introduced by [122, 123], utilises an infinite horizon to handle feasibility and optimisation problems without defining specified constraints and terminal regions. Employing variable horizon is more reliable than using infinite horizon because the assumption made on infinite horizon reduces its feasibility of application.

An alternative idea to solve nonlinear MPC is called contractive MPC which is first mentioned in [124]. The complete algorithm and proof on stability have been further developed in [125]. The key of this approach is to introduce an additional constraint to the usual formulation. The formulation aims to force actual states contracting at the following time steps. However, it is difficult to derive a proper constraint for defined formulation.

All the techniques mentioned above are utilised to solve the nonlinear MPC in overcoming the nonlinear dynamic model directly. However, each method has its specified conditions or extra controllers or extra constraints. The effort is inefficient and much more difficult when compared to solving the linear case [96]. It is recognised that making the system linearized initially can reduce the computational effort immensely. Therefore, several approaches have been proposed for solving such linearized nonlinear MPC problem.

1) The feedback linearization has been applied first in [126]. The MPC with feedback linearization was implemented in a linear system with cascade arrangement. The optimisation problem in the MPC approximately became a quadratic program. However, this approach is limited to low order systems which satisfied the conditions needed for feedback linearization.

2) Applying a different linear model obtained by implementing local linearization at each time step and also employing standard linear DMC to solve nonlinear MPC problem are introduced in detail by [127]. Because the linearization is implemented at each time step, the performance of this method is more accurate. However, the computation is much more demanding. In order to reduce the impact brought by disturbance, [128] and [129] proposed a developed method which added a developed Kalman filter to overcome the unstable dynamics for improving the disturbance estimation.. With further development based on this idea, [130] proposed an approach so that the explicit stability conditions can be achieved by adding contraction constraints.

3) Approximation on linear time-varying (LTV) system is applied in [131]. The approximation calculation is finished at each time step over the trajectory of predicted system which makes the computation tine-demanding.

4) The method of using a linear controller to approximate nonlinear MPC control law was proposed by [132] which emphasises on incorporating strategies of closed-loop control into the formulated MPC optimisation function. And then, the on-line computational demand can be significantly reduced.

2.2.3 Robust Model Predictive Control

MPC, based on feedback control method, has inherent robustness which has been analysed in [133-135]. Robust control means the system stability can be maintained and the performance specification can be satisfied within an uncertain range [96]. In other words, the minimum close-loop requirement is that robust stability can be guaranteed in the existence of uncertainty.

The robust performance is calculated by considering the worst performance under the specified uncertainty over a certain horizon [96] and the robust MPC optimisation problem is formulated as a min-max problem at the start of analysing robust MPC [97]. The extension definition of robust performance is based on measurement of the worst performance. The worst performance can be considered as an augmented ’robust’ MPC objective which aims to obtain the optimised control action by minimise the worst value calculated by analyzing the defined objective function. This describes the initial purpose of robust MPC algorithm. And the original robust

MPC algorithm was proposed in [136] by utilising the finite impulse response (FIR) models with uncertain coefficients. However, the algorithm proven by [137] indicated that robust stability cannot be guaranteed. It fails to obey the MPC algorithm that only the first component of the optimal control action is implemented and the min-max optimisation process is repeated at each control time step with the feedback update which causes uncertainties in the system.

Contraction principle was employed in [138] to obtain the sufficient necessary conditions for achieving stability robustly. Since these conditions are conservative, [139] addressed a new method that guaranteed robust stability by determining weights. In contrast to the literature which focuses on accessing robust performance, [140] proposed a new method to achieve robust stability by optimising nominal performance with an enforced robust contraction constraint which requires the states of the worst-case prediction to be contract.

Based on previous literature, the MPC design procedures for achieving robust stability can be summarised in two ways: 1) one is directly enforcing a specified robust contraction constraint to guarantees the state for all plants will converge in the presence of uncertainty, 2) the other is specifying description on uncertainty and performance objective so that the controlled optimisation leads to robust stability [141].

However, a new theory of a robust MPC control method has been proposed in [142]: both stability and offset- free set point tracking can be guaranteed under model uncertainty. Computation has also been proven in [142], and its application to examples can be found in [143].

Achieving robust stability is still a tough problem for implementing robust MPC in specified models, several approaches on how to access robust performance have been reviewed in this section. This literature contributes to the following research on robust MPC.

2.2.4 Optimisation Overview in Model Predictive Control

As described in previous sections, the theory of MPC is established one however is limited in performance and applicability because the areas modeling, sensing, state estimation, optimisation and fault detection, need to be improved [96]. The improved optimisation will be reviewed in this section because it is the most important issue on accessing control objectives.

As the feedback updates online are the basic premise behind MPC, the optimisation problem is required to be solved on-line as well. Based on the performance specification and the characteristics of the model, Linear Programming (LP), Quadratic Programming (QP) and Nonlinear Programming (NP) are usually described for the optimisation problems. The interior-point (IP) methods originally developed in the 1980s have drew research attention in solving LPs because they can be converge within 5-50 iterations depending on the size of problem [96], and they also are attractive for online use.

The extension of such methods for solving QPs were addressed in [144]. NP is the hardest case among the three. It is solved by applying sequential quadratic programming (SQP). SQP has a large demand on computation and has no convergence guarantee to global optimum solution. In order to improve the efficiency of computation, Genetic Algorithm (GA) has been proven to be another reliable solver for MPC [2, 13, 26].

A further approach of increasing the reliability and efficiency is to make the most of the problem structure. Take the Hessian matrices, highly-structured in the QPs, as an example. By utilising orders of magnitude in the structure of Hessian matrices, the computation can be increased dramatically in QPs [145]. Similar efforts have also been made in [146] for solving highly-structured large-scale LPs.

2.3 Review on Genetic Algorithm

As mentioned in the previous section, genetic algorithm (GA) has been considered as the possible solution of the optimisation solver in MPC.

GA is one kind of adaptive heuristic research based on population evolution and natural selection [147] which was introduced by John Holland in the early 1970s [148]. GA started with a possible solution called initial population with specified population size which remains the same during the whole process of the algorithm. New generation contains the possible solutions which are represented by chromosomes or strings [149] created by calculating a so called fitness value.

Fitness of each chromosome is evaluated at each generation, and some of them will be selected for constituting the next generation based on their fitness values. Matching the randomly selected chromosomes produces the offspring. While producing offspring, crossover and mutation happens at random. High fitness values mean chromosomes have a high possibility of selection, as a result the new generation created by the selected chromosomes may have a higher average fitness value than the previous one.

This evolution process is repeated until the prescribed condition is satisfied. The methodology of GA contains initialisation, selection, reproduction and termination [147]. The selection element is really important in GA because it determines the evolutionary search spaces, the selection mechanisms were introduced in [150].

GA has been widely applied as the optimisation solver in solving the optimising control problem in DWDS. [151] has employed GA to solve the optimal scheduling of multiple chlorine sources in DWDS. A hybrid GA has been utilised for optimisation of integrated quantity and quality control in DWDS [152]. Furthermore, a parallel multi-objective GA has been implemented in [74] for optimising the allocation of booster stations in DWDS. Furthermore, the reliability-based optimisation problem in DWDS was also solved by GA [153].

As a result of much experience applying GA to solve optimisation problem in DWDS, GA is also selected as the optimisation solver in this thesis for MPC controller.

2.4 Summary

This chapter has critically reviewed previous research related to operational control on DWDS, including quantity control, quality control and integrated quantity and quality control in DWDS. As the quality control associated with DBPs became a hot topic during recent years, the history, formation, regulation and control methods regarding DBPs were also reviewed in regards to previous researches. Joint control of DBPs and chlorine in DWDS is the main topic of this thesis. Joint control of chlorine and DBPs in the control of quality in DWDS is still a challenge in the DWDS control field, and will be discussed later in this thesis. In addition, the placement of booster stations and monitors, including hard sensors and soft sensors, were reviewed because they are the most important part of operational control in DWDS.

Furthermore, the literatures on MPC, including linear MPC, nonlinear MPC and robust MPC have been discussed. MPC is the main control strategy in this thesis for joint control of chlorine and DBPs in DWDS. The most important part of the MPC control problem contains the optimisation progress, therefore, several optimiser solvers have been reviewed based on previous research. Finally, GA, was selected as the optimisation solver for the MPC controller of this thesis, it has been reviewed in regard to its history and applications in DWDS.

Based on the above review, this thesis will conduct further study on the joint control of quality in DWDS while considering DBPs with MPC control algorithm. In addition, the related robust parameter estimation and output prediction regarding nonlinear quality dynamic model containing chlorine and DBPs will be discussed later.

CHAPTER 3 OPERATIONAL CONTROL AND MODELLING IN DRINKING WATER DISTRIBUTION SYSTEMS

This thesis mainly considers the water quality control in DWDS. However, water quality control and quantity control constitute the main aspects of operational control in DWDS. It is important to understand the fundamental knowledge of operational control of DWDS. Moreover, as hydraulic information is part of the inputs for water quality control, it is necessary to understand how hydraulic components work and their physical operational laws.

In this chapter, fundamentals of operational control of DWDS are introduced at the first. Then, the hydraulic components, including pipes, control valves pump stations and reservoirs, in the DWDS will be described. Furthermore, physical laws of operation in DWDS are given in detail. Finally, the path analysis algorithm for control of water quality in DWDS in the form of input-output models is introduced.

The overview of an example DWDS is shown in Figure 3-1:

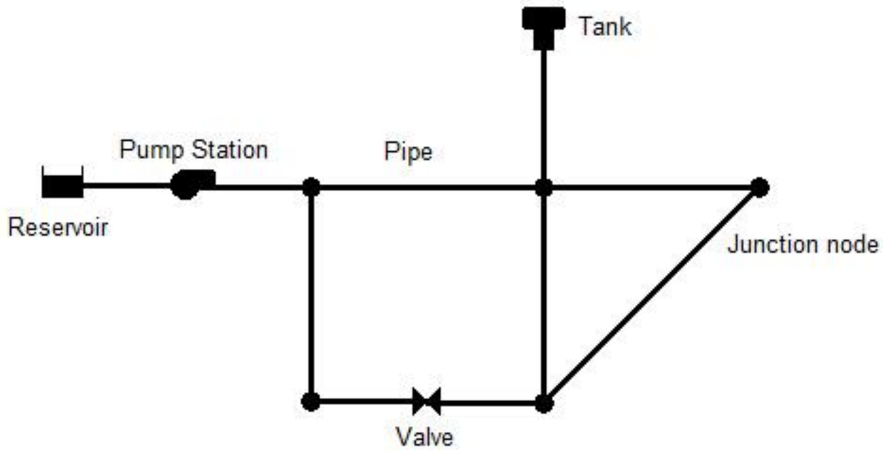

Figure 3-1 Overview of an Example DWDS

3.1 Fundamentals of operational control in Drinking Water Distribution Systems

Operation of water distribution systems require a number of decisions, which include development decisions concerning system development; management decisions for concerning system management and operational decisions for concerning system operation [1]. For example, system management needs to construct the regulations such as water pricing rules, water quality standards, consumer’s rights and obligations, and system operation specifies pump station configuration, water transportation, positions of monitor and booster station.

Operational decisions are different from two other types of decision because they change more frequently. Demand changes in the network or a security problem in the system require a new operational decision to be made.

3.1.1 Objectives of Operational Control

The specific objectives of operational control in DWDS vary depending upon the category of the water system. However, one of the common objectives is to satisfy the physical constraints. For example, in terms of physical components in DWDS, there are limitations on a retention reservoir which can be described as the maximum and the minimum levels of the reservoir. In the viewpoint of water quality control, maintaining the free disinfectant concentration (normally chlorine concentration) at a prescribed value or range can also be formulated as a set of equalities or inequalities constraints.

In this thesis, satisfying the objective of quality control not only considers the constraints on disinfectant, but also considers the minimisation of DBPs concentration in the specified network because DBPs are dangerous to people's health. Minimisation of operational cost is another control objective in the operational control of DWDS [1]. Electricity costs due to pumping constitute the major operational cost in DWDS. Moreover, the most important objective is to meet water demand generated by every consumer in the DWDS.

Therefore, the overall objective of operational control in DWDS can be summarised as: meeting water demand, satisfying the system constraints and minimising the operating cost.

3.1.2 Handling Uncertainties

It is significant to note that any operational decision making process is uncertain [1]. The time horizon in the operational control of DWDS is great when compared to other systems. Water demand is unknown at each hydraulic time step, values of parameters in pipes is unknown (for example, roughness coefficient), leakage is unknown regarding to time and position. Any of uncertainties mentioned above may require a redesign for obtaining a desired operational performance under such uncertainty.

A fundamental tool used by a system operator when making operational decisions is a predictive model of the specified system [1]. Predicting the uncertainty in systems over the considered time periods is a typical approach to handling uncertainty. The operational control problem becomes deterministic when the prediction of uncertainty is produced. There are a number of prediction methods using different descriptions of uncertainty which can be found in [1].

3.1.3 Basic Control Mechanisms

Two principle control mechanisms are utilised in the operational control of DWDS: control rules and repetitive control, respectively [1].

The control rule embeds available measurements into a control signal or decision, and the rule can be set up in the form of a table, formula, sets of written instruction, or even a computer program [1].

The repetitive control is based on the internal model principle. And it emphasise to reject or track arbitrary periodic signals during a fixed period [154]. The introduction of the repetitive control theory and its application to operational control of water systems can be found in [155].

3.2 Characteristics of Hydraulic Components and Physical Laws in Drinking Water Distribution Systems

The characteristics of water quality on transportation and mixing are mainly determined by the water flows, flow velocities and detention times from reservoirs. The hydraulic operation has a significant impact on the water quality modelling however the effect brought by chlorine injections can be ignored under certain accuracy. Modelling, simulation and operational control of water distribution systems are presented in [1].

However, the characteristics of hydraulic components and their related physical laws in DWDS are described here for better understanding the establishment of the water quality model and uncertain sources in water quality control.

The following assumptions are made for the following models which are also applied in the operational control of DWDS [2]:

1. The inertia effect of the water in the pipe is neglected;
2. Water is treated as incompressible fluid;
3. Constant temperature and air pressure within the DWDS;
4. Constant density and viscosity. Changes caused by injection of chlorine are neglected;
5. Instantaneous dynamics of the water network components are neglected, e.g. pump and valve on/off, and water pressure propagation dynamics in long pipes.

The simplified instantaneous hydraulics will result in the above assumptions, however, the control problems in DWDS are investigated in a time-scale from several minutes to hours. Therefore, the inaccuracies caused by the above assumptions can be considered as small and can be ignored while designing the controller [2].

3.2.1 Pipes

Pipes are the main components for water transportation and they deliver water from the higher head nodes to the lower head nodes. The direction of water flow is determined by the head of the junction nodes, if the head changes, the direction may change. The node with a higher head in a pipe is called the upstream node and the lower head node is called the sink node, the head-flow relationship for a pipe can be written as [1]:

$$q_{ij} = \phi_{ij}(h_i - h_j) \tag{3-1}$$

where q_{ij} denotes the flow from node *i* to node *j*, and $\phi_{ij}(\cdot)$ denotes the function between head loss and flow. The positive direction of q_{ij} is $i \to j$, if $q_{ij} \le 0$, the direction of the flow is $j \to i$. The flow q_{ij} is also called the discharge from node *i* to node *j*. Figure 3-2 [1] provides a graphical illustration of a single pipe.

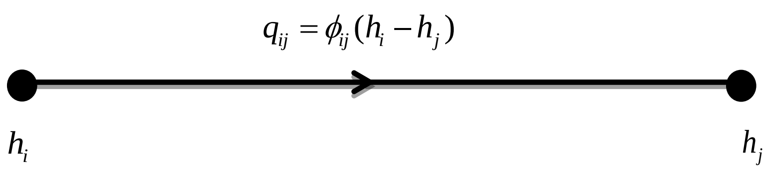

Figure 3-2 Model of a Single Pipe

By applying the Hazen-Williams formula, the equation (3-1) can be also written as [1]:

$$\phi_{ij}(h_i - h_j) = \phi_{ij}(\Delta h_{ij}) = G_{ij}(h_i - h_j)\left|h_i - h_j\right|^{-0.46} \tag{3-2}$$

where $\Delta \mathrm{h}_{ij}$ defines the head drop from the upstream node to the sink node in a pipe, and the coefficient G_{ij} presents the pipe conductivity. The Hazen-Williams equation, the most frequently used method in modelling DWDS, is selected because it is simple to calculate with acceptable accuracy which can meet the requirements of operational control in DWDS.

The above equation can be solved by introducing the head drop across the pipe [2]:

$$\Delta h_{ij} = h_i - h_j = g_{ij}(q_{ij}) = R_{ij} q_{ij} \left| q_{ij} \right|^{\alpha - 1} \tag{3-3}$$

where R_{ij} is the pipe resistance and α denotes the flow exponent caused by the friction losses during the transportation. By applying the Hazen-Williams equation, the equation (3-3) can be written as [1]:

$$\begin{aligned} \Delta h_{ij} &= h_i - h_j = g_{ij}(q_{ij}) = R_{ij} q_{ij} \left| q_{ij} \right|^{0.852} \\ R_{ij} &= (1.21216 \times 10^{10} \times L_{ij}) / (C_{ij}^{1.852} \times D_{ij}^{4.87}) \end{aligned} \tag{3-4}$$

where L_{ij} , D_{ij} and C_{ij} denote the pipe length, diameter and Hazen-Williams roughness coefficient, respectively. The value of the Hazen-Williams coefficient is mainly determined by the material of the pipe, and it can be changed according to the age of pipe, the manufacturer, workmanship and other factors [2]. If the pipe length and diameter are in *m* and *mm*, and the heads are in *m*, then the resulting flow in equation (3-1) are in *litre/sec* [1].

3.2.2 Valves

There exist several different kinds of valves used in DWDS for performing different functions [156]:

- Pressure Reducing Valves: Reduce water pressure
- Pressure Sustaining Valves: Maintain the pressure at a specified value
- Pressure Breaker Valves: Create required head loss across the valve
- Check Valves: Control the flow direction in one way only
- Flow Control Valves: Maintain the flow rate at a specified value

Pressure modulating valves, variable control valves, head control valves and non-return control valves are normally used in DWDS. In this section, the variable control valves are described as a modelling example, and one variable control valve is illustrated in Figure 3-3 . The variable control valves can be modelled as a pipe with controlled conductivity and are described as [1]:

$$q_{ij} = V_{ij} G_{ij} (h_i - h_j) \left| h_i - h_j \right|^{-0.46} \qquad (3\text{-}5)$$

where V_{ij} is the valve control factor. The valve is closed if $V_{ij} = 0$, and fully opened if $V_{ij} = 1$.

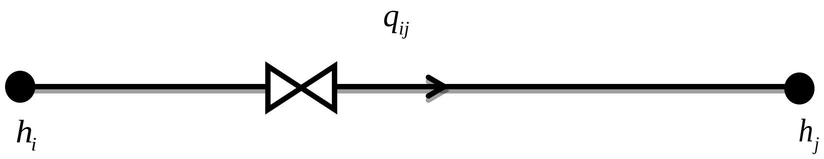

Figure 3-3 Model of Variable Control Valve Equipped in A Pipe

3.2.3 Pumps

Pumps are significant to water networks because they are the main energy consumption components in the DWDS. They transfer electricity energy to hydraulic energy and add energy into DWDS by increasing the hydraulic head of water. They provide the water supply from the water sources to the pipe distribution systems, and maintain the water head at a specified value throughout the whole network. There are three types of pump used in the DWDS, including fixed speed pumps (FSP), variable speed pumps (VSP) and variable throttle pumps (VTP) [1].

3.2.3.1 Fixed Speed Pumps

Considering a single fixed speed pump as an example, two nodes connected with the pump are called suction node and delivery node, respectively. The head-flow relationship of a fixed speed pump is called pump hydraulic characteristic curve, which can be written as [2]:

$$\Delta h_{ds} = g^{fs}(q_{sd}) \tag{3-6}$$

where $\Delta h_{ds} = h_d - h_s$ with $h_d \geq h_s$, h_s and h_d are called suction head and delivery head, respectively. q_{sd} denotes the flow from the suction node to delivery node. The superscript *fs* in $g^{fs}(q_{sd})$ presents ‘fixed speed’. Note that the pumping is always from the ‘lower head’ to the ‘higher head’ and this is why pumps are the active network elements and energy consumption components [1].

Equation (3-6) is a nonlinear function, and can be approximated by a quadratic function [157, 158]:

$$g^{fs}(q_{sd}) = A_{sd} q_{sd}^2 + B_{sd} q_{sd} + h_{so,sd} \tag{3-7}$$

where A_{sd} is the resistance coefficient with $A_{sd} \leq 0$, and B_{sd} is a coefficient normally taken as a value less than zero for guarantying a stable operating flow point with headloss. $h_{so,sd}$ is called the shut-off head [2].

