Chemical Product and Process Modeling

Volume 4, Issue 1

2009

Article 28

Modelling of Chlorine Contact Tank and the Combined Applications of Linear Model Predictive Control and Computational Fluid Dynamics

Abrar Muslim, *Syiah Kuala University, Indonesia*

Qin Li, *Curtin University of Technology, Western Australia*

Moses O. Tadé, *Curtin University of Technology, Western
Australia*

Recommended Citation:

Muslim, Abrar; Li, Qin; and Tadé, Moses O. (2009) "Modelling of Chlorine Contact Tank and the Combined Applications of Linear Model Predictive Control and Computational Fluid Dynamics," *Chemical Product and Process Modeling*: Vol. 4: Iss. 1, Article 28.

DOI: 10.2202/1934-2659.1307

Modelling of Chlorine Contact Tank and the Combined Applications of Linear Model Predictive Control and Computational Fluid Dynamics

Abrar Muslim, Qin Li, and Moses O. Tadé

Abstract

A dynamic model is developed to present chlorine decay in chlorine contact tank, and a single-input single-output (SISO) model that presents both chlorine dosing and decay process is developed in Simulink of Matlab software with considerations of the process disturbances of temperature and stagnant flow in the tank. A computational fluid dynamics (CFD) model of chlorine transport and decay in the tank is also developed with the use of mixture multiphase model to present the chlorine mixing and decay models in the tank. To optimally control free chlorine residual (FCR) concentration in the SISO system, a linear model predictive control (LMPC) is designed using the SISO system and LMPC control algorithm. The LMPC control objective is to regulate the optimal mass flow rates of gaseous chlorine to control the chlorine decay process inputs/outputs within the constraints. The results on the LMPC simulation using reference data from a real water plant show that the LMPC can control the FCR concentration in the tank within the constraint by regulating the optimal mass flow rates of gaseous chlorine. Commercial CFD software, FluentTM, has been used in this study to simulate the FCR distribution in the CCT channel based on the LMPC result.

KEYWORDS: chlorine contact tank, free chlorine residual, SISO model, linear model predictive control, computational fluid dynamics

Author Notes: Abrar Muslim is very grateful to Curtin University of Technology for the technical support and providing the Matlab 7.0.1, GAMBIT 2.2 and FLUENT 6.2 software used in this research. The authors would also like to thank the anonymous referees of Journal of Chemical Product and Process Modeling (CPPM) for their valuable suggestions.

INTRODUCTION

An ideal drinking water distribution system (DWDS) must supply safe drinking water with free chlorine residual (FCR) at the concentration of 0.2-0.6 ppm (AWWA, 2003). Meanwhile, the FCR is consumed in the bulk liquid phase and at the pipe walls of the DWDS as the result of chemical reactions (Dotson and Heltz, 1985, and Wooschlager and Soucie, 2003). According to the *Safe Drinking Water Act* (Government, 2006), surface water must be examined by a value known as CT that illustrates the effectiveness of the FCR to inactivate Giardia cysts. C represents the FCR concentration and T is contact time, and $CT = C \times T$. The actual CT of a DWDS must be computed using the water quality parameters (temperature, pH, and the FCR concentration at the first water consumer). Once the actual CT (CT_{calc}) is obtained, it must be compared to a minimum CT value ($CT_{99.9}$) set by the EPA, where $CT_{calc}/CT_{99.9}$ must be greater than 1. If the $CT_{calc}/CT_{99.9}$ is less than 1, a reservoir is required to be installed immediately after the chlorine booster for providing extra contact time, prior to being distributed to the first consumer.

A number of chlorine decay, consumption and residual models have been developed to predict the FCR in the pipes of DWDS (Johnson, 1978, Rossman et al., 1994 and Heraud et al., 1997). EPANet, which is a simulation platform based on a Lagrangian dynamic approach to track the fate of discrete parcels of water as they move along (Liou and Kroon, 1978), can be used in modelling of FCR in the DWDS (Sakarya and Mays, 2000, Wang et al., 2000, Rossman, 2000, and Chang, 2003). Muslim et al. (2006) developed discrete time distributed parameter models in Matlab to track the temporal and spatial variations of the FCR, which is based on a simpler model structure with a focus on addressing the reactive transport nature. However, a model that can represent the chlorine decay and mixing process within water flow and the chlorine injection for chlorine contact tank especially in the environment of Matlab SimulinkTM, have not been developed yet in the previous studies.

To control the FCR concentration in the DWDS with and without considering chlorine contact tank (CCT), adaptive and predictive controls had been proposed in the last decade where the chlorine control strategies were based on input/output chlorine concentration as the manipulated variable (MV) and controlled variable (CV) (Brdys et al., 2001, Wang et al., 2001, Polycarpou et al., 2002, Chang et al., 2003, Tarnawski et al., 2003, and Muslim et al., 2007). Model Predictive Control (MPC) which can predict the future behavior of a process over an extended prediction horizon under constraint concentration (Hangos and Cameron, 2001, Dougherty and Cooper, 2003, and Imsland et al., 2003) is a promising technique for chlorine control studies. It is noted that MPC has not been applied yet to generate mass flow rate of pure gaseous chlorine for the vital constraint of FCR concentration in the DWDS.