Furthermore, pumps installed in the pump station can be operated in series or in parallel. If the pumps are operating in series, the connected pumps have the same flow but the total increasing head from the original node to the destination node is the sum of increased heads generated by each pump. If the pumps are operating in parallel, the increased heads generated by each switched on pump are the same but the flow from original node to destination node is the sum of flows across each switched on pump.

For a group of U fixed speed pumps operated in parallel with u pumps switched on, the hydraulic characteristic curves are the same and can be written as [1]:

$$\Delta h_{ds} = g^{fs}(q_{sd}, u) \tag{3-8}$$

$$g^{fs}(q_{sd}, u) = \begin{cases} A_{sd}(\frac{q_{sd}}{u})^2 + B_{sd}(\frac{q_{sd}}{u}) + h_{so,sd}, & if \quad u \neq 0 \\ 0 \quad , & if \quad u = 0 \end{cases} \tag{3-9}$$

where $u \in [0, U]$ denotes the number of fixed speed pumps switched on.

3.2.3.2 Variable Speed Pumps

The pump speed of VSP can be continuously controlled over a certain speed range. Considering a single VSP as an example, the hydraulic characteristic curve can be written as:

$$\Delta h_{ds} = g_{sd}^{vs}(q_{sd}, s_{sd}) \tag{3-10}$$

where s_{sd} presents the pump speed and is defined as [1]:

$$s_{sd} = \frac{operating\ speed}{nominal\ speed} \tag{3-11}$$

The nonlinear equation (3-10) can also be approximated by a quadratic function and written as [157, 158]:

$$g^{vs}(q_{sd}, s_{sd}) = A_{sd} q_{sd}^2 + B_{sd} q_{sd} s_{sd} + h_{so,sd} s_{sd}^2 \tag{3-12}$$

For a group of U variable speed pumps running in parallel with u pumps switched on, the hydraulic characteristic curves of these pumps are the same and can be written as [1]:

$$\Delta h_{ds} = g_{sd}^{vs}(q_{sd}, s_{sd}, u) \tag{3-13}$$

$$g^{vs}(q_{sd}, s_{sd}, u) = \begin{cases} A_{sd}(\frac{q_{sd}}{u})^2 + B_{sd}(\frac{q_{sd}}{u})s_{sd} + h_{so,sd} s_{sd}^2, & if \quad s_{sd} \neq 0, and\ u_{sd} \neq 0 \\ 0 & otherwise \end{cases} \tag{3-14}$$

where $u \in [0, U]$ denotes the number of variable speed pumps switched on.

3.2.3.3 Variable Throttle Pumps

Based on the flow described in equation (3-1), the inverse function of equation (3-13) can be defined as [1]:

$$q_{sd} = \phi(\Delta h_{sd}, s_{sd}, u) \tag{3-15}$$

Then, the hydraulic characteristic curves for a group of U variable throttle pumps in parallel with u pumps switched on can be written as [1]:

$$\Delta h_{ds} = g^{fs}(q_{sd}, u) - \Delta h^t(q_{sd}, v) \tag{3-16}$$

where $u \in [0, U]$, variable v is control factor for the throttle conductivity.

The above equation describes the final head increase from the delivery node to suction node. There are two parts to the right side of equation (3-16), the first part presents the total increased head from the group of fixed speed pumps, and the second part presents the head drop across the throttle and can be modelled as a variable control valve.

3.2.3.4 Pump Station

In general, pumps installed in the network are considered as the form of pump stations. The structure of a pump station consisting of all types of pumps in parallel is illustrated in Figure 3-4 [1]. The figure illustrates the configuration of the i^{th} pump station in the total of I pump stations in a network, where M_i^f fixed speed pumps, M_i^s variable speed pumps and M_i^t variable throttle pumps are contained within the i^{th} pump station. Notations q_i or q_{pi} present the overall pump flow in the pump station. h_{si} and h_{di} are the suction head and delivery head, respectively.

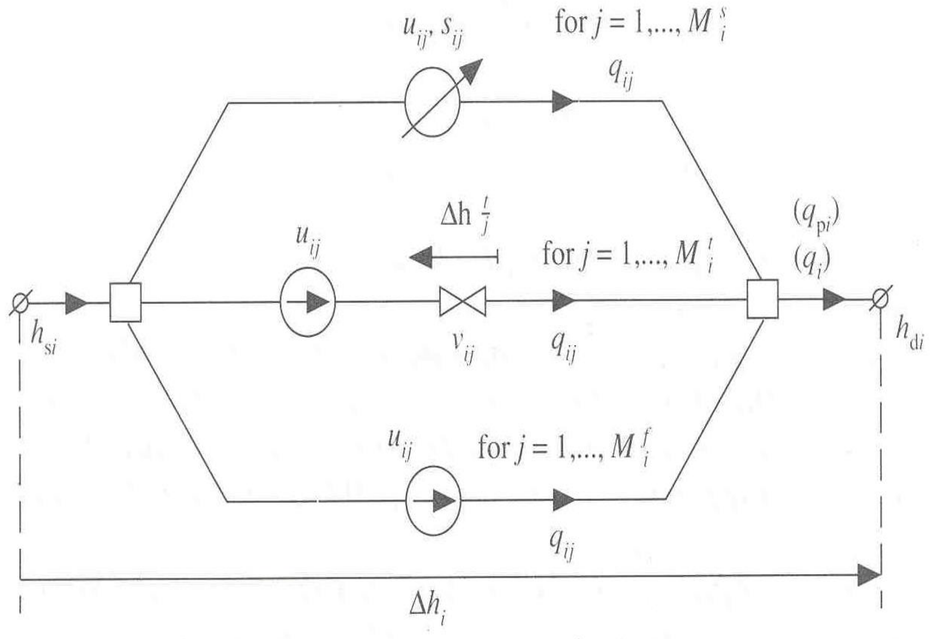

Figure 3-4 Generalized Pump Station Configuration [1]

3.2.4 Reservoirs

The distribution systems considered in this thesis are composed by pipes, control valves, pump stations, reservoirs (tanks) and consumers of drinking water, which are elements of the system. The pipes, control valves and pumps constitute the network branches, while reservoirs and drinking water consumers constitute the network nodes [1]. The water consumer nodes (non-reservoir nodes) are called junction nodes, which are different to reservoir nodes. Reservoirs are the dynamic elements in DWDS which can be considered as the energy stores. Figure 3-5 illustrates the model of a reservoir in DWDS.

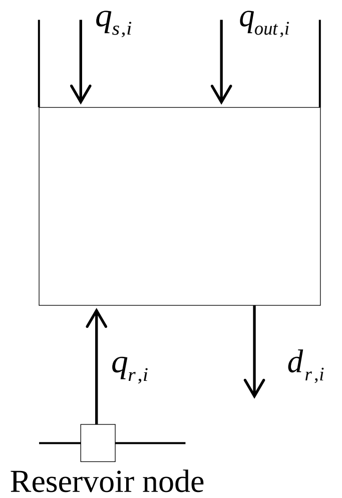

Figure 3-5 Model of a Reservoir

Denote q_s as the vector of flows from supply networks, denote q_{out} as the additional inflow which can be considered as the disturbance and it is different from q_s. Let us consider the i^{th} reservoir node in the network. The total water load $q_{lr,i}$ of reservoir i can be described as [1]:

$$q_{lr,i} = q_{s,i} - d_{r,i} + q_{out,i} \,, \quad for \;\; i \in [1,\, n_r] \;\; and \; i \in Z \tag{3-17}$$

where $q_{s,i}$ and $q_{out,i}$ denote the i^{th} components of the vectors q_s and q_{out}, respectively, and $d_{r,i}$ presents the i^{th} components of the reservoir demand d_r, and n_r denotes the number of reservoirs in the network.

Denote the flow vector delivered from the DWDS into the reservoir i as $q_{r,i}$. Then, the mass balance in the reservoir i can be described as [2]:

$$\frac{d\,w_i(t)}{dt} = \rho[q_{r,i}(t) + q_{lr,i}], \quad for\ i \in [1,\ n_r]\ and\ i \in Z \tag{3-18}$$

where ρ is the water density, $w_i(t)$ denotes the mass of water stored in the reservoir i at time instant t. Then, substituting the water head and cross-sectional area of the reservoir into equation (3-18) yields [2]:

$$\frac{d\,x_i(t)}{dt} = \frac{1}{S_i(x_i(t))}[q_{r,i}(t) + q_{lr,i}], \quad for\ i \in [1,\ n_r]\ and\ i \in Z \tag{3-19}$$

$$h_{r,i}(t) = x_i(t) + E_i, \quad for\ i \in [1,\ n_r]\ and\ i \in Z \tag{3-20}$$

Substituting equation (3-20) into equation (3-19) yields:

$$\frac{d\,h_{r,i}(t)}{dt} = \frac{1}{S_i(h_{r,i}(t))}[q_{r,i}(t) + q_{lr,i}], \quad for\ i \in [1,\ n_r]\ and\ i \in Z \tag{3-21}$$

where $x_i(t)$, $S_i(x_i(t))$ and $h_{r,i}(t)$ presents level of reservoir i, the cross-sectional area at this level and reservoir head, respectively. E_i is the reservoir elevation.

3.2.5 Physical Laws

3.2.5.1 Flow Continuity Law

For every junction node (non-reservoir node) j in the network, the following holds (see Figure 3-6):

$$\sum_{i \in J_j} q_{ij} = d_j \tag{3-22}$$

where J_j denotes set of nodes linked to the junction node j, and d_j are the water demand allocated to the junction node j. For reservoir nodes, $d_j = 0$ if no water demand is allocated to junction node j.

Furthermore, if j is a reservoir node in a steady state, which means the reservoir level at this node is constant, equation (3-22) is also satisfied at node j. The flow continuity law states that the sum of inflows and outflows is equal to zero for each junction node, and it is also holds for the reservoir nodes when they are in the steady state.

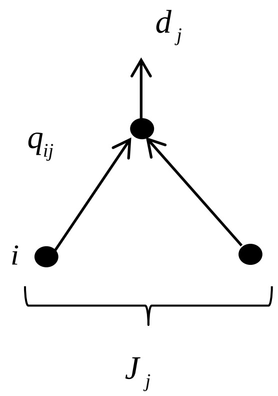

Figure 3-6 Connection Node

3.2.5.2 Energy Conservation Law

The energy conservation law is usually expressed in terms of the head change (increases or drops) along a loop or an energy path. The following holds:

$$\sum h_{ij} = \partial E_r \tag{3-23}$$

where $h_{ij} = h_i - h_j$ is the head change (increases or drops) across an arc (link) in r^{th} network path, and ∂E_r denote the energy difference between the starting node and final node on this path.

If the starting node is the same as the final node, which means the path existed as a loop in a network, the following holds:

$$\sum h_{ij} = 0 \tag{3-24}$$

The energy conservation law is applicable to all network paths that can produce the number of equations of the type described in equation (3-23) [1].

3.3 Path Analysis Algorithm

Only the input-output (IO) model is considered in this thesis, therefore, it is important to consider the transportation path from the injection node (input) to the monitored node (output) and the time delay associated with the path. In this section, the detention time in a pipe is calculated by utilising a back-tracking method and the detention time in a path is also calculated for the IO model [159]. The analysis on time delay calculation is called path analysis algorithm for quality transportation in the DWDS.

The path analysis algorithm contains a set of algorithms based on the quality transportation differential equations and its solutions [159] The transportation partial equations will be described in the following chapter, only the back-tracking algorithm and associated time delay calculation are introduced in this section.

A recursive backward tracking algorithm performed within a single pipe with a certain tracking time step starts from the downstream node until the upstream node is reached. A transportation path composes of several pipes; therefore, the backward tracking algorithm within a path normally starts at the monitored node and ends at the upstream node of this path. The recursive tracking is repeated independently in each pipe contained in the quality transportation path. The overall backward tracking finishes when every injection node is reached. After performing the algorithm at each monitored node, the IO model structure regarding the network can be obtained. The input and time delay numbers are the main two components of the IO model structure in terms of water quality.

3.3.1 Detention Time Calculation in a Pipe

Consider a pipe flow illustrated in Figure 3-7, where i and j are the upstream node and downstream node, respectively, L_{ij} denotes the length of the pipe, $v_{ij}(t)$ presents the flow velocity in the pipe. As the hydraulic dynamic is normally slow, the flow velocity with a hydraulic time step in a pipe is assumed as a constant.

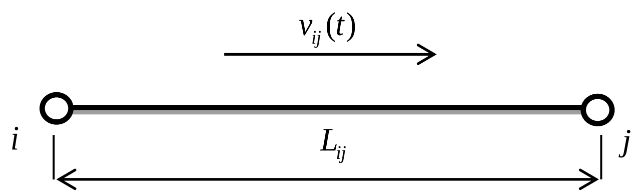

Figure 3-7 Water flow velocity in a pipe

In this calculation, the tracking time step should be selected appropriately. Let ΔT_h denote the hydraulic time step, ΔT_q as the quality time step and ΔT_D as the discretization time step. The relationship among these values can be described as [2]:

$$\Delta T_h \geq \Delta T_q \geq \Delta T_D \tag{3-25}$$

Then, tracking time step τ should follow the restrictions:

$$\begin{aligned} &\tau \leq \Delta T_q \\ &\tau v(t) \leq L_{ij},\ \textit{for any } t \textit{ and } L_{ij} \end{aligned} \tag{3-26}$$

The backward tracking in a pipe is illustrated in Figure 3-8. The backward tracking starts at downstream node j at time instant t. During each tracking time step τ, the flow can travel a distance $\tau \times v_{ij}(t)$. The tracking distance is the sum of the travelled distances generated in every tracking time interval τ. x_{ij} denotes the tracking distance from the downstream node j to the current tracking position.

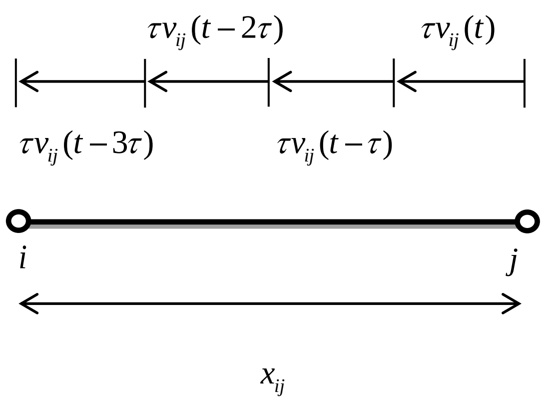

Figure 3-8 Backward Tracking in A Pipe

The detention time in the pipe described in Figure 3-8 can be expressed as:

$$DT_{ij} = \tau + \tau + \tau + \frac{L_{ij} - \tau\left|v_{ij}(t)\right| - \tau\left|v_{ij}(t-\tau)\right| - \tau\left|v_{ij}(t-2\tau)\right|}{\left|v_{ij}(t-3\tau)\right|} \tag{3-27}$$

Note that the direction of flow could change, but the positive direction defined for the flow in a pipe remains the same.

The backward tracking algorithm in a pipe can be described as [159]:

1. Set $DT = 0$ and $x = 0$ at initial time instant t;
2. If the flow direction is positive (opposite to tracking direction)

$x = x + \tau v(t - DT)$;

else $x = x - \tau v(t - DT)$;

3. If $x < L$, set $DT = DT + \tau$, and go to step 2;

   else $DT = DT + \dfrac{L - x + \tau v(t - DT)}{|v(t - DT)|}$, set the current node to i, end.

3.3.2 Detention Time Calculation in a Path

An illustration of transportation paths for delivering water quality from source node (injection node) A to monitored node G in a DWDS is shown in Figure 3-9 [159].

As shown in Figure 3-9, A, B, C, D, E, F and G denote junction nodes in paths. There are 4 different paths transporting water quality from the injection node A to monitored node G, including path A-B-C-E-G, path A-D-E-G, path A-F-G and path A-C-E-G, respectively. Several single pipes are presented by a, b, c, d, e and f.

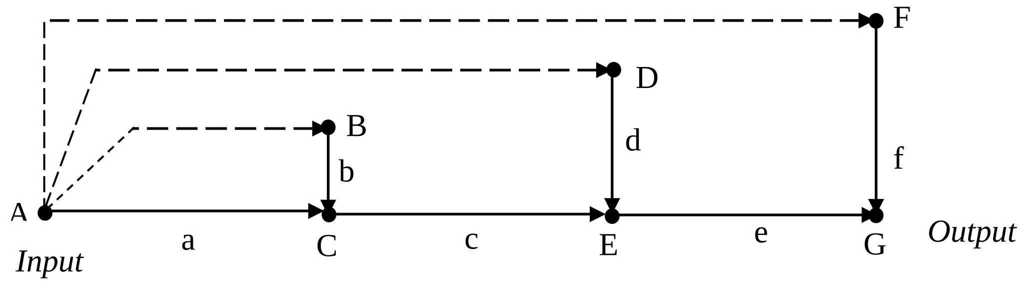

Figure 3-9 Illustration of Transportation Paths in a DWDS

Take detention time of path A-C-E-G as an example for calculation [2]:

$$
\begin{aligned}
d_1(t) &= d_e(t) \\
d_2(t) &= d_c(t - d_1(t)) \\
d_3(t) &= d_a(t - d_1(t) - d_2(t)) \\
d_{ACEGp}(t) &= d_3(t) + d_2(t) + d_1(t)
\end{aligned}
\tag{3-28}
$$

where detention time $d_1(t)$, $d_2(t)$ and $d_3(t)$ are calculated recursively, and sum of them is the detention time $d_{ACEGp}(t)$ of path A-C-E-G. The detention time at each path is required to be calculated independently.

3.3.3 Discretization of Time Delay

Based on the previous assumption that the flow velocity in the pipe is piece-wise constant with the tracking interval selected, the detention time is continuously time-varying within a min-max range during the modelling horizon T_h. As shown in Figure 3-10, the continuous time delay during the T_h is illustrated:

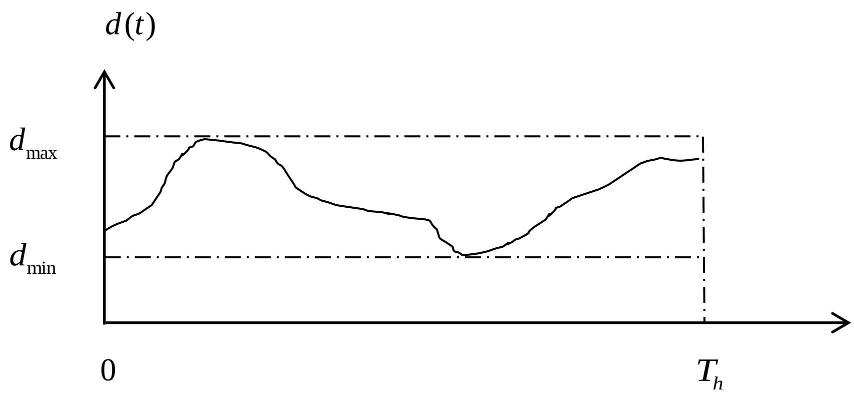

Figure 3-10 Continuous Time Delay during Modelling Horizon

The continuous variations in time delay are not applicable for modelling the water quality dynamic model numerically within the selected time interval or simulation time step. Therefore, the delay range is required to be discretized into a series of delay numbers and the continuous detention time can be approximated by these delay numbers [94, 160]. Delay numbers can be defined as:

$$
\begin{aligned}
&I_{ij} = \{n_{\min}, n_{\min}+1, ..., n_{\max}-1, n_{\max}\} \\
&n_{\min} = round(\frac{d_{\min}}{\Delta T_D}) \\
&n_{\max} = round(\frac{d_{\max}}{\Delta T_D})
\end{aligned}
\tag{3-29}
$$

where ΔT_D denotes the discretization time step, function $round(.)$ aims to find the closest real integer number, I_{ij} presents the delay number in pipe p_{ij} over the time period $[0, T_h]$. Normally, a structure error caused by discretization should be considered, which is to be discussed later in the following chapters.

3.4 Summary

This chapter explored the DWDS physical modelling and its operational control, and also explored the path analysis algorithm for detention time calculation.

The fundamentals of operational control in DWDS have been introduced under three main aspects, i.e. objectives, uncertainty handling and basic control mechanisms, respectively. The background of operational control of DWDS leads to a greater understanding of water quality control in DWDS.

The physical components installed in DWDS have also been described and illustrated, and each of them plays an irreplaceable role in water quality control. The physical laws, including flow continuity law and energy conservation law, were illustrated and described. Note that, hydraulic information is significant for the control of water quality in DWDS because it contains the input information for water quality control.

The path analysis algorithm has been introduced in this chapter, and the calculation of detention time in a pipe and in a path is formulated and will be applied in the following application to the deriving water quality IO model.

CHAPTER 4 APPLICATION OF NONLINEAR MODEL PREDICTIVE CONTROL ON WATER QUALITY IN DWDS WITH DBPS INVOLVED

This chapter develops a nonlinear model predictive controller to implement optimising control on water quality in DWDS. The water quality model utilised in the controller is based on the advanced nonlinear water quality dynamics model, which jointly considers the disinfection and the augmented control objective-DBPs. Based on the newly developed two time-scale architecture of the integrated control of quantity and quality in DWDS, the interest on analysing the impact brought by flow trajectories optimised by the upper level optimisation controller is increased. The applied nonlinear model predictive control (NMPC) is to operate in a fast time-scale as the same as the lower level quality controller within this architecture. The NMPC algorithm is to be applied to a comprehensive simulation study based on an example network with nonlinear water quality dynamics. The performance of the controller is validated by the related simulation results.

In this chapter, the hierarchical two-level structure for optimising integrated quantity and quality control will be introduced. The information from the upper level is considered as the priori known. Only the lower level controller for controlling water quality with DBPs is considered in this chapter. In addition, the MPC methodology is described in this chapter.

4.1 Introduction to the Hierarchical Two-Level Structure in DWDS

An increasing shortage of natural water resources around the world has been observed, due to climate change, a rising population and environment pollution[35, 36]. Therefore, meeting the demand for drinking water of a required quality requires advanced control technology to operate DWDS which are typically large scale complex network systems [1].

As described in Chapter 3, quantity and quality are the two primary aspects from the control viewpoint of DWDS. The quantity control aims to handle the flow of pipes and pressure of the junction nodes in water system by producing the optimised pump and valve control schedules. The main objectives of quantity control are: 1) meet the real water demand at the user nodes, and 2) minimise electrical energy cost due to pumping [1, 12].

As described in Chapter 2, one of quality control objectives aims to maintain the free disinfectant concentration at the monitored nodes. The maintained level of free disinfectant concentration must satisfy the user-defined limits prescribed in such a way that the bacterial re-growth over a whole DWDS is halted. However, the free disinfectant reacts with the organic matters over the DWDS producing so called disinfectant by-products (DBPs), which are dangerous to health [14].

Therefore, the DBP concentrations over the DWDS ought to be kept as low as possible and this is another objective of the quality control. Chlorine is considered as the disinfectant because of its low price and effectiveness. Therefore, the free chlorine concentration is often used for assessment of the water quality state [93]. In summary, the quality control aims to maintain free chlorine concentrations at the monitored nodes within the described lower-upper limits and minimising the DBP concentrations at these nodes.

The chlorine residuals are controlled by the treatment plant to ensure the water has the satisfied residual values when enter into the DWDS. However, with the water travelling throughout the whole network, the disinfectant reacts with bacteria and organic matters and it leads to its major decay and generation of DBPs so that the security of water may not be guaranteed, especially at several remote consumption nodes.

As a result, it is necessary to inject chlorine by employing booster stations located at selected intermediate junction nodes in DWDS. The chlorine injections are the only quality control inputs considered in this thesis because the hydraulic information is assumed as a priori known, while the booster stations are the corresponding quality actuators. The optimised allocation of the booster station problem was presented in [71, 74].

The quality concentrations can change rapidly because of the decay, mixing of water flows, even by consumption of physical materials during water transportation. The detention time described in chapter 3 from the source to the monitored nodes significantly depends on the hydraulic operation of the network. The quantity control has important effects on the quality control. However, the quality control inputs (injection) have no impact on the flows which are the hydraulic controlled outputs because the injected disinfectant mass can be negligible when compared to the mass of water. Nevertheless, the quality controlled outputs depend on the flows. Therefore, the quality and quantity interaction exists although it is only one way interaction from quantity to quality, and both quality and quantity are required to be controlled in an integrated manner.

In the operational control of DWDS, the quantity control problem is normally formulated based on the demand prediction over a certain control horizon, which is typically 24 hours. In general, the prediction step used in DWDS is 1 hour or 2 hours, and demand during the selected prediction step is assumed constant. This discrete time step is called hydraulic time steps. Quality has a quicker dynamic when compared to hydraulics in the DWDS, typically the quality time step is 5 or 10 minutes or even a smaller value.

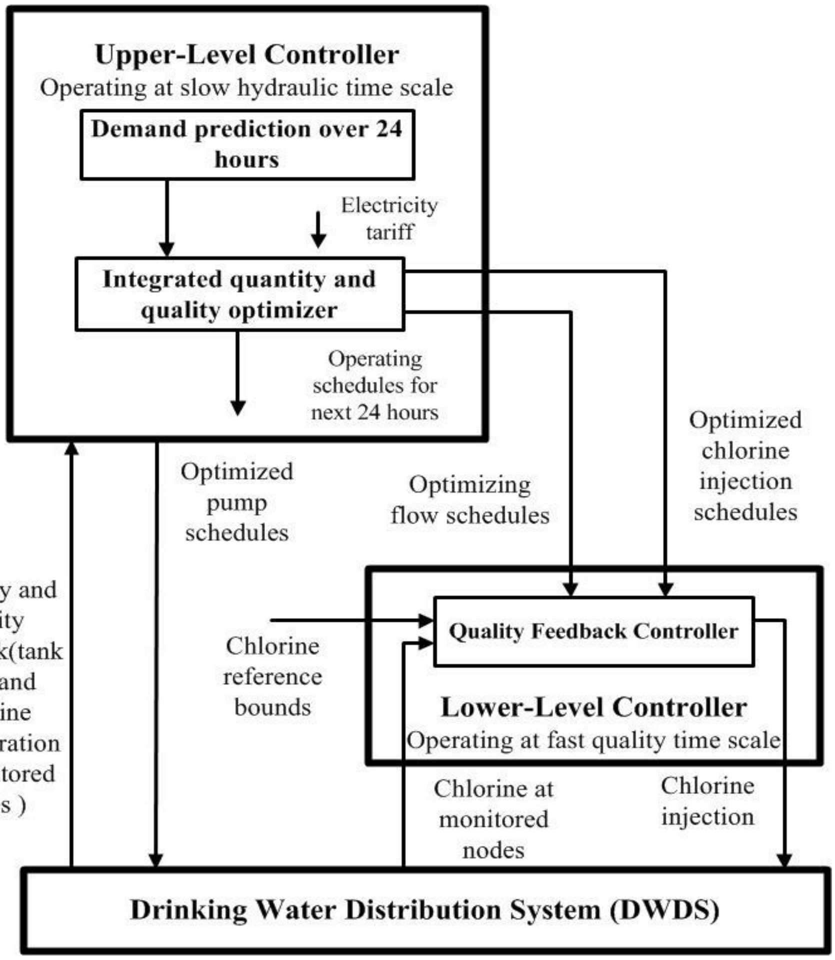

Figure 4-1 Hierarchical Two-Level Structure for Optimising Control of Integrated Quantity and Quality [13]

As a result of the multi time-scales in the dynamics of hydraulic and quality, which is slow and fast respectively, a dimension complexity of the integrated MPC optimisation task is large. This makes direct application of NMPC algorithm to integrated control of water quality and quantity even for a small size DWDS impossible [16]. Therefore, a two time-scale hierarchical control structure was proposed in [17] and [18] for jointly considering the two different time scale problems and the structure is illustrated in Figure 4-1.

The optimisation controller at Upper Control Level (UCL) operates in a slow hydraulic time scale based on the accurate hydraulic model and simplified quality model with one hour time step applied to both models. The models are used to predict the quantity and quality controlled outputs over the quantity prediction horizon of 24 hours.

Water quantity and quality are estimated or measured at beginning of a control period, and then sent to an integrated optimiser. Moreover, the water demand prediction is provided for the optimiser as well. Following the one way interaction between the quantity and quality, the hydraulic optimisation control resulting from solving the MPC optimisation task are truly optimal.

The quality dynamic model in the optimisation problem has the same time step as the quantity dynamic model. Although the problem dimension is decreased immensely, the error in modelling quality is extremely increased. Therefore, the quality controls need to be improved and this is done at the Lower Correction Level (LCL) by employing the fast quality feedback controller operating at the fast quality time scale. The hydraulic controlled outputs, which are flows, needed at the LCL by the fast quality controller are taken as determined at the UCL. The quality residuals are sampled at the rate required by the decay dynamics of the disinfectant [12, 16]and the growth dynamics of the DBPs [7, 161].

In order to achieve the operational objectives of DWDS described in chapter 3 in a robustly feasible and cost effective way, information about the DWDS states, including quantity and quality, is required on-line. Monitoring of the water quantity has been well developed in previous research, while the quality monitoring is also presented in [7, 92]. Optimised placement of hard chlorine sensors achieving the required balance between the estimation accuracy and sensor maintenance and capital cost is presented in [162].

Presently, only the bacterium objective is considered for the quality control under the MPC control methodology [2, 39]. In this thesis both the chlorine and DBPs are jointly considered and the MPC is applied to synthesize the Lower Level Controller (LLC) at LCL of the structure in Figure 4-1.

4.2 Quality Model Dynamics with Considering DBPs

The recently derived model of the quality state in [161] is too complex for the MPC applications. The model was simplified in [7] and applied for robustly monitoring the quality with DBPs and it is utilised in this thesis. As opposed to the previously used models for the quality control which is limited to the free disinfectant objective only, this model is highly non-linear due to the consideration of the non-linear dynamics of chlorine decay and DBPs build up reactions.

4.2.1 Dynamics of the quality kinetics

The chemical reactions generating the chlorine and DBPs are presented in [7, 8]. Based on the chemical reactions, the quality kinetics can be derived as follows [7]:

$$\begin{aligned} \frac{dc^1(t)}{dt} &= -k_{Cl}c^1(t) - s_{DBP}k_{DBP1}(DBP_{p1} - c^2(t))c^1(t) \\ \frac{dc^2(t)}{dt} &= k_{DBP2}(DBP_{p2} - c^2(t))c^1(t) \end{aligned} \tag{4-1}$$

where c^1 denotes the concentration of free chlorine in [mg/L] and c^2 denotes the total concentration of chlorine in DBPs compounds in [mg/L], k_{Cl}, k_{DBP1} and k_{DBP2} are the reaction kinetics parameters, DBP_{p1} and DBP_{p2} are the DBP formation potential parameters, s_{DBP} is the stoichiometric coefficient and meaningful bounds on the above parameters are known.

Denoting:

$$
\begin{aligned}
&c = [c^1, c^2];\\
&\Xi^1(c) = -k_{Cl}c^1 - s_{DBP}k_{DBP1}(DBP_{p1} - c^2)c^1;\\
&\Xi^2(c) = s_{DBP}k_{DBP2}(DBP_{p2} - c^2)c^1.
\end{aligned}
\tag{4-2}
$$

The quality kinetics (4-1) can be written in a compact form:

$$
\frac{dc(t)}{dt} = \Xi(c(t)), \Xi = [\Xi^1(c), \Xi^2(c)] \tag{4-3}
$$

4.2.2 Quality dynamic model

The following assumptions are made [7]:

1. DWDS is composed of water sources, pressure pipes, nodes and tanks.
2. The flow directions are constant over the considered modelling time horizon.
3. The flow rate and flow velocities are known.
4. Concentration of free chlorine and DBP at the external water sources are known.
5. Mixing at the nodes, pipes and tanks is instantaneous and complete and, in addition it is free of storage at the nodes.
6. A diffusive transport of chlorine and DBP is disregarded and only the advection transport is considered.

The quality dynamic model considers the change of chlorine and DBPs concentrations at junction nodes, tanks and along pipes. By applying (4-3) the quality advection transport along a pipe $p \in NP$ with length L_p can be described as [7, 163]:

$$\frac{\partial c_p(l,t)}{\partial t} + v_p(l,t)\frac{\partial c_p(l,t)}{\partial l} = \Xi(c_p(l,t)) \tag{4-4}$$

Equation (4-4) is constrained by the initial and boundary condition $c_p(l,0), l \in [0, L_p]$ and $c_p(0,t),\ p \in NP$ respectively, where $c_p(l,t)$ denotes the quality state at time *t* at distance *l* from the pipe flow entry point $l = 0$, $v_p(t)$ denotes the pipe flow velocity and *NP* is the number of pipes. Since the water is assumed incompressible and the pipes are of the pressure type, then $v_p(l,t) = v_p(t)$ for $l \in [0, L_p],\ p \in NP$.

After partitioning each pipe *p* into the NS_P segments with length Δl_p, and then defining $c_p(m,t) = c_p(m\Delta l_p, t)$, where $m = 1,..., NS_p$, equation (4-4) can be approximated in space as [7, 92]:

$$\frac{dc_p(m,t)}{dt} + v_p(l,t)\frac{c_p(m,t) - c_p(m-1,t)}{\Delta l_p} = \Xi(c_p(m,t)) \tag{4-5}$$

where: $c_p(m-1,t) = c_p(0,t)$ for $m = 1$.

The variables $c_p(m-1,t) = [c_p^1(m-1,t), c_p^2(m-1,t)],\ m = 1,..., NS_p$, are composed of the state variables of a quality model dynamics in pipe *p* and (4-5) are the state equations.

Next, in considering the water quality mixing at the pipe junction node $n \in NPJ$ at time instant *t*, the following denotations are made: *IIn*, *EIn* presents the sets of pipes delivering the water from the DWDS and external sources respectively, into the node *n* at time instant *t*; $c^1_{in,n}(t)$ denotes the free chlorine dosing into the node *n* by flow paced booster quality controlling devices [12].

The pipe junction nodes with the dosing are the quality control nodes (*CNPJ*). For practical reasons a set of these nodes *CNPJ* is limited to only achieving controllability of the quality [164]. The quality control inputs are $c^1_{in,n}(\mathrm{t})$, where $n \in CNPJ \subset NPJ$ .The resulting quality output $c_n(t)$ at the junction node *n* can be expressed as [7]:

$$c_n(t) = \frac{\sum_{p \in IIn} q_p(t) c_p(L_p, t) + \sum_{p \in EIn} q_p(t) c_p(L_p, t)}{\sum_{p \in IIn} q_p(t) + \sum_{p \in EIn} q_p(t)} + c_{in,n}(t) \qquad (4\text{-}6)$$

where $c_{in,n}(t) = [c^1_{in,n}(t), 0]^T$, $q_p(t)$ is the pipe flow at time instant *t*.

Furthermore, consider the quality dynamics in the tank. As for the pipe junction nodes, denoting *ITH(t)* as the set of pipes delivering water in the tank $h \in NT$ at time instant *t*, the quality model dynamics can be described as [7, 92]:

$$\frac{dc_{T,h}(\mathrm{t})}{dt} = \frac{\sum_{p \in ITh} q_p(t)(c_p(L_p, t) - c_{T,h}(\mathrm{t}))}{V_{T,h}(\mathrm{t})} + \Xi(c_{T,h}(\mathrm{t})) \qquad (4\text{-}7)$$

where: $c_{T,h}$(t) is the quality state in tank *h* and $V_{T,h}$(t) is the tank water volume at time instant *t*.

The quality monitored nodes with the prescribed concentration bounds are the quality control outputs and (4-6) are the output equations in the quality state-space model.

It is now clear that the quality state-space model described above is a non-linear time-varying dynamical system with the input and output constraints. As the free chlorine and DBP concentrations can be measured on-line by hard sensors located only at very limited number of elements of *NPJ*, the quality state must be estimated for control purposes.

4.3 Optimising Model Predictive Controller for Water Quality with Augmented DBPs Objective

Due to the nonlinear dynamics described in the quality model with DBPs involved, and the multivariable constrained optimisation control problems, the MPC methodology is selected as the core algorithm to implement the optimising quality control with considering the augmented DBPs objective at DWDS. Both chlorine and DBPs are considered as the control objectives in the nonlinear MPC controller. The details regarding to design the nonlinear MPC controller are to be presented in the following sections.

4.3.1 Model Predictive Control Methodology

As shown in Figure 4-2, the basic MPC control loop is made up of three core modules: plant model, output predictor/state estimator and solver of the MPC model based optimisation problem (MBOP).

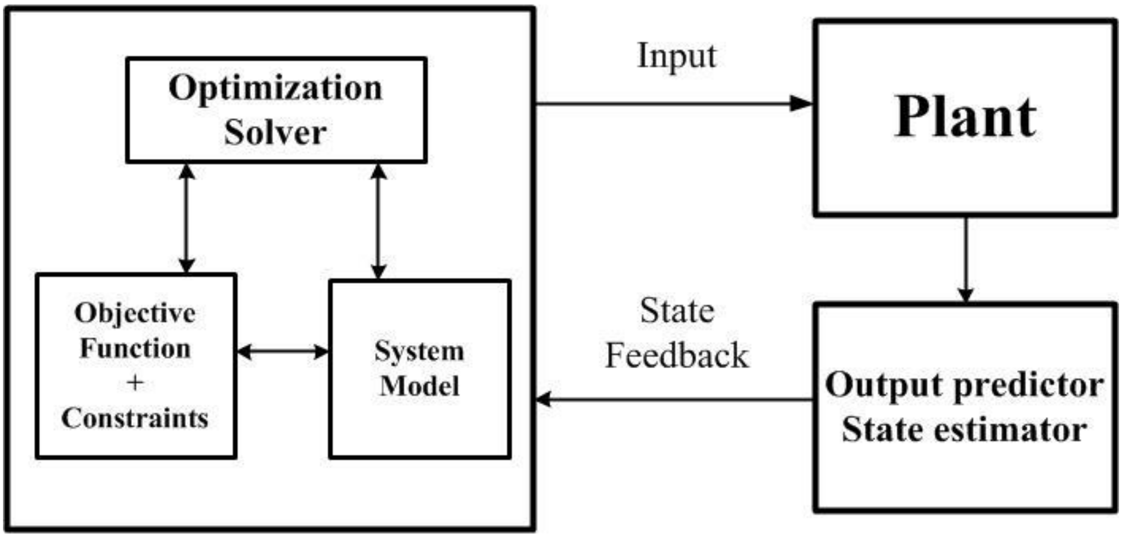

Figure 4-2 The Basic MPC Control Loop [13]

MPC, as an accepted standard and an advanced technology to solve the practical industries control engineering problems, belongs to one of the model based controller design methods. MPC has been widely used in the industry for solving multivariable constranined problems. The accuracy of the plant model determines the efficiency of MPC control performance. The basic idea of the MPC algorithm will not change no matter what kind of plant models are considered in the optimising problems.

The optimal control actions are determined by solving a prescribed objective function with defined constraints, which penalises the difference between the predicted output from the specified reference or limits. The control action at each MPC time step is calculated on-line by solving a finite-horizon open-loop optimisation problem [165]. The current states of the plant are used as the initial states of the optimisation problem for the next MPC time step. Only the first part of the optimised control sequence is utilised as the control action applied into the real plant. At a MPC control time step, the user-defined prediction horizon moves forward and the same procedure repeats till the modelling horizon ends.

Denote x_k as the states of the plant at time k, $\bar{u}_k$ as the first part of the optimised control action (input) applied to the plant, then the basic MPC algorithm can be expressed as:

1. Measure or estimate x_k at time k;
2. Determine the prediction horizon and control horizon based on the characteristics of target systems;
3. Obtaining $\bar{u}_k$ by solving the user defined objective functions, and applying $\bar{u}_k$ to the plant;
4. Set $k = k + 1$, go to step 1 till the modelling horizon ends.

4.3.2 Formulation of MBOP

Denote $u_i(t)$ and $\mathrm{y}_j(t)$ as the input and controlled output of the proposed control system respectively. The $u_i(t)$ is composed of the chlorine injections at the quality control nodes *CNPJ*, and $y_j(t) = [y_j^1(t), y_j^2(t)]$, $j \in MNPJ$ denotes the free chlorine and DBP concentrations, respectively, at the quality monitored nodes *MNPJ*. Based on analysis of the control objectives described in section 1, the constraints in the MBOP are formulated as:

$$\begin{aligned} &u_i^{\min}(t) \le u_i(t) \le u_i^{\max}(t); \\ &y_j^{1\min}(t) \le y_j^1(t) \le y_j^{1\max}(t). \end{aligned} \tag{4-8}$$

where $u_i^{\min}(t)$, $u_i^{\max}(t)$, $y_j^{1\min}(t)$ and $y_j^{1\max}(t)$ are the upper and lower bounds on inputs and outputs in *CNPJ* and *MNPJ*, respectively.