The use of computational fluid dynamics (CFD) modeling approaches to simulate chlorine/tracer decay and microbial inactivation and to predict flow structure, mass transport and mixing characteristics in the CCT, has generated credible results and good agreements with experimental data (see Wang and Falconer, 1998, Bellamy et al., 1999, Mahmood et al., 2002, Greene et al., 2004, and Templeton et al., 2006). The dosages of chlorine/tracer for the optimization of the FCR in the CCT were based on the CFD simulations as done by Greene et al. (2004) and Templeton et al. (2006). However, utilising CFD simulation to validate a control strategy design has not been investigated. In this study, we apply the CFD simulation to take into account the actual fluid-gas mixing and the distributed-parameter nature of a fluid flow, and further verify the control scheme performance.

The aim of our study is to develop a linear model predictive control (LMPC) by means of the mass flow rate of pure gaseous chlorine as the *MV*, which is applied into a developed single-input single-output model of CCT that presents both chlorine dosing and decay with the consideration of disturbances. Comparisons of the LMPC and a Proportional Integral (PI) performance have been carried out in this study. Matlab SimulinkTM is used in these studies. We also used commercial CFD software, FluentTM, to simulate the FCR distribution in the CCT based on the LMPC result.

METHODS

Model Development

Table 1: List of Parameters used for Model Development

Parameter	Unit
Density (ρ)	kilogram/meter ³ (kg/m ³)
Effectiveness of FCR to Inactivate Giardia Cysts (CT , CT_{calc})	ppm-minutes
FCR concentration (C , C_0 , CV , SF , X_{iT} , X_{oT} , X'_w , X'_{ic})	ppm
FCR decay rate constant (k_{bR} , k_R , k_{sc} , k , k_b , k_w)	/second (s ⁻¹)
Length (DT , LC , LT , PL , WC)	meter, kilometre (m, km)

Integral of the time-weighted absolute error (ITAE)	mins·ppm
Mass Flow Rate (MV, W_{ic}, W_{vws})	kilogram/second, kilogram/minute, (kg/s, kg/min)
Time ($T, t, tsc, \tau_p, \tau_{ic}, \theta_p$)	second (s), minute (min)
Temperature ($T1, T2$)	Degree Celsius ($^{\circ}\text{C}$)
Velocity (v)	meter/second (m/s)
Volume (CVL)	meter ³ (m ³)
Volumetric water supply (Q_T)	meter ³ /second (m ³ /s)

Figures 1.(a) and 1.(b) present the conceptual models of a CCT where Figure 1.(a) sketches the CCT layout, and Figure 1.(b) illustrates the control volume (CVL) for FCR computation in the CCT channel. The correlations of the dimensional parameters shown in Figure 1.(a) can be expressed as $PL = (B+1)*(LC+2WC)$; $LT = C*WC + B*WC$; and $v = Q / (A*DT)$ where PL denotes the distance needed by the FCR control volume to travel from the CCT inlet to the CCT outlet; v is the average water flow rate velocity in the CCT channels; B represents the number of baffles; C is number of channels; DT is the channel thickness; LC is the channel overlap; LT is the CCT length; WC is the width of channel slot; WT is the CCT width, and $WC1$ stands for the first water consumption.

Figure 1. a) the CCT layout, b) the FCR control volume (abbreviated as ‘FCR CVL’ in the figure) in a CCT channel

A dynamic model of the FCR decay in the CCT can be developed from both the CCT models shown in Figure 1, based on the overall mass balance for the FCR in the CVL at the total residence time t (see Nauman, 2002, Seborg et al., 2004). The CVL in the CCT is assumed to be constant, the FCR in the CVL diminishes as the CVL travels along the CCT at the total residence time t . By considering the CVL length (noted as the CCT length) from the point just after the chlorine injection to a certain point along the CCT, the overall mass balance equation can be rearranged as;

$$MC_{Acc} = MC_{OF} - MC - MC_R \quad (1)$$

where, MC_{Acc} denotes the total FCR mass accumulation in the CVL over the total residence time; MC_{OF} is the total FCR mass in the inlet stream coming into the CVL at the total residence time t ; MC is the total FCR mass in the outlet stream leaving the CVL at the total residence time t ; and MC_R indicates the total FCR mass consumed due to chemical reactions in the CVL at the total residence time t . Then, the overall mass balance for the FCR in the CVL at the total residence time t is derived to be Equation (2):

$$CVL \frac{d}{dt} X_{oT}(t) = Q_T X_{iT}(t) - Q_T X_{oT}(t) - k V_{CVL} X_{oT}(t) \quad (2)$$