Moreover, maintaining the DBP concentrations as small as possible is vital. Hence, the objective function is formulated as:

$$f(t) = \min \sum_{t \in H_P} \Big(\sum_{j \in MNPJ} y_j^2(t) \Big) \tag{4-9}$$

where H_P presents the defined prediction horizon in MBOP.

4.3.3 State Feedback

Given control sequence over the prediction horizon, the forced output is determined by applying the state-space quality model. However, as the states are not measurable, they must be estimated. The newly derived state estimator in [7] is applied to produce the robust state estimates on-line. DWDS state variables like 1) the free chlorine and DBP concentrations along pipes, 2) tank heads and 3) free chlorine and DBP concentrations in tanks are required to measured or estimated. Denoting the state vector at time instant *t* as [18]:

$$X(t) = \{H_{T,h}(t), c_{T,h}(t), h \in NT; c_p(l,t), l \in [0, L_p], p \in NP\} \tag{4-10}$$

where: $H_{T,h}(t)$ presents as tank head of tank *h* at time instant *t*.

Then the MPC controller operates at *kT* as follows:

1. States of DWDS *X(kT)* is measured or estimated. While, the water demand and DWDS quality boundary conditions are predicted.
2. The optimisation problem (4-9) in nonlinear MPC controller is solved.
3. Apply the first optimised control action into DWDS.
4. Set $k = k + 1$ and return to step 1.

4.3.4 Solver of MBOP

The optimiser is designed as performing the search in the space of the control inputs. This is supported by employing a fast and reliable simulator of the quality at DWDS. Hence, the Genetic Algorithm (GA) is applied to solve the optimisation problem as faster non-linear optimisation algorithms such as SQP are hardly applicable to the chosen structure of the optimisation search (the gradients and second derivatives are not analytically available). The initial quality states are provided by the state estimator. GA begins with a random population of individuals and/or a designer-selected population. The algorithms stop when one or more of pre-established criteria, such as the number of generations or fitness tolerance, are met [165].

4.3.5 Model Simulator: EPANET AND EPANET-MSX

EPANET is a software package published by the National Risk Management Research Laboratory of United State Environment Protection Agency in 2000. Normally, it is used in water system simulation and hydraulic behaviour design with pressurized pipe networks. Constructing the distribution of water systems, calibrating and tuning the coefficients of water systems are the main functions of EPANET. Moreover, EPANET can generate the EPANET input file which stores the simulation data for the network and can be called directly by MATLAB.

However, EPANET cannot be used alone to meet the objective of different control requirements. This is because the calculation of EPANET does not include any optimisation functions. In addition, a multiple species DBPs are considered in the quality reaction dynamics presented in this thesis, but EPANET is limited in tracking the transport of multiple species. Therefore, the EPANET-MSX software package is required to solve these problems. EPANET-MSX allows the original EPANET to model any system with multiple, interacting chemical species. This capability has been incorporated into a stand-alone executable program and also a toolkit library of functions that programmers can employ to implement customer's applications [166]. MSX stands for Multi-Species Extension. In this thesis, both EPANET and EPANET-MSX simulators are used to generate the simulation data results of the water network, including node pressure, pipe flow, and quality concentration and so on.

4.4 Application to Case Study DWDS and Simulation Results

4.4.1 Case Study Network and Design of Nonlinear MPC controller

The topology of the case-study network is illustrated in Figure 4-3. There are 8 consumption nodes: node 11, node 12, node 13, node 21, node 22, node 23, node 3 and node 32, respectively. Node 9 represents the reservoir, and node 2 stands for a switching tank. The link between node 9 and node 10 is the pump which is the only energy-consuming component. The quality output constraints are set as $y_j^{1\min}(t) = 0.1(mg/L)$ and $y_j^{1\max}(t) = 0.3(mg/L)$, respectively.

The upper limits on inputs are requirements due to health regulations. A value of 4(*mg/L*) is defined by US EPA. In practice, the DWDS operates at lower value than this because of the usage of chlorine booster stations. Hence, for the purpose of the simulation study, the upper limit on chlorine injection is taken as $u_i^{\max}(t) = 1(mg / L)$ because the simulation is implemented on a small network. Furthermore, the lower limit on chlorine injection is set as $u_i^{\min}(t) = 0(mg / L)$.

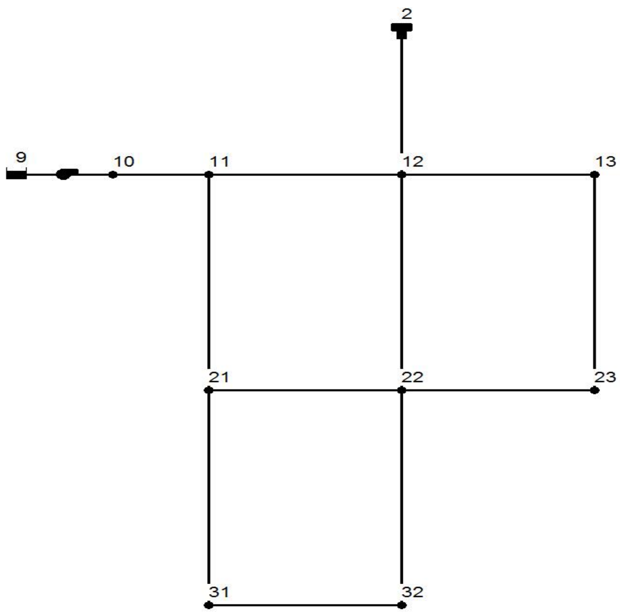

Figure 4-3 Case Study DWDS Network

For maintaining the chlorine concentration throughout the whole network within prescribed output constraints, *n32* is selected as the monitored node since it is the most remote node from the source. The booster station is installed at *n11*because it is the closest node to the reservoir.

The hydraulic time step is set as 1 hour, and quality time step is set as 10 minutes. The pump is operated by a simple rule according to the water head in the tank. The simple rule contains certain values for the water head in the tank which determines the tank operating status. The whole modelling horizon is 24 hours including filling cycle and draining cycle due to the operation of the tank.

The filling cycle operates in the first 13 hours, and then, the example DWDS switches to the draining cycle which takes 11 hours. Reservoir is the only source for supplying water to the DWDS in the filling cycle. During the draining cycle, the pump is closed and tank becomes the only water supplier of the DWDS. Due to the system needs two hours to initialise and the minimum delay between the node 11 and node 32 is around 2.5 hours, the control horizon is finally set as 6 hours based on a number of experiments made by using different control horizon in a range of 4 to 12 hours. Based on the path analysis algorithm, the maximum delay in the example network is around 5 hours. Hence, the prediction horizon is set as 11 hours.

The time step of the nonlinear MPC controller is the same as the quality time step (e.g.10 minutes), which means GA operates at every 10 minutes when measurement of states described in equation (4-10) transferred to the defined objective function from the model. The first action of the optimising sequence calculated by GA is then sent to the plant. Before the next MPC time step starts, the state of the current time is sent to the nonlinear MPC controller as the initial state for the model. The working procedure of the developed nonlinear MPC controller is presented in Figure 4-4 as follows:

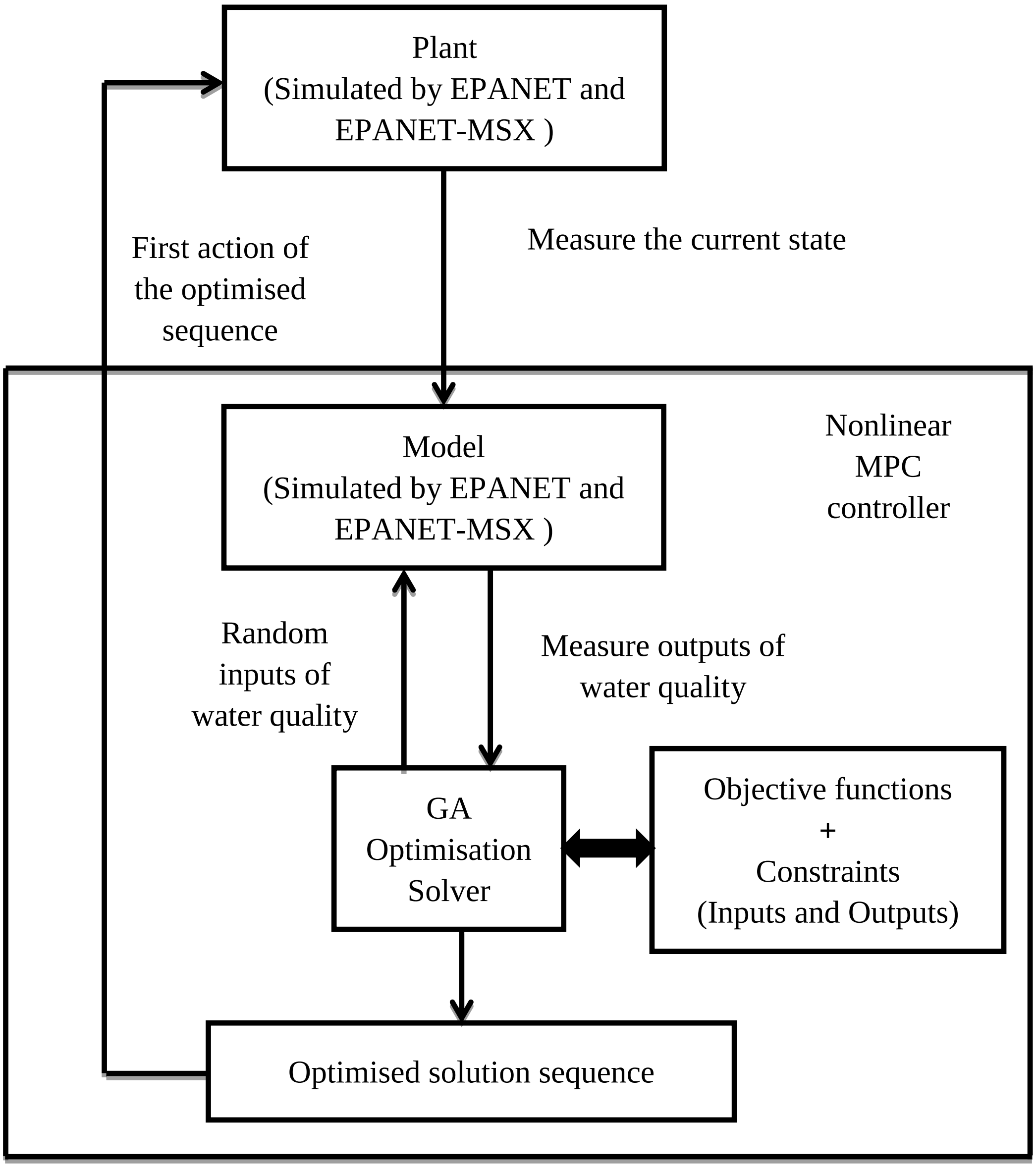

Figure 4-4 Working Procedure of Developed Nonlinear MPC Controller

The random inputs are generated by GA based on the performance of previous population which is calculated as the fitness value. Both model and plant are simulated by EPANET and EPANET-MSX but with different simulation data based on the selected modelling horizon, control horizon and prediction horizon.

4.4.2 Software Implementation

The simulation is based on the MATLAB environment. The GA toolbox in MATLAB is used to solve MPC optimising problems with connection to the EPANET software package and EPANET Multi-Species Extension (MSX) module.

The MPC controller is running by each quality time step, as is the GA optimiser. Therefore, in order to increase the optimiser computing efficiency, the optimised population obtained at current time step is to be used as the initial population for the next time step.

4.4.3 Simulation Results

As shown in the Figure 4-5, the trajectory of chlorine concentration at the monitored node is maintained within the upper and lower limits. Figure 4-6 illustrates the trajectory of minimised DBP concentration at the monitored node. Due to the system is controlled under zero initial condition at junction nodes, there is no output comes out in the first two hours because of initialising of the system. The output illustrated in

Figure 4-5 and Figure 4-6 are stable between the time period of 3 to 5 because a constant input is applied to the plant for bring the output of water quality into feasible solution area, otherwise, the feasible solution may not exist. From the results shown in Figure 4-5, it is obvious to see that the nonlinear MPC controller always try to bring the increased chlorine down to the lower limit level. This can reduce the dosage of chlorine and then reduce the budget of chlorine dosage。

As shown in Figure 4-6, the concentration of DBPs during most of the draining cycle period is at its saturation level. The reason of this phenomenon is that the tank becomes the only source of the DWDS, and the concentration of DBPs in tank has achieved its saturation level before draining period begins. As the method of removing DBPs from the DWDS during the water transportation is not considered in this thesis, DBPs within a high concentration level have been delivered to the other junction nodes from the tank.

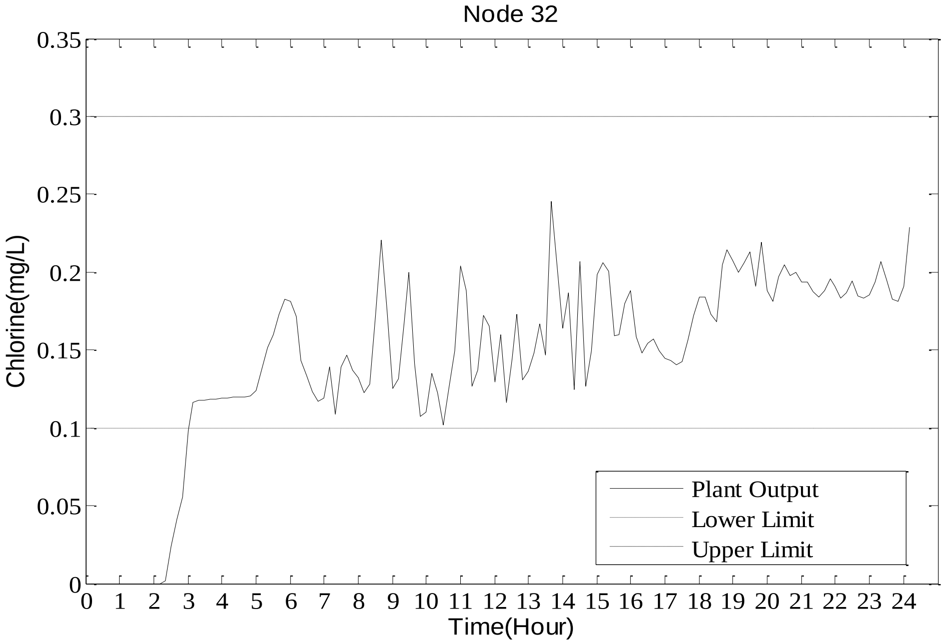

Figure 4-5 Chlorine Concentration at Monitored Node under 11 hours of Draining Cycle

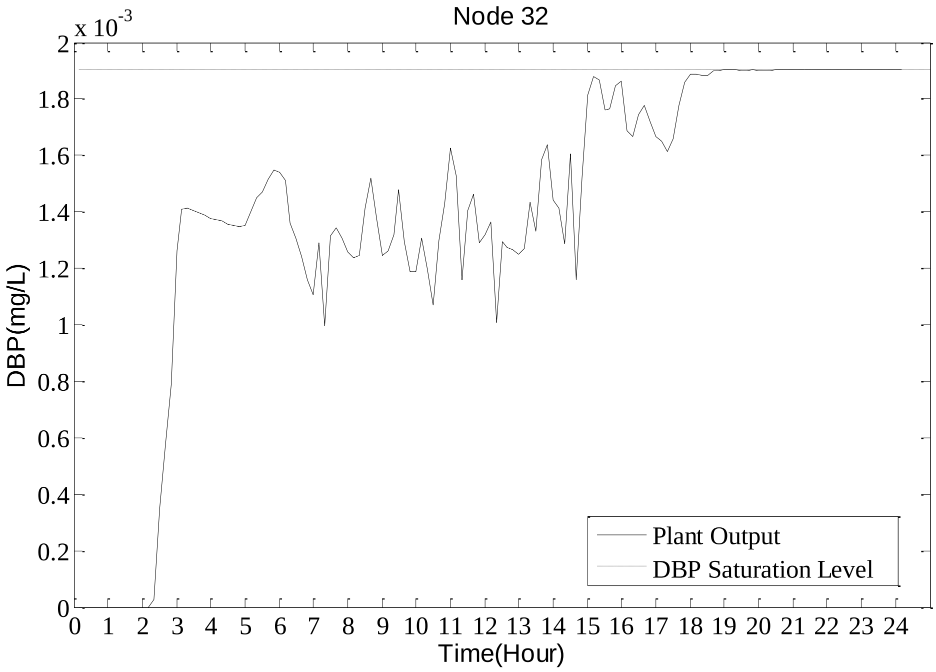

Figure 4-6 DBP Concentration at Monitored Node under 11 hours of Draining Cycle

In summary, due to the tank stores the DBPs produced there during the filling cycle, the high quantity of DBPs from the tank is transferred into the monitored node during the draining cycle. This makes the DBPs concentration at the monitored node high during the draining cycle. As the duration of these two cycles is determined by the network hydraulic operation, a significant impact of the hydraulics on the quality is demonstrated supporting relevance of the UCL in Figure 4-1. Figure 4-7 to Figure 4-10 illustrate the performance of quality control with different lengths of draining cycle (sum of the two cycles' duration is 24 hours).

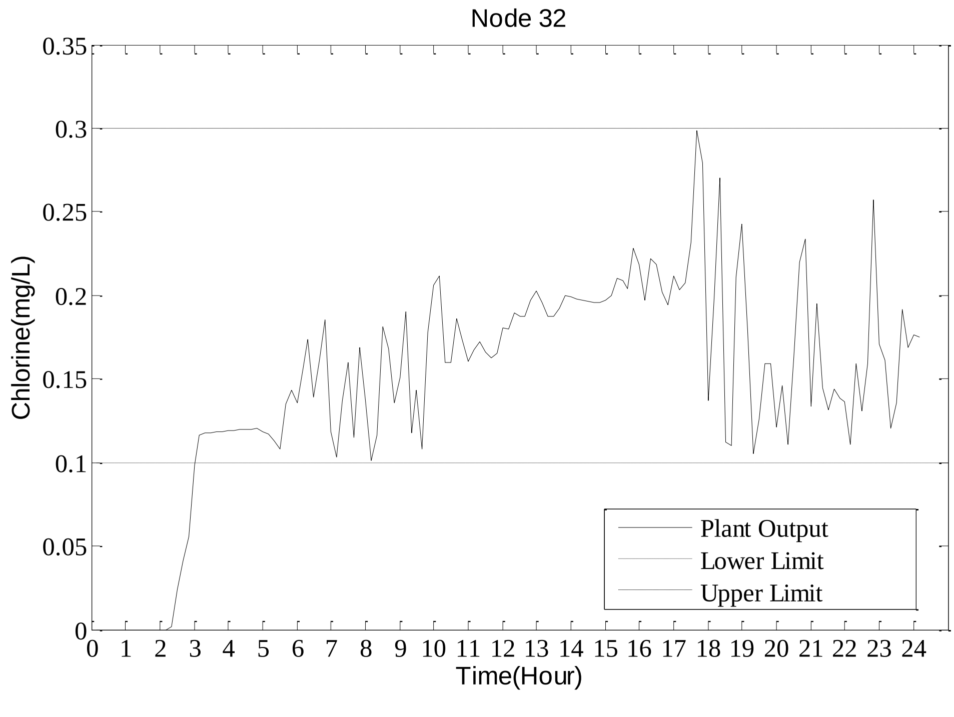

Figure 4-7 Chlorine Concentration at Monitored Node under 6.8 hours of Draining

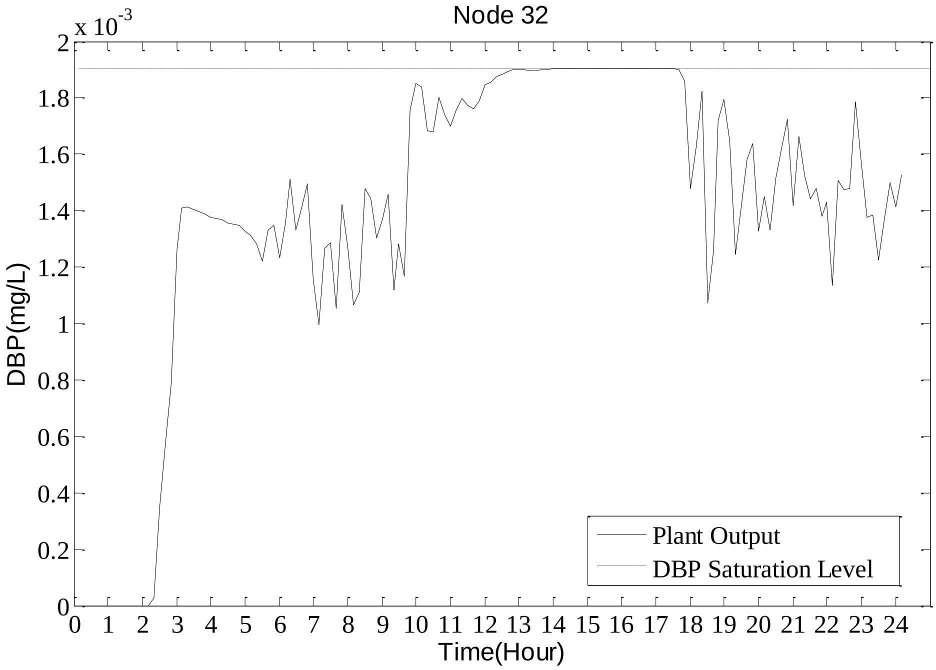

Figure 4-8 DBP Concentration at Monitored Node under 6.8 hours of Draining Cycle

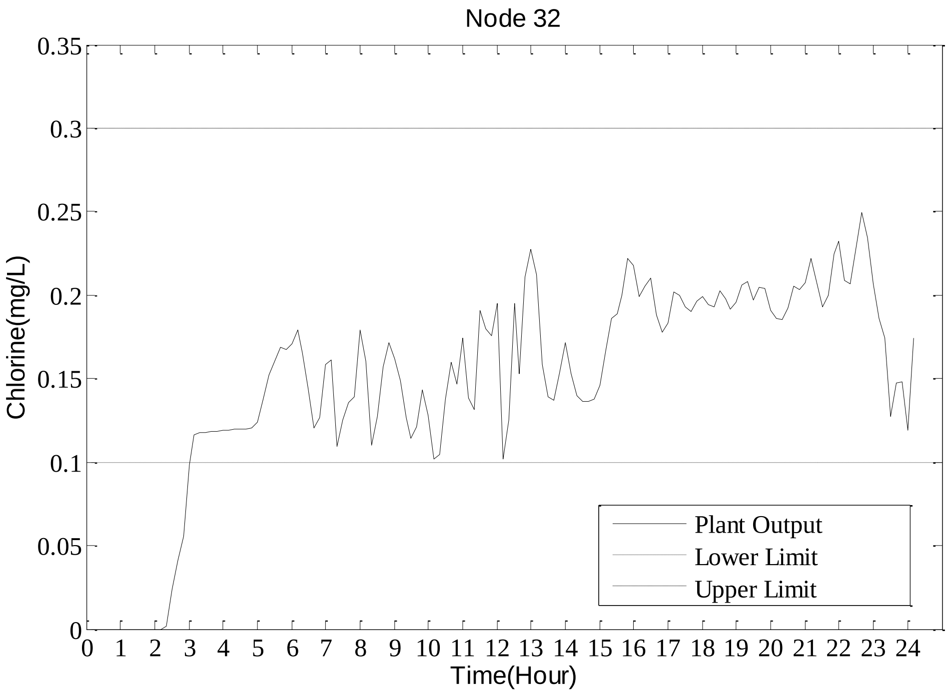

Figure 4-9 Chlorine Concentration at Monitored Node under 9.5 hours of Draining

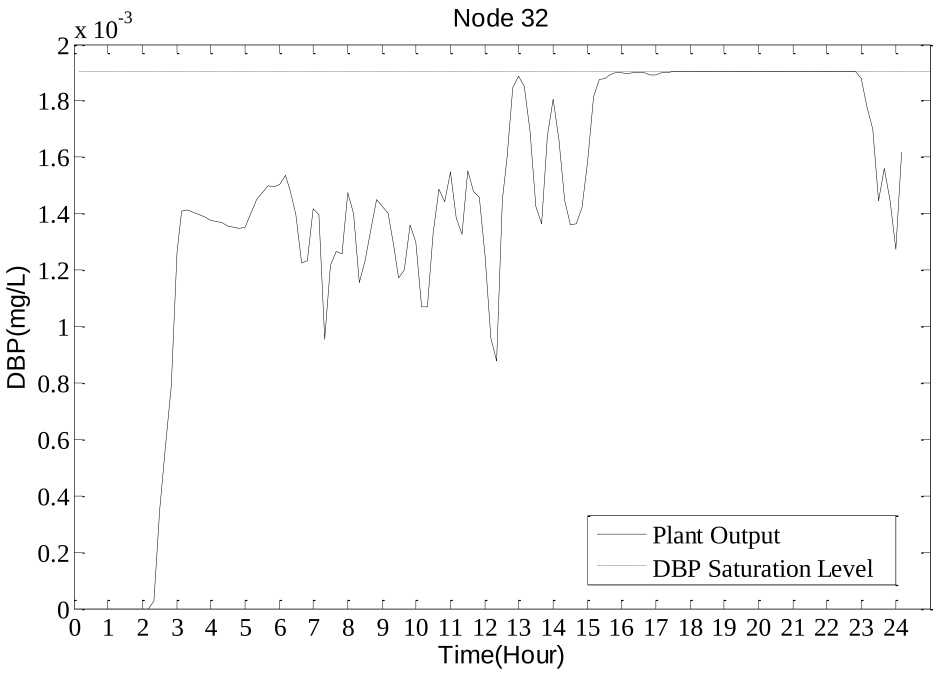

Figure 4-10 DBP Concentration at Monitored Node under 9.5 hours of Draining Cycle

The proposed MPC meets the quality control objectives very well. In order to assess an improvement of the proposed MPC with the DBP objectives directly incorporated into the performance index, the MPC was applied to control quality without DBP objective and the simulation results are illustrated in Figure 4-11 and. Figure 4-12.

Table 4-1 The Total Amount and Average Amount of DBP Concentration at Monitored Node under Different Scenarios

Scenarios	**Total amount**	**Average amount**
6.8 hours of draining cycle with considering DBPs	0.2031(mg/L)	0.001410(mg/L)
9.5 hours of draining cycle with considering DBPs	0.2055(mg/L)	0.001427(mg/L)

11 hours of draining cycle with considering DBPs	0.2025(mg/L)	0.001406(mg/L)
11 hours of draining cycle without considering DBPs	0.2128(mg/L)	0.001478(mg/L)

Clearly, the chlorine constraints are met but the chlorine profiles are different as shown in Figure 4-5 and Figure 4-11. The Table 4-1 presents the total and average amount of DBP concentration at the monitored node under different scenarios of controller and flow generated by UCL. According to the results listed in Table 4-1, the performance of quality controller without considering DBPs is worse than that considering DBPs since its high average amount of DBP concentration along the modelling horizon. Compare to the quality controller without considering DBPs, the quality controller considering DBPs can reduce the total amount of DBPs at 4.47%. Therefore, an advantage of the proposed controller can be clearly seen.

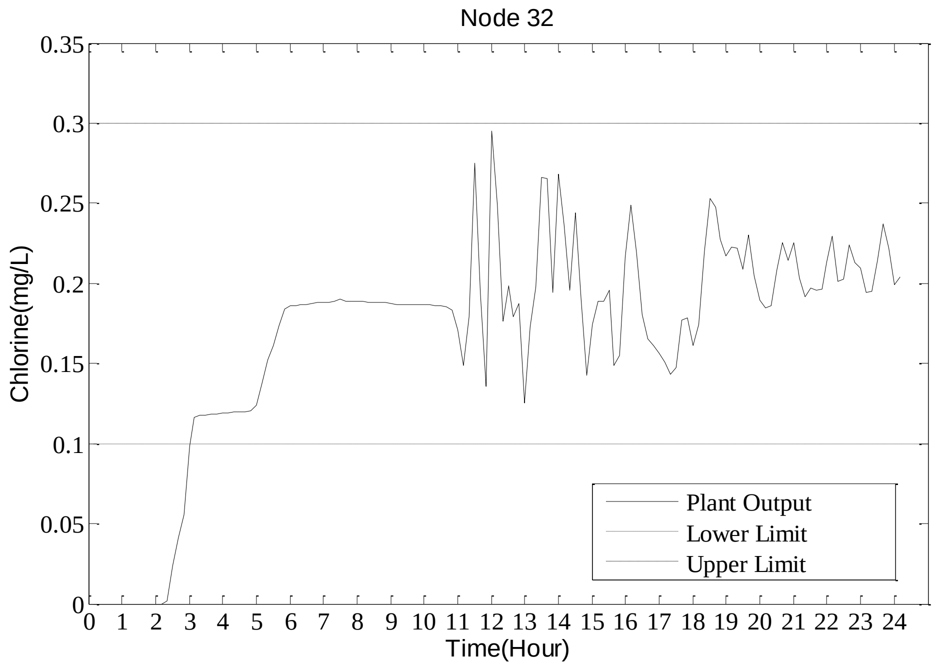

Figure 4-11 Chlorine Concentration at Monitored Node Obtained by MPC Controller without Considering DBP under 11 hours of Draining Cycle

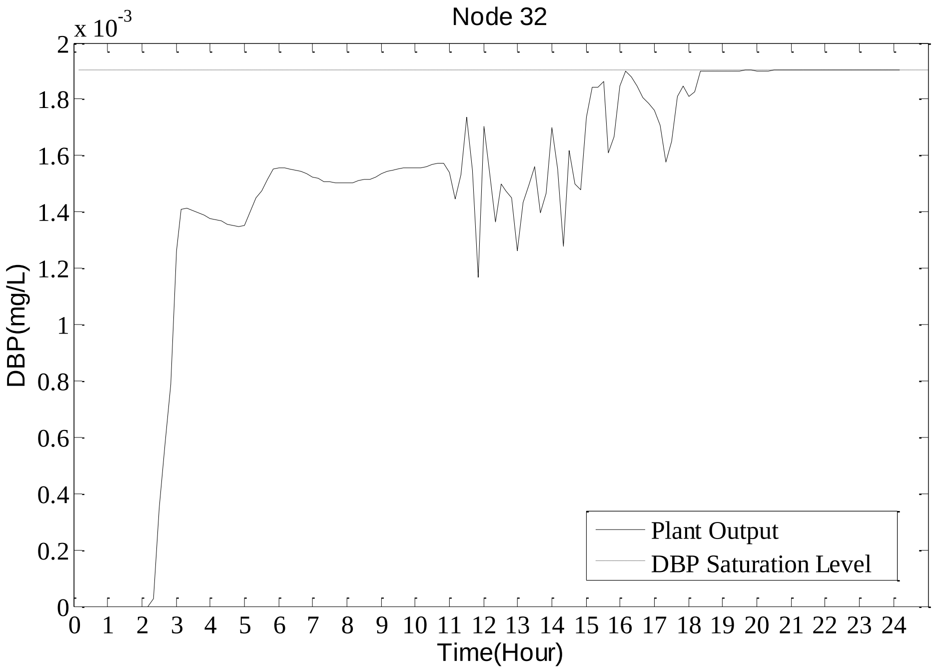

Figure 4-12 DBP Concentration at Monitored Node Obtained by MPC Controller without Considering DBP under 11 hours of Draining Cycle

4.5 Summary

This chapter has developed the nonlinear MPC control of water quality in DWDS based on the advanced non-linear water quality dynamics model considering DBPs objective. MPC has been considered as the control algorithm because it is widely used in solving such nonlinear, constrained with multivariable problem. The basic algorithm for MPC has been introduced and its application to a case study DWDS network has been implemented. This nonlinear MPC controller provided a practical solution for on-line control of water quality in DWDS considering DBPs. The simulation results illustrated regarding to the nonlinear MPC application on water quality control in DWDS have been shown a good and sustainable performance at LCL with the fast quality feedback. Furthermore, an importance of the hydraulic support as the quality control input was demonstrated.

CHAPTER 5 ROBUST PARAMETER ESTIMATION AND OUTPUT PREDICTION ON NONLINEAR WATER QUALITY MODEL IN DWDS WITH CONSIDERING DBPS

Chapter 4 developed a nonlinear MPC controller based on nonlinear water quality model which is modelled by EPANET and EPANET-MSX simulators. However, the uncertainty is not considered in these simulators. Because uncertainty can be explained by bounded parameters in the nonlinear water quality model, it is really important to derive a bounded parameter model with uncertainty considered.

This chapter mainly describes the implementation of robust parameter estimation and output prediction advanced algorithm based on nonlinear water quality model for the purpose of estimating and predicting the water quality states in DWDS. The advanced algorithm was tested for robustly predicting the outputs of a nonlinear water quality model in DWDS incorporating DBPs. The application of point-parametric model (PPM) for robustly estimating parameters of a nonlinear water quality model considering DBPs by utilising multi-input multi-output (MIMO) model structure is stretched.

The piece-wise constant parameters within the time-varying parameter model structure explaining the dynamics of water quality considering DBPs in DWDS under input disturbance is acquired by applying modified piece-wise continuity algorithms. This chapter describes the robustness of the PPM framework on MIMO nonlinear water quality model under multi-hydraulic operation status with advanced operating procedures. The developed MIMO Point-Parametric Model is utilised to present uncertainty and structure error in the nonlinear water quality model

5.1 Introduction

Climate change has a significant impact on continually growing systems, i.e. highly complex and interconnected systems, such as power systems, transportation systems, social networks, and drinking water systems, which are commonly known as a special group of large-scale complex systems, namely critical infrastructure systems (CIS) [167]. Some of the CIS, e.g. power grids and DWDS, constitute one group of systems that can be described as reactive carrier-load nonlinear dynamic networks systems (RCLNDNS) [167]. The monitoring, control and security of RCLNDNS-CIS has been given great attention by both academics and industries for security and protection purposes since September 11, 2011.

MPC technology has been widely applied in RCLNDNS-CIS to achieve complex control objectives. However, in terms of nonlinear MPC, it is still insufficient to solve those special defined optimisation tasks. This is the main reason that the control strategies based on linear MPC become attractive while the internal model of linear MPC still has large inaccuracies with regards to a real plant.

Managing MPC internal models working with uncertainties in the structure, unknown parameters, and complex varying operational conditions has become the most crucial task which requires proper mechanisms to guarantee the feasibility and veracity of the internal models at all times. The application of PPM is expanded from multi-input single-output (MISO) into multi-input multi-output (MIMO) because DBPs is considered in this thesis and its piece-wise continuity advanced algorithm is then further modified to be suitable for the MPC mechanism, especially for a robustly feasible model predictive control (RFMPC) framework.

DWDS, as a typical RCLNDNS-CIS, are highly nonlinear systems not only because of the multiple time-scale dynamics between the quantity operation and quality dynamics [17, 18] but also due to the complex biochemical process which contains consuming bacteria and limits its re-growth, the decay of disinfectant, and generation of DBPs [161].

The characteristics listed above makes DWDS a good selection for investigating such robust parameter estimation and output prediction technology for the purpose of achieving the application of RFMPC on the nonlinear systems. In order to achieve a proper working PPM, hydraulic information and the DWDS quality states including both free chlorine concentration (disinfectant) and DBPs is required on-line. Robust monitoring chlorine concentration in DWDS was well developed in [92], while the quality monitoring with DBPs was presented in [7].

An PPM based approach utilised to deliver a linear structure quality model with time-varying parameters and the related algorithms for robustly estimating parameters and predicting outputs were presented in [2]. The structure of PPM was developed by applying backward path tracking algorithm, described in Chapter 2.

5.2 MIMO Structure of PPM in IO Model

5.2.1 IO model of water quality in DWDS with Considering DBPs

The entire junction nodes and storage equipment in the DWDS are contained in the water quality model and result in a distributed model within pipe transportation. In fact, no explicit relationship exists between the chlorine injections and the concentrations of chlorine and DBPs at the monitoring nodes in the DWDS, which represent the inputs and outputs of the system in terms of water quality control.

As described in Chapter 4, the nonlinear water quality model used for the MPC controller is modelled by EPANET simulator. However, for designing a control system, an explicit relationship between the inputs and outputs is essential. As presented in [2], the water quality transportation paths in the network and time delay associated with paths connected between the injection nodes and monitored nodes were calculated by applying a backward tracking algorithm, which was also known as the path analysis for water quality transportation in the DWDS and described in the previous.

Throughout the water quality transportation, chlorine consumes the bacteria and generates decay. Furthermore, it reacts with organic matter in the water to generate DBPs. Following that, both chlorine and DBPs mix with other flows at junction nodes, the process of which is described by a series of impact coefficients in the final obtained IO model. The time-delay existing in the input-output model which occurs due to the transportation is time continuous and time varying.

In order to obtain the explicit IO water quality model with DBPs, the range of these continuous time delays over the entire modelling horizon is discretized and approximated by several delay numbers. The discrete IO model is normally obtained in a moving average (MA) format. However, the existence of storage facilities increases the detention time of water quality transportation from the input nodes to output nodes. The increased detention time must be taken into consideration when processing the dynamic of model. Therefore, the model parameters which can explain the quality dynamics are required. The IO model with tanks in the DWDS is derived in an autoregressive moving average (ARMA) format:

For Chlorine:

$$y_{n,1}(t)=\begin{cases}\sum_{j=1}^{n_I}\sum_{i\in I_{n,j}(t)} a_{n,j,i,1}(t)u_j(t-i)+\varepsilon_{n,1}(t),\ t\in \mathrm{S}_{n,f}\\ \sum_{h=1}^{n_T} b_{n,h,1}(t)y_{n,1}(t-h)+\sum_{j=1}^{n_I}\sum_{i\in I_{n,j}(t)} a_{n,j,i,1}(t)u_j(t-i)+\varepsilon_{n,1}(t),\ t\in \mathrm{S}_{n,d}\end{cases}\quad (5\text{-}1)$$
$$for\ \ n=1,...,n_M$$

For DBPs:

$$y_{n,2}(t)=\begin{cases}\sum_{j=1}^{n_I}\sum_{i\in I_{n,j}(t)} a_{n,j,i,2}(t)u_j(t-i)+\varepsilon_{n,2}(t),\ t\in \mathrm{S}_{n,f}\\ \sum_{h=1}^{n_T} b_{n,h,2}(t)y_{n,1}(t-h)+\sum_{j=1}^{n_I}\sum_{i\in I_{n,j}(t)} a_{n,j,i,2}(t)u_j(t-i)+\varepsilon_{n,2}(t),\ t\in \mathrm{S}_{n,d}\end{cases}\quad (5\text{-}2)$$
$$for\ \ n=1,...,n_M$$

where $t\in[t_0,t_0+T_M]$, t_0 is the initial time and T_M is the modelling horizon; $y_{n,1}(t)$ are chlorine concentrations and $y_{n,2}(t)$ are DBPs concentration at the monitored node, for $n=1,...,n_M$; $u_j(t)$ are chlorine concentrations at injection nodes, $j=1,...,n_I$; n_M

and n_I present number of monitored nodes and number of injection nodes, respectively; $S_{n,f}$ and $S_{n,d}$ present time-slots in filling and draining cycle, respectively; $I_{n,j}(t)$ denotes the delay number set that corresponds to output $y_n(t)=[y_{n,1}(t),y_{n,2}(t)]$ associating with the j^{th} input $u_j(t)$; $a_{n,j,i}(t)=[a_{n,j,i,1}(t),a_{n,j,i,2}(t)]$ are the model parameters corresponding to the n^{th} output $y_n(t)$ and the j^{th} input $u_j(t)$ associating with the delay number i ; $b_{n,h}=[b_{n,h,1},b_{n,h,2}],\ h=1,...,n_T$ are the parameters corresponding to the n^{th} output $y_n(t)$ that described dynamics caused by n_T tanks; $\varepsilon_n(t)=[\varepsilon_{n,1}(t),\varepsilon_{n,2}(t)]$ denotes structure error in output $y_n(t)$.

5.2.2 MIMO Point-Parametric Model

5.2.2.1 Mathematical Model of MIMO Point-Parametric Model

Due to the fact that the IO model is discretized and linearized, the structure error is inevitable and cannot be ignored. Meanwhile, the parameter uncertainty caused by hydraulic information is unknown. Therefore, parameter estimation on bounding the structure error and parameters is essential to build up a complete quality model for control purposes.