where X_{iT} is the initial FCR concentration in the CVL just after chlorine injection; X_{oT} is the FCR concentration in the CVL at the CCT outlet, which is known as the controlled variable; k is the FCR rate constant; and Q_T is volumetric water supply (VWS) in the CCT. Applying Laplace Transformation (Seborg et al., 2004), the time domain solution of Equation (2) is obtained as:

$$X_{oT}(t) = \frac{X_{iT}}{(1 + \tau_r k)} (1 - e^n), n = -(t - \theta_p) / \tau_p \quad (3)$$

where the residence time, τ_r is predicted from PL/v ; the time constant, τ_p equals to $1/(PL/v + k)$; θ_p is the time delay of the FCR decay process and can be also calculated by $\theta_p = PL/v$. It can be observed that the FCR concentration, $X_{oT} = 0$ when $t = 0$, and $X_{oT} = X_{iT} / (1 + \tau_r k)$ when $t \rightarrow \infty$ (time approaches infinity), the steady state gain (K) of the process is equal to $1/(1 + \tau_r k)$, and the transfer function of Equations (3) can be derived as:

$$G_T(s) = K_T e^{-\theta_p s} / (1 + \tau_p s), K_T = \frac{\Delta X_{oT}}{\Delta X_{iT}} = \frac{\left(\frac{X_{iT}}{1 + k \tau_r} \right)}{X_{iT}} = \frac{1}{1 + k \tau_r} \quad (4)$$

where $G_T(s)$ is the transfer function of the FCR decay process in the CCT, and K_T is the process gain.

The dynamic model for the mixing process of water flow and chlorine injection (see Figure 1.b) can be derived from the steady state component balance of $W_{VWS} X'_w + W_{ic} X'_{ic} = (W_{VWS} + W_{ic}) X_{iT}$, and by applying Laplace Transformation of the steady state model, the chlorine mixing process is described by:

$$G_{ic}(s) = \frac{X'_{ic} - X_{iT}}{W_{VWS} + W_{ic}}, G_{VWS}(s) = \frac{W_{VWS}}{W_{VWS} + W_{ic}}, \tau_{ic} = \tau_{VWS} = \frac{\rho V_C}{W_{VWS} + W_{ic}} \quad (5)$$

where $G_{ic}(s)$ is the transfer function of chlorine injection process; $G_{VWS}(s)$ is the transfer function of the VWS just before chlorine injection; W_{ic} is the average mass flow rate of pure component gaseous chlorine injected by the chlorine booster, as the MV; W_{VWS} is the VWS mass flow rate before passing the boosters; X'_w is the average FCR concentration in the VWS; τ is the process time constant; X'_{ic} is the average FCR concentration just after the injection of pure component gaseous chlorine; and ρ is the density of solution after the mixing process.

The chlorine decay of stagnant flow denoted as SF , in the CCT needs to be considered as the first disturbance in the system, symbolised as $G_{dv}(s)$ shown in Figure 2. The SF value can be obtained using the SF equation of $SF = psc \cdot C_0 \exp(-ksc \cdot tsc)$, where C_0 is the initial chlorine concentration; ksc is the overall chlorine decay in the SF ; psc is the portion of stagnant flow; and tsc is the residence time for chlorine decay process in the SF .

The effect of temperature change in drinking water along the CCT and the DWDS main pipe over time is considered as the second disturbance in the system, denoted as $G_{Temp}(s)$ shown in Figure 2. The k is dependent on the wall (the CCT wall or main pipe wall) chlorine decay rate constant, k_w and bulk chlorine decay rate constant, k_b , i.e. $k = k_b + k_w$ (AWWA, 2003), and k_b rises by 2.05 fold with a temperature increase of 10-20°C (Kiene et al., 2008). To simplify the CCT system calculation, the relationship between the k and k_b is $k_b = k k_R / k_{bR}$ based on the model by Rossman et al. (1994) where k_{bR} and k_R is denoted as the k and k_b in model. Thus, the k at the temperature of T2, k_{T2} , can be obtained as $k_{T2} = k_{T1} [1 - (i_T - 1) k_{bR} / k_R]$ where k_{T1} is the k at the temperature of T1 and i_T is the increase coefficient of k_b , e.g. 2.05 (10-20°C). Thus, the transfer function can be modelled as $G_{Temp}(s) = [C(k_{T2}) - C(k_{T1})] / (\tau_{Temp}s + 1)$.

Figure 2. A SISO system with LMPC designed in Simulink Matlab software.

The CV in the system is the FCR concentration at the first water consumption point, which should be at the upper end of the permitted FCR level, i.e. close to 0.6 ppm. Therefore, the FCR concentration in the CCT should be adjusted in accordance with the chlorine decay process between the CCT outlet point and the first water consumption point, denoted as $G_{MP1}(s)$. $G_{MP1}(s)$ can be derived using Equation (4), which is $G_{MP1}(s) = K_{MP1}e^{-\theta s} / (1 + \tau_p s)$ where the parameters are related to the chlorine decay process in the DWDS main pipe. The SISO model of the FCR decay process for the CCT system is shown in Figure 2.

Linear Model Predictive Control

In this research, a model predictive control toolbox of Matlab is used to develop the LMPC. With the functions given by the Matlab toolbox, LMPC can deal with linear model presented in Simulink models (Bemporad et al., 2005). The LMPC control objective is to regulate optimal mass flow rate of pure gaseous chlorine as the MV of the CCT input order to control the FCR concentration at the first water consumption at the required level based on $G_{VWS}(s)$, $G_T(s)$, $G_{ic}(s)$, $G_{Temp}(s)$ and $G_{MPI}(s)$. In order to ensure the CV is regulated within the required range, the CV is constrained within the range of 0.2-0.6 ppm. The control action can also be computed subject to hard constraints on the MV and the CV : $MV_{min}(i) \leq MV(j+i) \leq MV_{max}(i)$; the MV rate constraints: $|\Delta MV(j+i)| \leq \Delta MV_{max}(i)$; $CV_{min}(i) \leq CV(j+i) \leq CV_{max}(i)$ where i is the step input; j the step output; and k is the sampling interval of prediction horizon.

The LMPC control performance is also dependent on the design parameters that can be tuned, the model horizon, N (typically, $30 \leq N \leq 120$), moving horizon, M (typically, $5 \leq M \leq 20$ and $N/3 \leq M \leq N/2$), prediction horizon, P ($P = N + M$), output weight (OW), input weight (IW), rate weight (RW) and control interval (CI) (Seborg et al., 2004).

Figure 2 shows the block diagram of LMPC designed using Matlab Simulink to deal with the SISO system. Sp is the setpoint for the CV ; $K_V I(s)$, $K_I(s)$, and $M(s)$ are the control elements of control valve, transducer, and transmitter transfer function, respectively which are based on Seborg et al., (2004), the chlorine injection process (www.usfwt.com) and the assumptions made. The simulation time is denoted as t (s); IT , I_v , and I_c are the inputs for $G_{Temp}(s)$, and $G_{dv}(s)$, respectively; $c(s)$ is the value of $\bar{W}_{VWS}$ based on the equation of the steady state component balance; and $gI(s)$ is the dynamic model for the FCR fluctuation input to $G_{VWS}(s)$ when there is a fluctuation in the VWS .

Computational Fluid Dynamics

The purpose of using CFD in this study is to cross-check the regulation of the optimal CV obtained by the LMPC in fluid dynamics simulation when actual fluid flow is considered. In the model development of LMPC, the CCT tank geometry is assumed to be a linear pipe line and it is informative to acquire the knowledge of the fluid flow pattern in a baffled tank shown in Figure 1.(a) and the possible consequence of the geometry on the FCR distribution.

In this research, the mixture multiphase model is used because it is suitable for the chlorine mixing process of the CCT. The concept of phase volume fraction is introduced. These volume fractions are assumed to be continuous function of space and time (Fluent, 2003). To simplify the CFD simulation of the CCT, 2D with steady-state condition solver is chosen, the SIMPLE (Semi-Implicit

Method for Pressure-Linked Equations) algorithm is a method for calculating pressure and velocities as proposed by Versteeg and Malalasekera (1995). The turbulence in this CCT phase has been modelled using a modified k - ϵ turbulence model available in FLUENT 6.2, which was used in the turbulence model of continuous flow reactor (Dennis et al., 2006).

In the first step of CFD simulation, GAMBIT 2.2 (pre-processor for FLUENT 6.2) was used to create 2D geometries of the CCT with 4 m additional main pipe at the CCT input and output as well as for its meshing. Small size quadrilateral mesh was created for the area close to the distributor.

In the simulations, water (phase-1), chlorine (phase-2) and ammonium (phase-3) were taken as liquid, gas and liquid phase, respectively, with an assumption that chlorine is instantly converted into FCR when dissolved in water. The velocity inlet condition was applied at the distributor and the velocities as well as volume fractions of both phases were specified appropriately. Based on the data used in the LMPC simulation (a main pipe of 0.3048 m diameter connected into the CCT input with the average VWS of 0.45 m³/s), the value of $X'_w + X'_{ic}$ (assumed as a volume fraction of 0.918 ppm) and the velocity inlet of 6.203 m/s as the boundary condition are applied with the operation condition of pressure being 2068427 Pa (300 psig) based on the chlorine capacity in the available literature (Filter, 2003) at the inlet point [2.4 m, -4 m]. Mass transfer rate of phase-2 into phase-3, 2.785E-5 /s, which is also used in the LMPC simulation, is applied to present the CCT chlorine decay process.