The above IO model results in the discrete MIMO model structure:

$$\begin{cases} y_{n,1}(k) = \sum_{h=1}^{n_T} b_{n,h,1}(k) y_{n,1}(k-h) + \sum_{j=1}^{n_I} \sum_{i \in I_{n,j}(k)} a_{n,j,i,1}(k) u_j(k-i) + \varepsilon_{n,1}(k) \\ y_{n,2}(k) = \sum_{h=1}^{n_T} b_{n,h,2}(k) y_{n,1}(k-h) + \sum_{j=1}^{n_I} \sum_{i \in I_{n,j}(k)} a_{n,j,i,2}(k) u_j(k-i) + \varepsilon_{n,2}(k) \end{cases} \tag{5-3}$$

$$n = 1, \ldots, n_M$$

Hence, the problem of parameter estimation is finally formulated as a time-varying dynamic model in a form of MIMO with delayed inputs under uncertainty, which is given as a general ARMA form: $\begin{cases} y_{n,1}(k) = \theta_{n,1}(k)\varphi(k-1) + \varepsilon_{n,1}(k) \\ y_{n,2}(k) = \theta_{n,2}(k)\varphi(k-1) + \varepsilon_{n,2}(k) \end{cases}$

(5-4)

Write above equations in a compact form yields:

$$y_n(k) = \theta_n(k)\varphi_n(k-1) + \varepsilon_n(k), k \in [k_0, k_0 + T_m]_Z \tag{5-5}$$

where $y_n(k) = [y_{n,1}(k), y_{n,2}(k)]$ denotes the outputs at n^{th} monitored node; $\theta_n(k)$ and $\varepsilon_n(k)$ presents the model parameters and structure error, respectively, which explains the uncertainties within the dynamics of the IO model; $\varphi_n(k-1)$ is the regressor vector; k_0 is the current time instant and T_m presents the modelling horizon length; Z denotes the integer field. The structure of elements in (5-5) is shown as follows:

$$\theta_n(k) = \begin{bmatrix} \theta_{n,1}(k) \\ \theta_{n,2}(k) \end{bmatrix} = \begin{bmatrix} b_{n,1,1}(k) \ldots b_{n,n_T,1}(k) & a_{n,I,1}(k) \\ b_{n,1,2}(k) \ldots b_{n,n_T,2}(k) & a_{n,I,2}(k) \end{bmatrix}, I = [i_l, \ldots, i_u] \tag{5-6}$$

$$\begin{aligned} \varphi_n(k-1) = [&y_{n,1}(k-1), \ldots, y_{n,1}(k-n_T), \ldots \\ &u_1(k-i_{n,l,1}), \ldots u_1(k-i_{n,u,1}), \ldots \\ &u_{n_I}(k-i_{n,l,n_I}), \ldots u_{n_I}(k-i_{n,u,n_I})] \end{aligned} \tag{5-7}$$

$$\varepsilon_n(k) = [\varepsilon_{n,1}(k), \varepsilon_{n,2}(k)] \tag{5-8}$$

Actually, $\theta(k)$ can have a sudden change at time instant $k_j \in [k_0, k_0 + T_m]$, $j \in Z^+$, but the change can be considered to be very slow over a shorter time horizon $[k_{j-1}, k_j]$ and can be considered as constant during this shorter time horizon. Therefore, the modelling time horizon T_m is partitioned into several time-slots [2] that results in the following definition of the j^{th} time-slot:

$$S_j \stackrel{\Delta}{=} \left\{ k \in Z^+ : k_{j-1} \le k \le k_j \right\}, j \in Z^+ \tag{5-9}$$

By using the data generated by the implicit model which is known as plant simulator, the values build up the regressor, i.e. past measurements parameters, can be obtained. The collection of the regressor under uncertainty in the model can be estimated by using the bounding approach which is explained in [2]. However, since the structure error is difficult to obtain in advance, it would be beneficial to bound parameters and structure error and uncertainty together, which results in the application of PPM.

Then the union containing the entire model parameters that need to be searched is expressed as:

$$\Theta\left(\theta_n{}^l, \theta_n{}^u, \varepsilon_n{}^l, \varepsilon_n{}^u\right) \stackrel{\Delta}{=} \left\{ \begin{array}{l} \left(\theta_n{}^{n_E}, \varepsilon_n{}^{n_E}\right) \in R^n : y_n{}^{n_E}(k) = \theta_n{}^{n_E} \varphi^{n_E}{}_n(k) + \varepsilon_n{}^{n_E}(k) \\ \theta_n{}^{n_E} \in \left[\theta_n{}^l, \theta_n{}^u\right]; \varepsilon_n{}^{n_E}(k) \in \left[\varepsilon_n{}^l, \varepsilon_n{}^u\right], \\ n_E = 1, \ldots, N_E, k \in \left[k_0, k_0 + T_m\right]_Z, \\ n = 1, \ldots, n_M \end{array} \right\} \tag{5-10}$$

where $\left(\theta_n, \varepsilon_n(k)\right) \in \Theta$, and N_E is the number of experiments required.

The final PPM structure is as follows:

$$\begin{aligned} & y_n(k) = \theta_n \varphi_n(k) + \varepsilon_n(k) \\ & \left(\theta_n, \varepsilon_n(k)\right) \in \Theta, k \in \left[k_0, k_0 + T_m\right]_Z, n = 1, \ldots, n_M \end{aligned} \tag{5-11}$$

The application of PPM on MIMO model structure is the main interest of this research which results in jointly bounding the parameters within two outputs with interactions.

5.2.2.2 Structure of information exchange

The information exchange structure for explaining the PPM framework is shown in Figure 5-1 [167]. The Calibrator is utilised for processing the initial information containing parameters and measurements and delivering them to implicit model, i.e. Plant Simulator in Figure 5-1 and build up plant information, i.e. Structure Information in Figure 5-1. The essential data are redistributed between Plant Simulator, Estimator and Explicit Model. The Model Structure Determination is required to establish the Explicit Model structure. Based on the estimated model parameters, the Explicit Model generates the robust output predictions, including output prediction of nominal model in a form of Chebyshev Centre and upper & lower bounds for real plant. The clear explanation of the aforementioned structure can be found in [167].

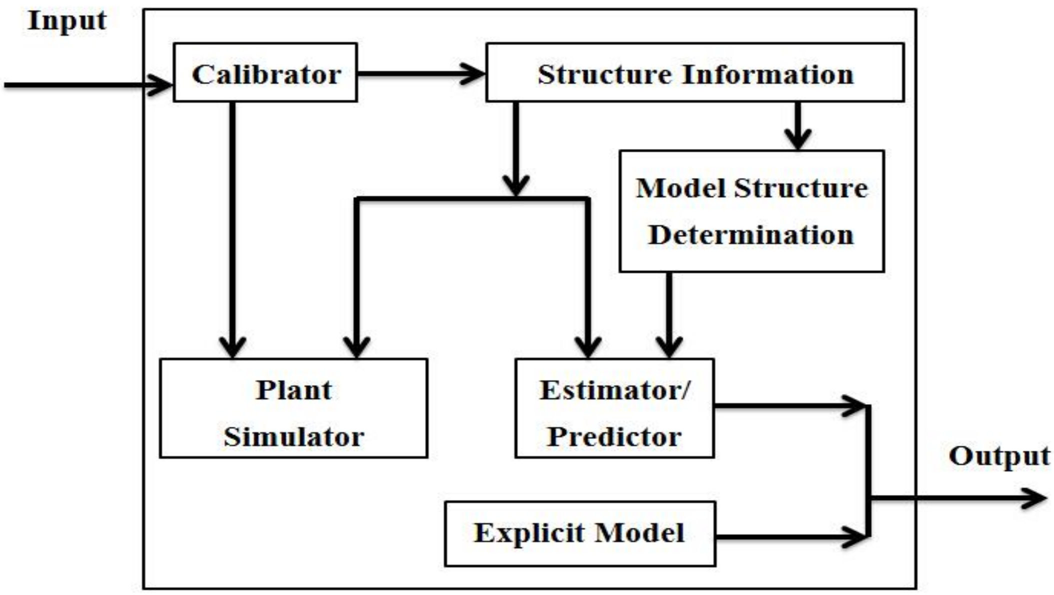

Figure 5-1 PPM Information Structure

5.2.2.3 Robust Parameter Estimation

According to previous analysis, the parameter estimation is implemented based on the collected input-output measurements as input-output pairs. The overall number of pairs is determined by the number of experiments conducted based on the plant simulator. For each of the input-output pair, a corresponding series of parameters involved in the model can be found. An example of parameter estimation that searched for two-dimension parameters experiment can be found in [2]. However, those experiments are based on MISO models structure. Regarding to the developed PPM on water quality in this thesis, bounding the parameters of the quality outputs should be jointly considered due to the interaction between two quality outputs.

Taking one monitored node as an example, the estimation of the set $\Theta^*\left(\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}\right)$ containing the least conservative parameter bounds is carried out by solving the following optimization task:

$$\begin{aligned}\left[\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}\right]=\underset{\left[\theta^{l},\theta^{u},\varepsilon^{l},\varepsilon^{u}\right]}{\arg\min}\left\{J\left(\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}\right)\right\}\\ s.t.\ \left(\theta^{n_E},\varepsilon^{n_E}\right)\in\Theta\left(\theta^{l},\theta^{u},\varepsilon^{l},\varepsilon^{u}\right)\end{aligned}\tag{5-12}$$

where for the clarity of presentation: $\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}$ are denoted as the least conservative lower and upper bounds on parameter vector and structural error respectively; pair ($\theta^{n_E},\varepsilon^{n_E}$) represents the coefficients that can explain the n_E^{th} experiment output; the cost function $J\left(\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}\right)$ is set up to find the minimal distance between the parameter and structure error bounds as:

$$J\left(\theta^{*l},\theta^{*u},\varepsilon^{*l},\varepsilon^{*u}\right)=\left(\theta^{*u}-\theta^{*l}\right)^T\mathbf{P}\left(\theta^{*u}-\theta^{*l}\right)+\left(\varepsilon^{*u}-\varepsilon^{*l}\right)^T\mathbf{Q}\left(\varepsilon^{*u}-\varepsilon^{*l}\right)\tag{5-13}$$

where weight matrices **P** and **Q** are assumed to be diagonal and positive defined. In this case that latter is equivalent to matrices having positive diagonal entries [2]. Since the weight coefficient matrices **P** and **Q** have significant impact on the uncertainty contained in the parameters and structure error over the estimation, it is vital to choose appropriate values for those matrices that can bring influential results by solving the given optimisation task. The impact brought by different weight coefficient matrices will be presented in the following section.

The optimization task in equation (5-12) is required to solve over the whole modelling horizon within each time instant to obtain the complete piece-wise PPM structure.

5.2.2.4 Experiment Design

The input for the system is normally affected by the actuator performance and limitations. For water quality control, the input constraints can be expressed as:

$$\begin{aligned} & u^{\min} \le u(t) \le u^{\max}, \quad for\ t \in [t_0, t_0 + T_c] \\ & u^{\min} \ge 0 \end{aligned} \tag{5-14}$$

where T_c is control horizon.

An input $u = [u(t_0)\ u(t_0+1) \ldots u(T_c)]$ over the horizon can be presented as a point in a T_c dimension of Euclidean space with N_v vertices, where $N_v = 2^{T_c}$. The theorem described in [168] is applicable for designing the input of experiments:

Theorem 5-1 Define $K \subset R^d$ to be a polytope, $K = \{v_1, v_2, ..., v_r\}$. Each $x \subset K$ can be presented in a form as:

$$x = \sum_{i=1}^{r} \lambda_i(x) v_i \tag{5-15}$$

where $\lambda_i(x) \ge 0$, and $\sum_{i=1}^{r} \lambda_i(x) = 1$. The proof of Theorem 5-1 can be found in [168].

Theorem 5-1 allows any point in the polytope space to be expressed by the convex combination of the polytope's vertices [2]. Then, any input satisfying (5-14(5-14) can be expressed as:

$$u(t)=\sum_{i=1}^{N_v}\gamma_i u^i,\ \ t=1,\ldots,T_c \tag{5-16}$$

where $\sum_{i=1}^{N_v}\gamma_i=1$ and $\gamma_i\geq 0$. And $u^i=[u^i(1),u^i(2),\ldots,u^i(T_c)]$ is the i^{th} vertex of the T_c-dimension cube and is so called base input. The component $u^i(k)$ in u^i is $u^{\min}$ or $u^{\max}$ defined in (5-14).

For each experiment in fact, the time horizon of output should be no longer than input horizon. In this thesis, the horizon of input and output is considered as the same. One experiment is implemented by applying one base input to obtain the two outputs at the same time horizon. The associated input-output pair is collected for estimating the parameter bounds in (5-11).

Note that the required number of experiments $N_E=2^{T_c}$, with large T_c, the difficulty of computation in solving (5-11) increases dramatically. In practice, the experiments start with certain base inputs, and calculate the responding bounds on parameters. Then they increase the number of base inputs until the model satisfies the prescribed constraints or requirements.

5.2.2.5 Validation of the MIMO PPM

The PPM described in equation (5-11) is composed of chlorine and DBPs. Due to these two models has the same structure, it is convenient to validate them separately.

The PPM for chlorine in continuous time can be presented as:

$$\begin{aligned} &y_{n,1}(t) = \theta_{n,1}\varphi_{n,1}(t) + \varepsilon_{n,1}(t) \\ &\left(\theta_{n,1}, \varepsilon_{n,1}(t)\right) \in \Theta, t \in [t_0, t_0 + T_m]_Z, n = 1, ..., n_M \end{aligned} \tag{5-17}$$

Consider only one monitored node exist, and then let $\left\{u^{n_E}(t), y_{1,1}^{n_E}(t)\right\}_{n_E=1}^{N_E}$ be the input-output pairs corresponding to the PPM defined as in (5-17), where $t = 1, ..., T_c$. Let $\theta_{n,1}^1, ..., \theta_{n,1}^{N_E}, \varepsilon_{n,1}^1(t), ..., \varepsilon_{n,1}^{N_E}(t)$ be the parameter in $y_{1,1}^{n_E}(t) = \theta_{1,1}^{n_E}\varphi_{1,1}^{n_E}(t) + \varepsilon_{1,1}^{n_E}(t)$, where $\left(\theta_{1,1}^{n_E}, \varepsilon_{1,1}^{n_E}(t)\right) \in \Theta$, and Θ is defined as in (5-10). For each experiment for $n_E = 1, ..., N_E$:

$$y_{1,1}^1(t) = \theta_{1,1}^1\varphi_{1,1}^1(t) + \varepsilon_{1,1}^1(t) \tag{5-18}$$

$$y_{1,1}^{N_E}(t) = \theta_{1,1}^{N_E}\varphi_{1,1}^{N_E}(t) + \varepsilon_{1,1}^{N_E}(t) \tag{5-19}$$

where $\left(\theta_{1,1}^{n_E}, \varepsilon_{1,1}^{n_E}(t)\right) \in \Theta$. Due to the PPM is linear, its response to the input $u(t) = \sum_{n_E=1}^{N_E} \gamma_{n_E} u^{n_E}$ is $y_{1,1}(t) = \sum_{n_E=1}^{N_E} \gamma_{n_E} y_{1,1}^{n_E}(t)$, where $\gamma_{n_E} \geq 0$, and $\sum_{n_E=1}^{N_E} \gamma_{n_E} = 1$ .And $\varphi_{1,1}(t) = \sum_{n_E=1}^{N_E} \gamma_{n_E} \varphi_{1,1}^{n_E}(t)$. And then, define $\theta_{1,1}, \varepsilon_{1,1}(t)$ as [2]:

$$\theta_{1,1,m} = \sum_{n_E=1}^{N_E} \beta_m^{n_E}(t)\theta_{1,1,m}^{n_E}, \quad m = 1,\ldots,M \tag{5-20}$$

$$\varepsilon_{1,1}(t) = \sum_{n_E=1}^{N_E} \gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \tag{5-21}$$

where $\beta_m^{n_E}(t) = \dfrac{\gamma_{n_E}\varphi_{1,1,m}^{n_E}(t)}{\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1,m}^{n_E}(t)}$ where M is the dimension of the parameter vector, $\theta_{1,1,m}$ is the m^{th} component of vector $\theta_{1,1}$, $\varphi_{1,1,m}$ is the m^{th} component of vector $\varphi_{1,1}$. In our application, $u(t) \geq 0$ and $y_{1,1}(t) \geq 0$, $\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1,m}^{n_E} = 0$ is equivalent to $\varphi_{1,1,m}^{n_E}(t) = 0$. Therefore, $\theta_{1,1,m}$ can be defined as $\theta_{1,1,m} = \sum_{n_E=1}^{N_E}\gamma_{n_E}\theta_{1,1,m}^{n_E}$ when $\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1,m}^{n_E} = 0$ [2]. This does not change the following calculation:

$$
\begin{aligned}
\theta_{1,1}\varphi_{1,1}(t)+\varepsilon_{1,1}(t) &= \theta_{1,1}\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1}^{n_E}(t)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{n_E=1}^{N_E}\sum_{m=1}^{M}\gamma_{n_E}\theta_{1,1,m}\varphi_{1,1,m}^{n_E}(t)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{m=1}^{M}\frac{\gamma_{n_E}\theta_{1,1,m}^{n_E}\varphi_{1,1,m}^{n_E}(t)}{\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1,m}^{n_E}(t)}\left(\sum_{n_E=1}^{N_E}\gamma_{n_E}\varphi_{1,1,m}^{n_E}(t)\right)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{m=1}^{M}\sum_{n_E=1}^{N_E}\gamma_{n_E}\theta_{1,1,m}^{n_E}\varphi_{1,1,m}^{n_E}(t)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{n_E=1}^{N_E}\sum_{m=1}^{M}\gamma_{n_E}\theta_{1,1,m}^{n_E}\varphi_{1,1,m}^{n_E}(t)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{n_E=1}^{N_E}\gamma_{n_E}\sum_{m=1}^{M}\theta_{1,1,m}^{n_E}\varphi_{1,1,m}^{n_E}(t)+\sum_{n_E=1}^{N_E}\gamma_{n_E}\varepsilon_{1,1}^{n_E}(t) \\
&= \sum_{n_E=1}^{N_E}\gamma_{n_E}\left\{\sum_{m=1}^{M}\theta_{1,1,m}^{n_E}\varphi_{1,1,m}^{n_E}(t)+\varepsilon_{1,1}^{n_E}(t)\right\} \\
&= \sum_{n_E=1}^{N_E}\gamma_{n_E}y_{1,1}^{n_E}(t) \qquad (5\text{-}22) \\
&= y_{1,1}(t)
\end{aligned}
$$

Thus, it has been proved that equation (5-17) is existent. The validation on PPM of DBPs can be proved in a similar way.

5.2.3 Robust Output Prediction by Implementing Piece-Wise Constant Continuity in Model Parameters

In order to achieve RFMPC control purpose, the optimisation task of obtaining robust output prediction needs to be solved.

Define:

$$W = \max\left\{Y_{1,p}{}^{u} - Y_{1,p}{}^{l}\right\}, \text{under}\, u(\mathrm{t}) = 1(\mathrm{t}) \tag{5-23}$$

where W is the model uncertainty radius which presents the impact of model uncertainty on the output prediction accuracy and is calculated by applying a unit step input. $Y_{1,p}$ represents output prediction of disinfectant at one monitored node. The explanation of applying unit step input to determine uncertainty radius can be found in [2].

As DBPs are considered as the second output, the interaction between chlorine and DBPs cannot be ignored. Apart from the objective of maintaining chlorine within the prescribed limits, the second objective of the MPC water quality control is to keep DBPs concentration as small as possible. Hence, there is no need to define the uncertainty radius for DBPs. However, DBPs saturation level exists when considering the upper bound of output prediction on DBPs [13]. Moreover, with the increasing of the time instant, the lower bound of output prediction on DBPs should be kept no less than zero, which means another condition for determining the time-slot is required:

$$Y_{2,\mathrm{p}}^{l} \geq 0 \tag{5-24}$$

The upper and lower bounds for outputs are defined as:

$$
\begin{aligned}
&Y_p^{\,u} = \left[y_p^{\,u}\left(k+1|k\right) \ldots y_p^{\,u}\left(k+T_m\,|\,k\right) \right] \\
&Y_p^{\,l} = \left[y_p^{\,l}\left(k+1|k\right) \ldots y_p^{\,l}\left(k+T_m\,|\,k\right) \right] \\
&where\, Y_p = [Y_{1,p}, Y_{2,p}]
\end{aligned} \tag{5-25}
$$

where $y_p^{\,u}\left(k+1|k\right)$ and $y_p^{\,u}\left(k+1|k\right)$ are calculated based on solving the following optimisation problems [2]:

$$
\begin{aligned}
y_p^{\,u}\left(k+i\,|\,k\right) &= \max_{V_{p,t+i}} \left\{ y\left(k+i\,|\,k\right) \right\} \\
&\quad s.t.\; y\left(k+i\,|\,k\right) \in Y_p \\
y_p^{\,l}\left(k+i\,|\,k\right) &= \min_{V_{p,k+i}} \left\{ y\left(k+i\,|\,k\right) \right\} \\
&\quad s.t.\; y\left(k+i\,|\,k\right) \in Y_p
\end{aligned} \tag{5-26}
$$

where $V_{p,t+i}$ is given by:

$$
V_{p,k+i} = \left\{ \begin{array}{l} y\left(k+1|t\right),..,y\left(k+i\,|\,t\right), \\ \varphi\left(k+1|t\right),..,\varphi\left(k+i\,|\,t\right), \\ \theta, \varepsilon\left(k+1|t\right),..,\varepsilon\left(k+i\,|\,t\right) \end{array} \right\} \tag{5-27}
$$

The robust output prediction is calculated by the following algorithm: A priori partitioning is produced based on the path analysis;

Step 2. Starting estimation at t_0 with N=1, the parameter bounds are calculated by solving Equation (5-16);

Step 3. If $t_0 + N$ is within the a priori slot and corresponding obtained W satisfies with the selected W^{max} and Equation (5-24) is satisfied, set N=N+1, back to Step 2;

Or set $t_0 = t_0 + N$ as the new partitioning point, back to Step 2 until the whole modelling horizon is completed.