RESULTS AND DISCUSSIONS

Matlab/Simulink Simulation

The simulated DWDS is assumed to have a main pipe of 0.3048 m diameter with the average VWS of 0.45 m³/s which is 97.2% of Townsville water supply (NQWater, 2006). The chlorine overall decay rate constant, k , is taken from Rossman et al. (1994) related to the pipe diameter size of 0.3048 m, and the bulk chlorine decay rate constant is taken as 0.55 mg/L per day. It is also assumed that the first water consumption is located at 0.5 km from the chlorine booster with the required FCR concentration of 0.6 ppm at which the chlorine disinfection of Giardia cyst reaches 0.5-log reduction.

The CT_{calc} value is obtained as 0.806 ppm-minutes. The $CT_{calc}/CT_{99.9}$ values are 0.0048, 0.0059 and 0.0039 for the plant with conventional filtration, slow sand filter and membrane filtration value, respectively. The water temperature is assumed to range from 5°C to 25°C. Therefore, the simulated DWDS needs a reservoir, i.e. CCT, after the chlorine booster for extra contact time, prior to being distributed to the first consumer. The CCT domain description

is $B = 9$ ($C = 10$), $LC = 20.8$ m, $LT = 48.9$ m, $WC = 4.8$ m, $WT = 30.4$ m and $DT = 3$ m (Government, 2006). With this CCT capacity, the CT_{calc} is obtained to be approximately 162.1 minutes, which is 42.1 minutes longer than that the maximum $CT_{99.9}$ value required.

With regard to SISO system with the disturbances of $G_{Temp}(s)$ and $G_{dv}(s)$, and the LMPC elements, $G_{VWS}(s)$, $G_{ic}(s)$, $G_T(s)$ and $G_{MPI}(s)$ are obtained using Equation (5) and the state component balance based on simulated data with the assumption of X'_w being 0.25 ppm. The VWS is assumed to be constant, being $0.45 \text{ m}^3/\text{s}$ because the velocity inlet/boundary condition for CFD simulation should be constant, so that $g_1(s)$ is equal to 1. To obtain $G_{Temp}(s)$, the FCR deviation is about $0.00220 \text{ ppm}/^\circ\text{C}$ based on a simulation with the bulk decay k_b being 2.1, the assumed ratio k_b/k rises at a rate of 0.14 with a temperature change from 5°C to 25°C per day with the repeating sequence input with time value of $[0, 720]$ and output of $[0, 20]$ used for the simulation. $G_{dv}(s)$ is found through a CFD study that the portion of stagnant flow being 1.5% in the CCT gives 0.1 ppm changes in the FCR concentration at the CCT outlet. $K_I(s)$ I/P transducer (*Current-to-Pressure Transducer*) is assumed to act as a linear device with negligible dynamics (Seborg et al., 2004). The output signal from 3 to 300 psi when input signal changes full-scale from 4 to 20 mA are assumed for the feedback control, and these are normal scales in post-chlorination (Filter, 2003) that yields $K_I(s) = 18.5625$. To obtain $K_{VI}(s) = 90.909/(0.0833s + 1)$, the zero and span of each composition transmitter is assumed to be 0-6 ppm (the FCR mass fraction, $0 - 6 \times 10^{-6} \text{ kg FCR/kg chlorine solution}$) with the output range assumed to be 4-20 mA, and the time delay associated with measurement is assumed to be 0.5 minutes.

Figure 3 shows the FCR concentrations at various positions as a result of PI controls and LMPC application over a period of 7 days. Because the dynamic model is a fourth-order process, PI control with Ziegler-Nichols (ZN) tuning setting; $K_c = 20.83$, $\tau_I = 0.105$ (Seborg et al., 2004) is applied to get the better performance. As can be seen in Figure 3.(a), in controlling the CV (the FCR concentration at 0.55 km from the CCT outlet), the PI (ZN) control generated no offset, and the CV settling time is about 3200 minutes. The decay ratio of the CV is about 2/5, which is generally acceptable in terms of a controller performance assessment (greater than 1/4). However, the CV at the time of approximately 960-1320 minutes and 1680-2030 minutes is greater than the required upper level of 0.6 ppm, exceeding the upper limit of safe drinking water requirement. We can also observe that the FCR concentration is still present until the point of 4.55 km from the CCT outlet in the period between 245 and 705 minutes.

Figure 3. The FCR concentration; (a) PI control (ZN tuning setting; $K_c = 20.83$, $\tau_i = 0.105$), (b) PI control (ITAE method; $K_c = 12.04$, $\tau_i = 0.083$), (c) LMPC ($CI = 15$, $M = 30$, $P = 20$, $RW = 0.85$, $IW = 0.15$, $OW = 1$).

The integral of the time multiplied by the absolute error (ITAE) was also used to tune the PI control where the ITAE usually marks in the most conservative controller setting (Seborg et al., 2004). As can be viewed in Figure 3.(b), the PI (ITAE) control results in a more stable CV compared to the CV by PI (ZN) control, and the settling time is approximately 890 minutes which is 570 minutes faster than the one by PI (ZN) control. The maximum value of CV, 0.6612 ppm (see the peak of the CV in Figure 3.b) is only slightly higher than the required FCR upper level, which is 0.4588 ppm less than the overshoot (1.1200 ppm) generated by PI (ZN) control (see the peak of the CV in Figure 3.(a)).

Compared to the PI (ZN) and PI (ITAE) control strategies, the LMPC control performance appears superior. The CV controlled by the LMPC is much more stable, the settling time is approximately 410 minutes which is 2790 minutes faster than the one by PI (ZN) control, and 480 minutes faster than PI (ITAE). Moreover, the fluctuation of FCR concentration is very small. The FCR concentration is always within the required level of 0.2-0.6 ppm up to the point of 4.55 km from the CCT output (see the dot curve in Figure 3.a and Figure 3.b).

Figure 4. The LMPC performance ($CI = 15$, $M = 30$, $P = 20$, $RW = 0.85$, $IW = 0.15$, $OW = 1$); (a) the mass flow rate of pure gaseous chlorine (MV), (b) the X_{iT} and X_{oT} profiles.

In comparison, LMPC strategy provides the most stable control among the 3 methods. As justified by obtaining the CV ITAE values (Seborg et al., 2004), the 3 control strategies can be ranked as LMPC > PI (ITAE) control > PI (ZN) control. Their CV ITAE values are approximately 1572, 1643, 2214 mins·ppm, respectively. The disturbances of temperature and stagnant flow cause the decrease in the FCR concentration at the CCT output which is approximately 1.0044 ppm less than the situation without the disturbances. This amount is contributed by the 0.0044 ppm on the effect of increasing temperature and by the 0.1 ppm on the effect of stagnant flow based on the LMPC and PI simulations.

The stable responses of LMPC (see the solid line in Figure 4.a) is attributed to one of the key features of LMPC in which we can put a constraint of $5.931\text{E-}6$ to $1.067\text{E-}5$ kg/minute at the LMPC output when designing the LMPC to optimally adjust MV , a constraint of 0.2 to 0.6 ppm at the CV (see the solid line in Figure 3.b). Therefore, if the upper constraint value of $1.067\text{E-}5$ is multiplied by both numerators of $K_{IP}(s)$ and $K_V(s)$, it yields the LMPC MV value of 0.018 kg/minute as shown in Figure 4.a. This LMPC MV value results in the FCR concentration at the CCT input (X_{iT}) and CCT output (X_{oT}) of approximately 0.918 ppm and 0.638 ppm, respectively, as can be seen Figure 4.b. In contrast, we cannot put any constraint in any PID control, so that the PI MV is oscillating as can be seen by the dash line in Figure 4.a.

CFD Simulation

The CFD simulation results (steady-state profiles) are shown in Figure 5 when the convergence occurred at the time of approximately 9000 s. As can be seen in Figure 5.a, the CFD result is able to present the FCR decay and transport in the CCT as the FCR travels along the CCT channel, the FCR concentration diminish in proportion to its residence time from the CCT input to the CCT output. By applying the FCR initial concentration of 0.918 (the LMPC X_{iT}) obtained as the optimal MV regulated by the LMPC, we are able to justify the SISO model accuracy in presenting the FCR decay process and the LMPC performance which is shown by the FCR concentration at the CCT outlet (the CFD X_{oT}) as 0.618 ppm. The CFD X_{oT} value of 0.618 ppm is reasonable because the disturbance of temperature change of 0.0044 ppm cannot be included in the CFD simulation. When the FCR concentration change of 0.0044 due to the disturbance is added into the CFD X_{oT} , the CFD X_{oT} becomes 0.6224 ppm which is close to the LMPC X_{oT} of 0.638 ppm.

(a)

(b)

Figure 5. The CFD simulation results of the LMPC X_{IT} ; (a) contour of phase-2 (the available FCR concentration along the CCT channel) volume fraction, (b) contour of phase-3 (the consumed FCR concentration by the organic compound along the CCT channel) volume fraction.

Figure 5.b shows the mass transfer of phase-2 into phase-3 to represent the FCR consumption by the organic compound in the CCT with the initial phase-3 volume fraction of 0.001 ppm. As can be seen in Figure 5.b, the phase-3 at the CCT outlet is approximately 0.272 ppm. Compared to the reduced FCR concentration being 0.28 ppm in the LMPC simulation, which is from 0.918 to 0.638 ppm, the CFD total mass change is consistent. The difference between the LMPC results and the CFD results discussed above is approximately only 3.2 %. The CFD simulation results confirm that the LMPC performance in controlling the FCR in the CCT is very reasonable. Moreover, the CFD results indicate that the fluid dynamics in such a baffled configuration of a CCT under the applied flow rates has no noticeable effect on the FCR distribution. In real industrial scenarios, the CFD simulations can be useful in control strategy design in achieving the optimal control solution by taking the hydrodynamic distributed parameters into account.