5.3 Simulation Results and Discussions

5.3.1 Example network with one switching type tank

The topology of the case study network is illustrated in Figure 5-2. There are 8 consumption nodes in the DWDS as the same as described in Chapter 4. Node 9 is the reservoir, and node 2 is a switching tank operating by user-defined control rules. A pump connected between node 9 and node 10 is the only energy-consumed component in the network. The hydraulic time-step is set to 1 hour and quality time step is set to 10 minutes. The pump is operated by a simple rule according to the water head in the tank. The simple rule contains specified values for the water head in the tank which determines the tank operating status.

The whole modelling horizon is 35 hours including filling cycle and draining cycle due to the operation of the tank. In the first 13 hours, the example DWDS is in a filling operation, and then it switches to a draining cycle which takes the next 11 hours, after that it switches back to the filling cycle lasting 11 hours. This multiple hydraulic operation status increases the complexity of the PPM application on water quality control. In addition, since two outputs are involved, in the parameter estimation, more estimated parameters are introduced, which further increases the complexity of the application of PPM on MIMO.

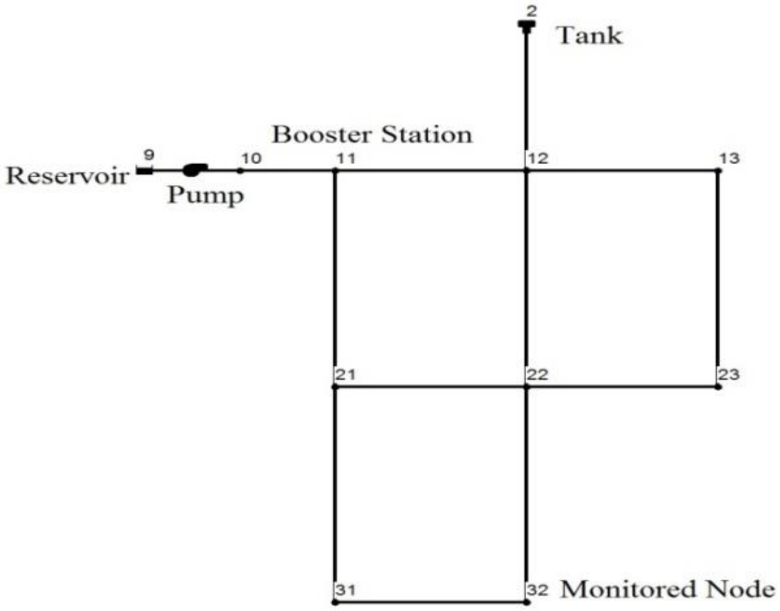

Figure 5-3 The Case Study Network with a Switching Tank

The junction node *n32* is selected as the monitored node since its location is considered to be the most remote from the source. The booster station is installed at *n11* (Injection node). The algorithms on determining allocation of booster stations are presented in [71, 74].

The constraints of control input in this network can be expressed as:

$$0(\mathrm{mg/L}) \le u(t) \le 1(\mathrm{mg/L}), \quad for\ t \in [0, T_m] \tag{5-28}$$

5.3.2 Illustration of Path Analysis Algorithm

The IO model of water quality is described by equations (5-2) and (5-3). During the filling cycle, three paths are active from the injection node to the monitored node, which can be denoted by the sequences of the pipe ID, i.e. Path I (111-121-31), Path II (111-21-122), and Path III (11-112-122). Only one path is active when the tank switches to the draining period which is Path I. Algorithms of calculating the detention time of quality transportation in DWDS were described in Chapter 3. The water quality transportation delay in paths and associated delay number can be calculated by applying a backward tracking algorithm, and the tracking time step is set to 1 minute. The path analysis result is shown in Figure 5-4. Figure 5-5 illustrates the time delay in 3 active paths. The delay number corresponding to the associated paths can be calculated.

The simulation is based on MATLAB with a connection to EPANET software package and EPANET Multi-Species (MSX) Module.

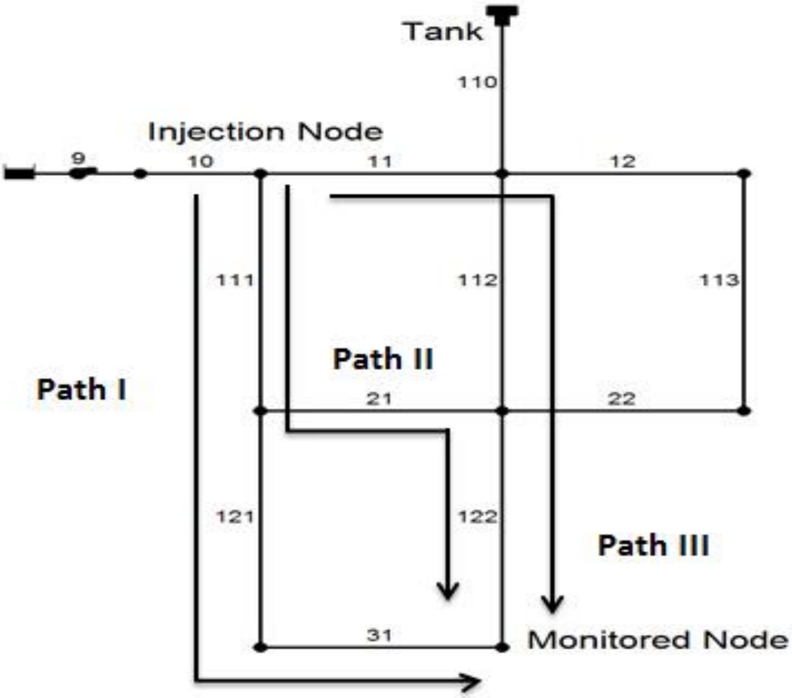

Figure 5-4 Path Analysis to the Case Study Network

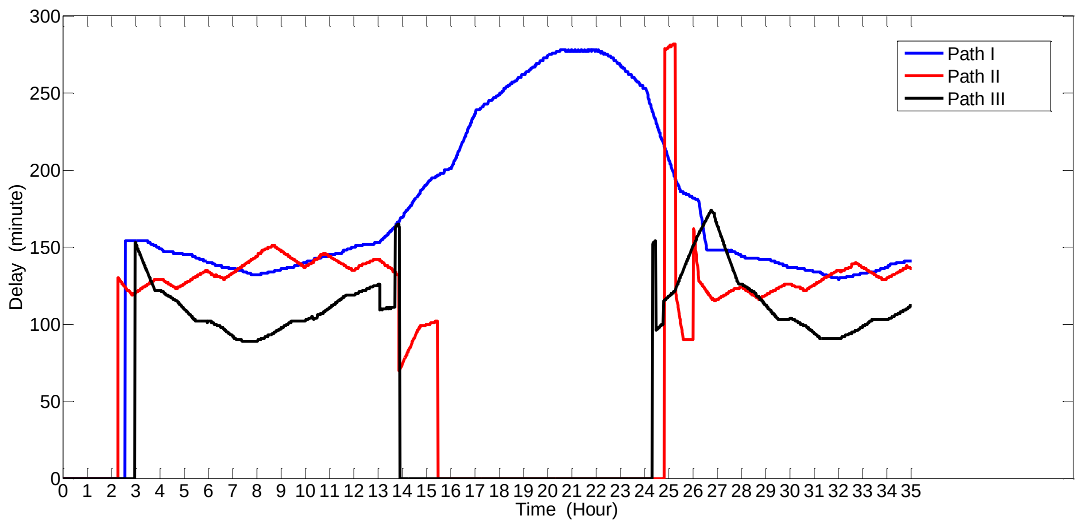

Figure 5-5 Detention Time in Three Active Paths during the Whole Modelling Horizon

5.3.3 Simulation Results and Discussions

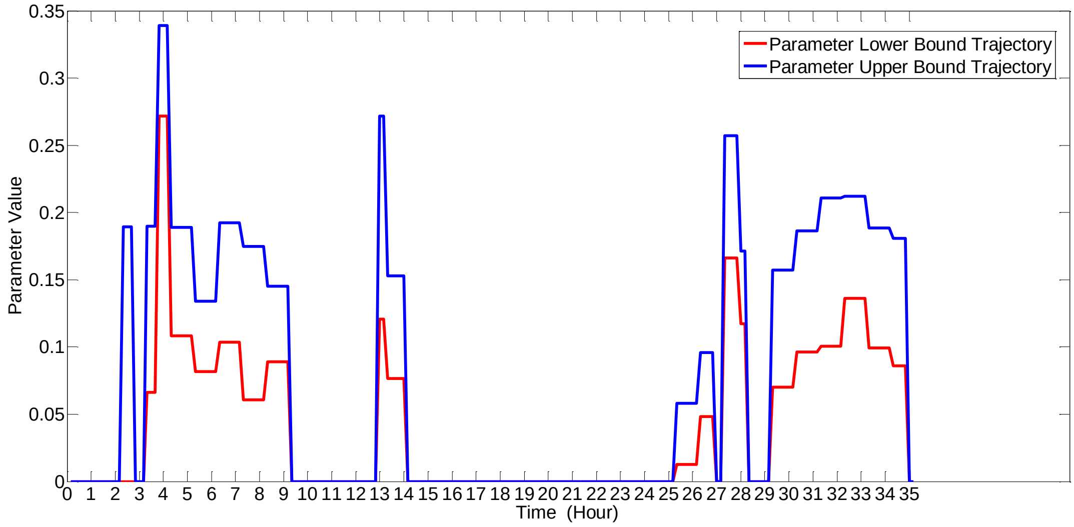

Figure 5-6 Parameter Bounds Corresponding to Delay Number 13 in Chlorine

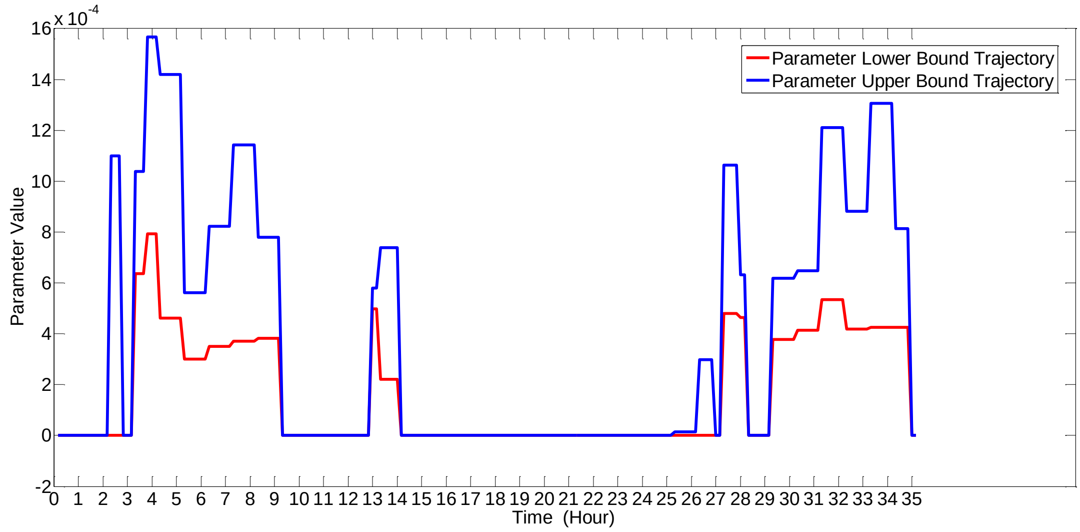

Figure 5-7 Parameter Bounds Corresponding to Delay Number 13 in DBPs

Figure 5-6 and Figure 5-7 illustrate the example of bounded piece-wise constant parameters corresponding to delay number 13 for the model of chlorine and DBPs, respectively. These parameters are active at certain periods based on the hydraulic operation. Envelops of the parameter bounds are similar due to the existence of such interactions between free chlorine and DBPs in the nonlinear water quality dynamic model.

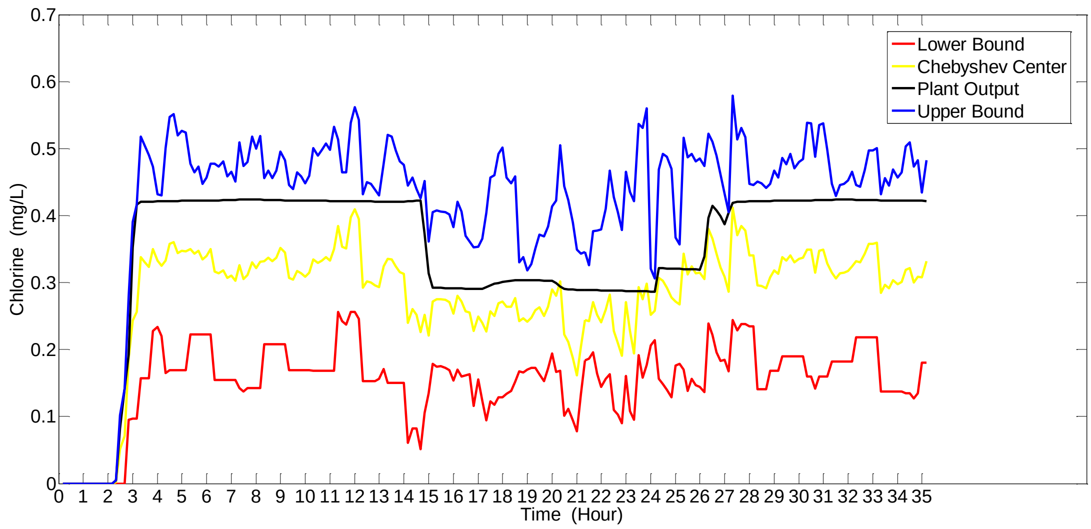

Figure 5-8 Robust Output Prediction on Chlorine under Unit Step Input

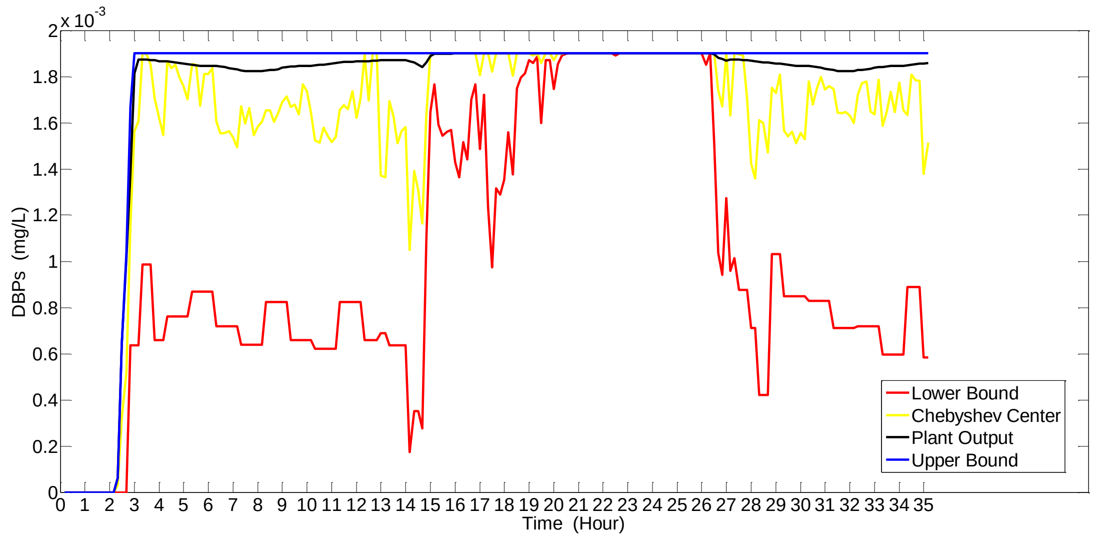

Figure 5-9 Robust Output Prediction on DBPs under Unit Step Input

The robust output predictions for chlorine and DBPs at the monitored node obtained by applying unit step input are illustrated in Figure 5-8 and Figure 5-9, respectively. It can be seen that real plant output is covered by the robustly predicted upper and lower bounds on chlorine concentration and DBPs concentration at the monitored node within such a complex hydraulic operation status. The upper bound of predicted DBPs concentration remains constant during such a period as the DBPs concentration cannot exceeds its saturation level.

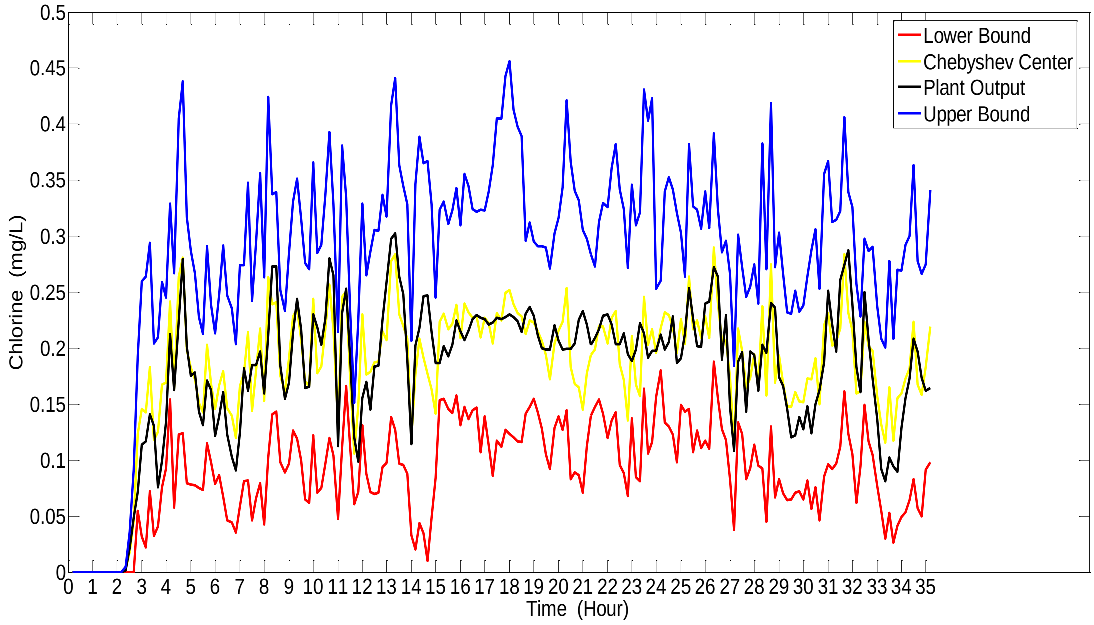

Figure 5-10 Robust Output Prediction on Chlorine under Random Input

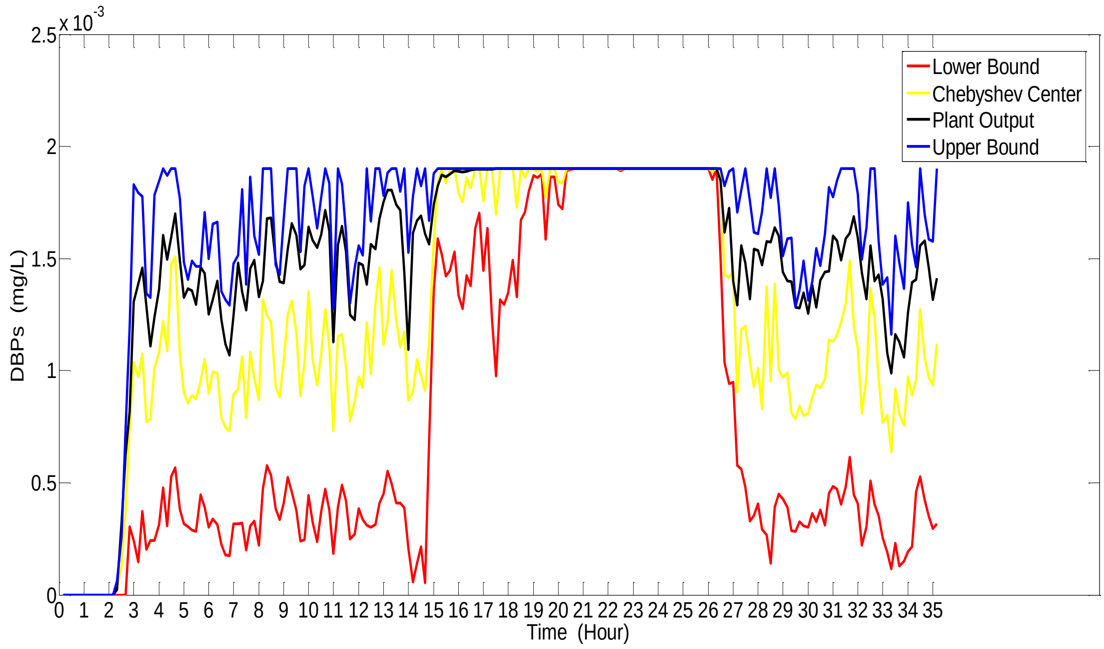

Figure 5-11 Robust Output Prediction on DBPs under Random Input

Figure 5-10 and Figure 5-11 illustrate the robust output prediction on chlorine and DBPs concentration at the monitored node under random input. Even if the input considered is selected at random, the real plant output covered by its upper and lower prediction bounds is still valid. Hence, the PPM framework is verified to be appropriate for such MIMO model structure.