CONCLUSIONS

A SISO model has been developed in Matlab Simulink to present chlorine dosing and chlorine decay processes in a CCT with considerations of the process disturbances of temperature and stagnant flow in the CCT. To optimally control FCR concentration in the SISO system, a LMPC has been designed. The LMPC control objective is to regulate the optimal mass flow rates of gaseous chlorine to control the FCR at water distribution points within the safe drinking water requirements (0.2 – 0.6 ppm). A CFD model of chlorine transport and decay in the CCT was also developed to cross-check the effects of initial chlorine concentration, the disturbances, as well as the hydrodynamics.

The results on the LMPC and CFD simulations using a CCT in a simulated DWDS, which has almost the same volumetry water supply (VWS) as the reference real water plant, showed that the LMPC can control the FCR concentration in the water distribution line within the constraints by regulating the optimal mass flow rates of gaseous chlorine. The simulation results demonstrated that the LMPC control strategy is superior to the conventional PI controls. Moreover, the combination of CFD with control strategy simulations presents a new direction in evaluating a control scheme particularly pertinent to fluid mixing problems.

REFERENCES

- American Water Works Association (AWWA), *Treatment - Principles and Practices of Water Supply Operation*, 3rd ed. AWWA: Denver, Colorado, USA, 2003, pp. 161-165.
- Bellamy, W.D., Finch, G.R., and Haas, C. N., *Integrated Disinfection Design Framework*, AWWA Research Foundation, Denver, CO., 1999.
- Bemporad, A., Morari, M., and Ricker, N. L., *Model Predictive Control Toolbox: For Use with MATLAB*, The MathWorks, Inc., Natick, 2005.
- Brdys, M. A., Chang, T., and Duzinkiewicz, K., Intelligent Model Predictive Control of Chlorine Residuals in Water Distribution Systems, *Bridging the Gap: Meeting the World's Water and Environmental Resources Challenges* (eds. Don Phelps and Gerald Sehlke editor) Orland, Florida, May 20-24, 2001.
- Chang, T., Brdys, M. A., and Duzinkiewi, K., Decentralized Robust Model Predictive Control of Chlorine Residuals in Drinking Water Distribution Systems, *Proceedings of World Water and Environmental Resources Congress, World Water and Environmental Resources Congress and Related Symposia* (eds. Paul Bizier and Paul DeBarry), Philadelphia, Pennsylvania, June 23-26, 2003.
- Dennis, J. G., Charles, N. H., and Bakhtier, F., "Computational Fluid Dynamic Analysis of the Effect of Reactor Configuration on Disinfection Efficiency," *Water Environment Research*, vol. 78(9), 2006, pp. 909-919.
- Dotson, D., and Heltz, G. R., Chlorine Decay Chemistry in Natural Waters, *In Water Chlorination: Environmental Impact and Health Effects* (eds. R. L. Jolley, W. A. Brungs and R. B. Cumming), Ann Arbor Science Publisher, Inc., 1985, pp. 713-722.
- Dougherty, D., and Cooper, D., *A Practical Multiple Model Adaptive Strategy for Single-Loop MPC*, Control Engineering Practice, 2003, pp. 141-159.
- Fluent, *Fluent 6.1 User Guide*, Lebanon, 2003.
- Gas Chlorine Education Committee (GCEC), 2001. Available: <http://www.wwdmag.com/Gas-chlorine-Education -article 2620>.
- Government, O., *Procedure for Disinfection of Drinking Water in Ontario: (As adopted by reference by Ontario Regulation 170/03 under Safe Drinking Water Act)*, Ontario, 2006. Available: http://www.ontario.ca/drinkingwater/stel01_046942.pdf.