By changing the weight of the P and Q expressed in equation (5-16), the uncertainty allocation in the parameter part and structure error part can be varied. Table 5-1 shows the uncertainty radius obtained by selecting different sets of weight coefficients. It can be found that the uncertainty radius W is at the minimum at P=1.0 and Q=0.1 according to the data. However, the optimal values of P and Q that result in a global minimum *W* still remain unanswered.

Table 5-1 Uncertainty Radius within Different Weight Coefficient Sets

Values of Weight Coefficients	**Uncertainty Radius**
P=1.0 Q=0.1	0.3762
P=1.0 Q=0.2	0.3785
P=1.0 Q=0.1	0.3843
P=1.0 Q=0.5	0.4330
P=1.0 Q=10.0	0.4330

The performance of PPM can be further improved by applying appropriate hydraulic information since the water demand (input disturbance for water quality) and flow (another quality input in the hydraulic part) have significant impact on control of water quality.

5.4 Summary

In this chapter, an extension of applying PPM framework from MISO to MIMO model structure on nonlinear dynamic water quality model with considering DBPs has been presented. The MISO output prediction algorithm has been incorporated with MIMO in order to robustly estimate parameters of the quality model.

The piece-wise constant parameters for such a MIMO model have been obtained for the purpose of robust feasible control on water quality considering DBPs. The explicit structure of the water quality model has been also presented in the form of a input-output model by implementing a back-tracking algorithm.

The simulation results above described the piece-wise constant parameters within the MIMO PPM and also illustrated that the real plant outputs can be explained by their upper and lower prediction bounds. In addition, this chapter has developed the MISO model structure into the MIMO model structure. The capability of PPM of processing a wider range of system identification problems has been proved. The importance of the hydraulic support to the quality control has been highlighted. The MIMO model and the algorithm presented in this chapter will be beneficial for robust feasible model predictive control of water quality in DWDS considering DBPs.

CHAPTER 6 CONCLUSION AND FUTURE RESEARCH WORK

6.1 Conclusions

Quantity and quality control are the two main interests in the operational control of DWDS. The quality control problem has been discussed in this thesis within a newly derived nonlinear water quality model. Compared to the linear water quality model, the advanced nonlinear water quality model considering dynamic of DBPs is more close to the real DWDS application. Objectives of the water quality control problem have been replenished when considering the existences of DBPs. Conclusions for this thesis are summarised as follows:

1. One of the main objectives in this thesis is to develop a nonlinear MPC controller for optimising water quality in DWDS with DBPs under defined constraints. Firstly, according to the work been done in Chapter 4, MPC has been proved as the core control driver in solving such nonlinear, constrained, multivariable problem. This nonlinear MPC controller successfully provided a practical solution for on-line control of water quality in DWDS considering augmented DBPs objective. Furthermore, the simulation results illustrated in Chapter 4 have been shown a good

MPC controller performance on dealing with water quality optimisation control problem. It has been proved that chlorine and DBPs can be jointly controlled by formulating the proper objective functions and applying nonlinear MPC controller. Moreover, MPC control algorithm can be considered as a reliable method to handle nonlinear control problem in DWDS. And GA is also a good optimisation solver in solving the multi-objective optimisation control problem when no gradient exist. In addition, the impact brought by hydraulic can be clearly observed, especially in output dynamic of DBPs during the draining cycle.

2. Because the uncertainty is not considered in the simulators employed in Chapter 4 for designing the nonlinear MPC controller, the other objective is to take uncertainty into consideration when modelling the advanced nonlinear water quality model. Hence, the research conducted in Chapter 5 is necessary in analysing nonlinear water quality model with considering uncertainty. Firstly, the bounding approach so call point-parametric model has been successfully applied in this thesis for analysing nonlinear water quality model. Although PPM has been applied to the liner water quality model in the previous research work, the complete piece-wise PPM in a form of MIMO on nonlinear water quality control has been derived and proposed for the first time. Furthermore, the parameter estimation and output prediction of the nonlinear water quality model have been robustly implemented based on the derived the piece-wise constant bounded MIMO PPM model. Moreover, the results have been

clearly shown that plant outputs of water quality can be explained by derived piece-wise MIMO PPM, even under random inputs. The fact that influence caused by hydraulic information cannot be ignored has been proven again especially from the output prediction of DBPs.

Much work has been done on investigating the nonlinear water quality control problem, though further development is required which will be summarised in the following section as future research work.

6.2 Future Research Work

Based on the research work presented in this thesis, future studies can be continued under the following aspects:

Firstly, with MIMO PPM derived in Chapter 5, a reliable RFMPC controller is needed. The parameters explained the dynamic of the nonlinear water quality model in a form of MIMO PPM which was estimated robustly, and the output prediction of such a model has been implemented based on a defined ‘uncertainty radius’, the RFMPC controller can be designed in the future.

Secondly, in this thesis, only one node was considered as the monitored node that was selected properly in representing the quality distribution in the case study DWDS network. Monitoring more nodes on-line under the limitation of hard sensors will make the problem more complicated because more constraints are required to be satisfied in the control problem. Implementing such a MPC controller in a much more complicated case study network with several injection nodes or monitored nodes will benefit observation of the reliability of such a control mechanism under more uncertainties.

Thirdly, although GA is selected as the optimisation solver in the developed MPC controller because no gradient is provided in the formulated objective functions, its high demand on computation is observed. Further developing the derived water quality model so that a greater optimisation solver can be utilised in the MPC controller is a possible way to improve the computation efficiency.

LIST OF PUBLICATIONS

Journal Papers

[1] **Mingyu Xie**, Mietek Brdys, “Nonlinear Model Predictive Control of Water Quality in Drinking Water Distribution Systems with DBPs Objectives”, International Journal of Mathematical, Computational, Physical, Electrical and Computer Engineering, Vol:9, No:8, 2015.

[2] **Mingyu Xie**, Puyu Wang, Xiao-Ping Zhang and Dilan Jayaweera, “Robust Parameter Estimation and Output Prediction for Control of Water Quality in Drinking Water Distribution Systems with Considering Disinfectant By-Products,” (Submitted to the Journal of Water Resources Planning and Management)

APPENDIX A EPANET INPUT FILE FOR EXAMPLE NETWORK

```
[TITLE]
EPANET INPUT FILR FOR A CASE STUDY NETWORK

[JUNCTIONS]
;ID            Elev          Demand        Pattern
 10            710           0             1             ;
 11            710           150           1             ;
 12            700           150           1             ;
 13            695           100           1             ;
 21            700           150           1             ;
 22            695           200           1             ;
 23            690           150           1             ;
 31            700           100           1             ;
 32            710           100           1             ;

[RESERVOIRS]
;ID            Head          Pattern
 9             800                         ;

[TANKS]
;ID Elevation  InitLevel  MinLevel  MaxLevel  Diameter  MinVol  VolCurve
2   850        121        100       160       50.5      0                 ;

[PIPES]
;ID  Node1  Node2  Length  Diameter  Roughness  MinorLoss  Status
10   10     11     100     18        100        0          Open   ;
11   11     12     2640    14        100        0          Open   ;
12   12     13     2640    10        100        0          Open   ;
21   21     22     2640    10        100        0          Open   ;
22   22     23     2640    12        100        0          Open   ;
31   31     32     2640     6        100        0          Open   ;
111  11     21     2640    10        100        0          Open   ;
112  12     22     2640    12        100        0          Open   ;
113  13     23     2640     8        100        0          Open   ;
121  21     31     2640     8        100        0          Open   ;
```

```
122   22    32    2640   6    100    0    Open    ;
110   2     12    200    18   100    0    Open    ;

[PUMPS]
;ID        Node1        Node2        Parameters
 9         9            10           HEAD 1   ;

[VALVES]
;ID     Node1     Node2     Diameter     Type     Setting     MinorLoss

[TAGS]

[DEMANDS]
;Junction          Demand          Pattern          Category

[STATUS]
;ID                Status/Setting

[PATTERNS]
;Demand Pattern
;ID                Multipliers
 1      1       1       1       1       1       1
 1      1       1       1       1       1       1
 1      1.2     1.2     1.2     1.2     1.2     1.2
 1      1.2     1.2     1.2     1.2     1.2     1.2
 1      1.35    1.35    1.35    1.35    1.35    1.35
 1      1.35    1.35    1.35    1.35    1.35    1.35
 1      1.5     1.5     1.5     1.5     1.5     1.5
 1      1.5     1.5     1.5     1.5     1.5     1.5
 1      1.35    1.35    1.35    1.35    1.35    1.35
 1      1.35    1.35    1.35    1.35    1.35    1.35
 1      1.2     1.2     1.2     1.2     1.2     1.2
 1      1.2     1.2     1.2     1.2     1.2     1.2
 1      1.1     1.1     1.1     1.1     1.1     1.1
 1      1.1     1.1     1.1     1.1     1.1     1.1
 1      1       1       1       1       1       1
 1      1       1       1       1       1       1
 1      0.9     0.9     0.9     0.9     0.9     0.9
 1      0.9     0.9     0.9     0.9     0.9     0.9
 1      0.8     0.8     0.8     0.8     0.8     0.8
 1      0.8     0.8     0.8     0.8     0.8     0.8
```

```
 1      0.9    0.9    0.9    0.9    0.9    0.9
 1      0.9    0.9    0.9    0.9    0.9    0.9
 1      1      1      1      1      1      1
 1      1      1      1      1      1      1
;Injection for node 11
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0
 P11    0      0      0      0      0      0

[CURVES]
;PUMP: Pump Curve for Pump 9
;ID                X-Value          Y-Value
1                  1500             250

[CONTROLS]
LINK 9 OPEN IF NODE 2 BELOW 104.5
LINK 9 CLOSED IF NODE 2 ABOVE 150

[RULES]
```

```
[ENERGY]
 Global Efficiency        75
 Global Price              0
 Demand Charge             0

[EMITTERS]
;Junction            Coefficient

[QUALITY]
;Node                  InitQual
 9                     0
 2                     0.3

[SOURCES]
;Node          Type                Quality           Pattern
 11          FLOWPACED            0.5                P11

[REACTIONS]
;Type          Pipe/Tank              Coefficient


[REACTIONS]
 Order Bulk                1
 Order Tank                1
 Order Wall                1
 Global Bulk               -0.5
 Global Wall               -1
 Limiting Potential         0
 Roughness Correlation      0

[MIXING]
;Tank                  Model

[TIMES]
 Duration                  24:00
 Hydraulic Timestep         1:00
 Quality Timestep           0:10
 Pattern Timestep           0:10
 Pattern Start              0:00
 Report Timestep            0:10
 Report Start               0:00
```

```
 Start ClockTime        12 am
 Statistic              None

[REPORT]
 Status                 No
 Summary                No
 Page                   0

[OPTIONS]
 Units                  GPM
 Headloss               H-W
 Specific Gravity       1
 Viscosity              1
 Trials                 40
 Accuracy               0.001
 CHECKFREQ              2
 MAXCHECK               10
 DAMPLIMIT              0
 Unbalanced             Continue 10
 Pattern                1
 Demand Multiplier      1.0
 Emitter Exponent       0.5
 Quality                Chemical mg/L
 Diffusivity            1
 Tolerance              0.001

[COORDINATES]
;Node                   X-Coord           Y-Coord
 10                     20.00             70.00
 11                     30.00             70.00
 12                     50.00             70.00
 13                     70.00             70.00
 21                     30.00             40.00
 22                     50.00             40.00
 23                     70.00             40.00
 31                     30.00             10.00
 32                     50.00             10.00
 9                      10.00             70.00
 2                      50.00             90.00
```

```
[VERTICES]
;Link              X-Coord              Y-Coord

[LABELS]
;X-Coord           Y-Coord              Label & Anchor Node

[BACKDROP]
 DIMENSIONS        7.00           6.00           73.00          94.00
 UNITS             None
 FILE
 OFFSET            0.00           0.00

[END]
```

APPENDIX B EPANET-MSX INPUT FILE FOR EXAMPLE NETWORK

```
[TITLE]
 EPANET-MSN INPUT FILE FOR A CASE STUDY NETWORK

[OPTIONS]
   RATE_UNITS HR                   ;Reaction rates are concentration/hour
   SOLVER          RK5             ;5-th order Runge-Kutta integrator
   TIMESTEP        600             ;600 sec (10 min) solution time step
   RTOL            1.0e-11         ;Relative concentration tolerance
   ATOL            1.0e-6          ;Absolute concentration tolerance

[SPECIES]
   BULK   CL2    MG                ;Dissolved free chlorine
   BULK   DBP    MG                ;Dissolved total chlorine in DBP


[COEFFICIENTS]
   CONSTANT kCL      0.0049256     ;Reaction kinetics parameter
   CONSTANT kDBP1    4.0397        ;Reaction kinetics parameter
   CONSTANT kDBP2    4.0397        ;Reaction kinetics parameter
   CONSTANT sDBP     39.541        ;Stoichiometric coefficient
   CONSTANT DBPp1    0.0019023     ;DBP formation potential parameter
   CONSTANT DBPp2    0.0019023     ;DBP formation potential parameter

[PIPES]
   RATE     CL2     -kCL*CL2-sDBP*kDBP1*(DBPp1-DBP)*CL2

   RATE     DBP      kDBP2*(DBPp2-DBP)*CL2


[TANKS]
   RATE     CL2     -kCL*CL2-sDBP*kDBP1*(DBPp1-DBP)*CL2

   RATE     DBP      kDBP2*(DBPp2-DBP)*CL2

[SOURCES]
```

[QUALITY]

NODE	10	CL2	0
NODE	11	CL2	0
NODE	12	CL2	0
NODE	13	CL2	0
NODE	21	CL2	0
NODE	22	CL2	0
NODE	23	CL2	0
NODE	31	CL2	0
NODE	32	CL2	0
NODE	9	CL2	0
NODE	2	CL2	0.3

NODE	10	DBP	0
NODE	11	DBP	0
NODE	12	DBP	0
NODE	13	DBP	0
NODE	21	DBP	0
NODE	22	DBP	0
NODE	23	DBP	0
NODE	31	DBP	0
NODE	32	DBP	0
NODE	9	DBP	0
NODE	2	DBP	0

LINK	10	CL2	0
LINK	11	CL2	0
LINK	12	CL2	0
LINK	21	CL2	0
LINK	22	CL2	0
LINK	31	CL2	0
LINK	111	CL2	0
LINK	112	CL2	0
LINK	113	CL2	0
LINK	121	CL2	0
LINK	122	CL2	0
LINK	110	CL2	0
LINK	9	CL2	0

```
   LINK     10          DBP     0
   LINK     11          DBP     0
   LINK     12          DBP     0
   LINK     21          DBP     0
   LINK     22          DBP     0
   LINK     31          DBP     0
   LINK     111         DBP     0
   LINK     112         DBP     0
   LINK     113         DBP     0
   LINK     121         DBP     0
   LINK     122         DBP     0
   LINK     110         DBP     0
   LINK     9           DBP     0

[PATTERNS]


[REPORT]
Report results for all nodes
   NODES      10   11   12   13   21   22   23   31   32   9   2;
Report results for all nodes
   LINKS     10   11   12   21   22   31   111   112   113   121   122   110   9;
Report results for each specie
   SPECIES   CL2     YES     5                ;
   SPECIES   DBP     YES     7                ;
```

APPENDIX C AN EXAMPLE C-MEX FILE FOR CALLING EPANET IN MATLAB

```
#include "mex.h"
#include "epanet2.h"
/*
  *   an example of C-MEX function that allows to retrieve the
  *   pressures in all nodes of the network and flows in all pipes.
/*
void ErrorCode(int error)
{
        if (error > 100)
        {
                ENclose();
                mexPrintf(" Error code: %d \n",error);
                mexErrMsgTxt("There was an error using Epanet");
        }
}

/* Main MEX gateway function */
void mexFunction(int    nlhs, mxArray *plhs[],int nrhs, const mxArray *prhs[])
{
        // Variable declaration
        //aux variables to help copy the network name
        int fileLen, reportLen, status;
          //name of the epanet network file and report file
        char *file, *report;
        //time of the simulation, hydraulics step
        long simTime, hydStep;
        //variables for iterational solving of hydraulics
        long t, tstep, temp;
        //no. of nodes, pipes, tanks
        int nNodes, nPipes, nTanks;
        int i,j, k;
        // variable used to read p(pressure) and f(flow) and q(quality) in nodes and pipes
and source and tank
        float pressure,flow,velocity;
        // pointers to pressures and flows (output),and quality
```

```
double *presPtr, *flowPtr;

    // checking for the no of inputs
if (nrhs != 2)
        mexErrMsgTxt("Two input required");
// Checking if inputs are strings
if( !mxIsChar(prhs[0]) || !mxIsChar(prhs[1]))
        mexErrMsgTxt("Input 1 and 2 must be a string.");
//determining the lenght of the file name
fileLen = (mxGetM(prhs[0]) * mxGetN(prhs[0])) + 1;
//memory allocation for the filename
file = mxCalloc(fileLen, sizeof(char));

reportLen = (mxGetM(prhs[1]) * mxGetN(prhs[1])) + 1;
report = mxCalloc(reportLen, sizeof(char));

      // Copy sting from prhs[0] to C variable file
status = mxGetString(prhs[0], file, fileLen);
if (status != 0)
        mexWarnMsgTxt("Not enough space. String is truncated.");

status = mxGetString(prhs[1], report, reportLen);
if (status != 0)
        mexWarnMsgTxt("Not enough space. String is truncated.");

// Opening epanet
ErrorCode(ENopen(file, report, ""));

// Getting the time parameters of the simulation
ErrorCode(ENgettimeparam(EN_DURATION, &simTime));
ErrorCode(ENgettimeparam(EN_HYDSTEP, &hydStep));

// getting the parameters of the network
ErrorCode(ENgetcount(EN_NODECOUNT, &nNodes));
ErrorCode(ENgetcount(EN_TANKCOUNT, &nTanks));
ErrorCode(ENgetcount(EN_LINKCOUNT, &nPipes));

// creating matrices for outputs
  plhs[0] = mxCreateDoubleMatrix(nNodes, (simTime / hydStep)    + 1,
mxREAL);
  plhs[1] = mxCreateDoubleMatrix(nPipes, (simTime / hydStep)    + 1,
```

```
mxREAL);
   // assigning the outputs to pointers
    presPtr = mxGetPr(plhs[0]);
    flowPtr = mxGetPr(plhs[1]);

    // initialising the hydraulics epanet solver
    ErrorCode(ENopenH());
    ErrorCode(ENinitH(1));

    j = 0;
    temp = 0;

    do{
        ErrorCode(ENrunH(&t));
        // condition for reading the data only on full hydraulics step
        if ((temp == hydStep) || (temp == 0))
        {
            temp = 0;
            for( i = 1; i <= nNodes ; i++)
            {
                ErrorCode(ENgetnodevalue(i, EN_PRESSURE, &pressure));
                presPtr[j*(nNodes)+i-1] = pressure;
            }
            for (k = 1; k <= nPipes; k++)
            {
                ErrorCode(ENgetlinkvalue(k,EN_FLOW, &flow));
                flowPtr[j*nPipes + k-1] = flow;
            }

            j++;
        }
        ErrorCode(ENnextH(&tstep));
        temp += tstep;
    }while( tstep > 0);

     ErrorCode(ENcloseH());
    ErrorCode(ENclose());
}
```

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