- Greene, D. J., Farouk, B., and Haas, C. N., "CFD Design Approach for Chlorine Disinfection Processes", *Journal AWWA*, vol. 96(8), August 2004, pp. 138-150.
- Hangos K. M., and Cameron I. T., *Process Modelling and Model Analysis*, Academic Press, London, 2001.
- Heraud, J., Kiene, L., Detay, M., and Levi, L., "Optimized Modeling of Chlorine Residual in a Drinking Water Distribution System with a Combination of On-line Sensors," *J. Water SRT-Aqua*, vol. 46(2), 1997, pp. 59-70.
- Imsland, L., Findeisen, R., Bullinger, E., Allgöwer, F., and Foss, B. A., "A Note on Stability, Robustness and Performance of Output Feedback Nonlinear Model Predictive Control," *Journal of Process Control*, vol. 13, 2003, pp. 633-644.
- Johnson, J. D., Measurement and Persistence of Chlorine Residual in Natural Waters, *Water chlorination: Environmental impact and health effects (ed. in Jolle W R. L)*, Ann Arbor Science, Ann Arbor, Michigan, 1978, pp. 37-63.
- Kiene, L., Lu, W., and Levi, Y., "Relative Important of the Phenomena Responsible for Chlorine Decay in Drinking Water Distribution System," *Wat. Sci. Tech.*, vol. 38 (6), 2008, pp. 219-227.
- Liou, C.P., and Kroon, J.R., "Modeling the Propagation of Waterborne Substances in Distribution Networks," *J. AWWA*, vol. 79(11), 1978, pp. 54-58.
- Mahmood, F., Pimblett, J., Grace, N., and Grayman, W., Evaluation of Mixing Characteristics of Water Storage Tanks, *Water Quality Technology Conference*, Seattle, WA USA, 10-14 Nov. 2002, pp. 2002.
- MathWorks, Inc., *MATLAB Release 7.0.1 Help Guidelines*, 2005.
- Muslim, A., Li, Q., and Tadé, M. O., Discrete Time-Space Model for Free Chlorine Concentration Decay in Single Pipes of Drinking Water Distribution System, *Proceeding of Chemeca 2006 Conference in Auckland-New Zealand* (eds. B. R. Young, D. A. Patterson, and X. D. Chen), ISBN; 0-86869-110-0, 18 September 2006, Paper No. 129/450.
- Muslim, A., Li, Q., and Tadé, M. O., "Simulation of Free Chlorine Decay and Adaptive Chlorine Dosing by Discrete Time-Space Model for Drinking Water Distribution System," *Journal of Chemical Product and Process Modelling*, vol. 2(2), 2007, article 3.
- Nauman, E.B., *Chemical Reactor Design, Optimization, and Scaleup*, New York, McGraw-Hill, 2002.

- NQWater, Townsville/Thuringowa Water Supply Upgrade Project, 2006.
Available: <http://www.nqwater.com.au/?page=38>.
- Polycarpou, M. M, Uber, J. G., Wang, Z., Hang, F., and Brdys, M., "Feedback Control of Water Quality, IEE Control System Magazine," vol. 2, June 2002, pp. 68-87.
- Rossman, L. A., Clark, R. M., and Grayman, W. M., "Modelling chlorine residual in drinking water distribution system," *J. Environmental Engineering*, vol. 120(4), July/August 1994, pp. 803-820.
- Rossman, L. A., *EPANET2 Users Manual*, EPA US: Cincinnati, USA, 2000.
- Sakarya, B. A., and Mays, L. W., "Optimal Operation of Water Distribution Pumps Considering Water Quality," *Journal of Water Resources Planning and Management*, August 2000, pp. 210-220.
- Seborg, D. E., Edgar, T. F., and Mellichamp, D. A., *Process Dynamic and Control*, USA, John Wiley & Son Inc., 2004.
- Tarnawski, J., Brdys, M. A., and Duzinkiewicz, K., Supervised Model Reference Adaptive Control of Chlorine Residuals in Water Distribution Systems, *Proceedings of World Water and Environmental Resources Congress and Related Symposia (eds. Paul Bizier and Paul DeBarry)*, Philadelphia, Pennsylvania, June 23-26, 2003.
- Templeton, M. R., Hofmann, R., and Andrews, R. C., "Case Study Comparisons of Computational Fluid Dynamics (CFD) Modeling Versus Tracer Testing for Determining Clearwell Residence Times in Drinking Water Treatment", *Journal of Environmental Engineering and Science*, vol. 5(6), 1 November 2006, pp. 529-536.
- U.S. Filter; S2K Sonic Chlorinator, 2003. Available: <http://www.wallaceandtiernan.usfilter.com>.
- Versteeg, H. K., and Malalasekera, W., *An Introduction Fluid Dynamics: The Finite Volume Method*, Pearson Education Limited, England, 1995.
- Wang, H., and Falconer, R. A., "Simulating Disinfection Processes in Chlorine Contact Tanks Using Various Turbulence Models and High-Order Accurate Difference Schemes", *Water Research*, vol. 5, 1998, pp. 1529-1543.
- Wang, Z., Polycarpou, M.M., and Uber, J.G., Decentralized Model References Adaptive Control of Water Quality in Water Distribution Networks, *Proceedings of the 15th IEEE International Symposium on Intelligent Control*, Rio, Patras, Greece, July 2000, pp. 127-132.

- Wang, Z., Polycarpou, M M., Shang, F., and Uber, J. G., Design of Feedback Control Algorithm for Chlorine Residual Maintenance in Water Distribution Systems, *Proceedings of World Water and Environmental Resources Congress, Bridging the Gap: Meeting the World's Water and Environmental Resources Challenges* (eds. Don Phelps and Gerald Sehlke), Orlando, Florida, May 20-24, 2001.
- Woolschlager, J., and Soucie, W. J., Chlorine Reactivity with Concrete Surfaces, *Proceedings of the World Water and Environmental Resource Congress, World Water and Environmental Resource Congress and Related Symposia* (eds. P. Bizier and P. DeBarry), Philadelphia, Pennsylvania, USA, June 2003, pp. 23-26.