

Special Theme Research Article

Simultaneous model of chlorine dosing and decay in drinking water distribution system and model predictive control application

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ABSTRACT: The most commonly applied active disinfectant in drinking water distribution system (DWDS) is free chlorine residual (FCR) in the form of hypochlorous acid and hypochlorite ion. The concentration of FCR decreases along the transport pipeline. Controlled replenishment of chlorine at various sites in DWDS is critical to maintain the FCR in the safe range of 0.2–0.6 ppm. This study proposed a multiple-input multiple-output (MIMO) model (developed in Simulink of Matlab 7.0.1) that simultaneously takes into account chlorine dosing and decay process with the considerations of process disturbances. The model is further implemented into a centralised model predictive control (CMPC) system. The advantages of our CMPC system in controlling multiple outputs are its robustness and short settling time, compared to the conventional process-data-based proportional integral (PI) control strategies. Moreover, the simplicity of this reactive-transport-model-based MIMO control system and the use of Matlab promise an easy adaptation to field test and plant implementation. It addresses an important need in water quality management, particularly for developing countries. © 2008 Curtin University of Technology and John Wiley & Sons, Ltd.

KEYWORDS: free chlorine residual; MIMO system; Simulink; model predictive control

INTRODUCTION

On the one hand, the free chlorine residual (FCR), hypochlorous acid (HOCl) and hypochlorite ion (OCI⁻) decreases along the pipes of drinking Water distribution system (DWDS) due to chemical reactions in the bulk phase and at the pipe wall.^[1] On the other hand, the DWDS must ideally supply safe drinking water with the FCR at a concentration of 0.2–0.6 ppm that must be presented at the points of water consumption.^[2]

A number of models have been developed to predict the FCR in the pipes of DWDS. Steady-state time-domain models for the FCR decay were proposed by Johnson^[3] and Heraud *et al.*^[4] A mass transfer-based model for the FCR decay was developed by Rossman *et al.*^[5] EPANet, which is a simulation platform based on a Lagrangian time-based approach to track the fate of discrete particles of water as they move along,^[6] can be used in the modelling of FCR in the DWDS.^[7–11] Muslim *et al.*^[12] developed discrete time-space models (DTSM) using explicit finite difference method in

Matlab 7.0.1, and Muslim *et al.*^[13] proposed adaptive chlorine dosing based on the DTSM simulation.

In controlling the FCR concentration in the DWDS, control schemes (adaptive and predictive controls) were proposed by Wang *et al.*,^[14] Polycarpou *et al.*,^[15] Brdys *et al.*,^[16] Chang *et al.*,^[10] Tarnawski *et al.*^[17] and Biscos *et al.*,^[18] and these chlorine dosing control strategies were all based on input and output chlorine concentration (ppm). So far, there is no model-based predictive control (MPC) scheme that is developed on the basis of mass flow rate of pure gaseous chlorine (kg/s) as the manipulated variables (MVs). Meanwhile, gaseous chlorine is generally injected for post-chlorination of the DWDS.^[19,20]

This study proposed a multiple-input multiple-output (MIMO) model (developed in Simulink of Matlab 7.0.1) that simultaneously takes into account chlorine dosing and decay process with the considerations of process disturbances. The model is further implemented into a centralised model predictive control (CMPC) system. The advantages of our CMPC system in controlling multiple outputs are its robustness and short settling time, compared to the conventional process-data-based proportional integral (PI) control strategies. Moreover, the simplicity of this reactive-transport-model-based

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concentration after mixing in the mass flow rate of \bar{w} (kg/s); τ is the process time constant (s); ρ (kg/l) is the density of solution after the mixing process. Owing to the time-varying diurnal VWS, $G_1(s)$ is the main disturbance in $G(s)$, and $G_1(s)$ also contains the dynamic models of diurnal VWS, $g_i(s)$. For multiple mixing and decay process, the model is shown in Fig. 2.

The chlorine decay in the reservoir (CDR) and the chlorine decay in short circuit (CDSC) need to be considered and calculated. The value of CDR and CDSC can be obtained using the following equations:

$$CDR = C_0 \exp(-kr \cdot tr) \tag{9}$$

$$CDSC = pscC_0 \exp(-ksc \cdot tsc) \tag{10}$$

where C_0 (ppm) is the initial chlorine concentration, kr and ksc (s^{-1}) are the overall CDR and short circuit, respectively, psc is the portion of solution of short-circuit flow, and tr and tsc (s) are the residence time for chlorine decay process in the reservoir and short circuit, respectively.

Temperature change affects the FCR decay process. Parameter k is dependent on the wall chlorine decay rate constant, k_w and the bulk chlorine decay rate constant, k_b , i.e. $k = k_b + k_w$ according to AWWARF,^[22] and k_b rises as 2.05-fold with a temperature increase of 10–20 °C. The relationship between k and k_b is $k_b = kk_R/k_{bR}$ for certain pipe diameter size, as described in Rossman.^[5] Thus, we obtain k at the temperature of T_2 (°C), denoted as k_{T2} :

$$k_{T2} = k_{T1}[1 - (i_T - 1)k_{bR}/k_R] \tag{11}$$

where k_{T2} is k at the temperature of T_1 (°C) and i_T is the increase coefficient of k_b . Thus, the transfer function for the temperature change can be modelled as

$$G_T(s) = \frac{C(k_{T2}) - C(k_{T1})}{(\tau_T s + 1)} \tag{12}$$

where $C(k)$ is obtained using the equation in Muslim *et al.*,^[13] by changing k to be k_{T2} and k_{T1} , respectively, and τ_T is the time constant of $G_T(s)$.

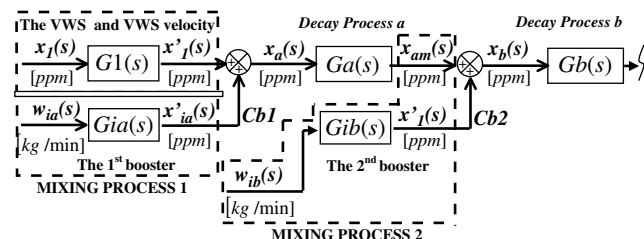


Figure 2. A model of the mixing process (chlorine dosing) and FCR decay process for two chlorine boosters in a single pipe of the DWDS.

The change in the FCR concentration due to water consumption and circuiting flows in closed loops (see the loops in Ref. [23]) along the DWDS main pipe can be modelled as $G_{dv}(s)$ and obtained by the same way as $G_T(s)$. Average water velocity after the consumption, μ_2 (m/s), is obtained from $\mu_2 = \mu_{1VWS} \left(1 - x \frac{d\mu}{dx}\right)$, where μ_{1VWS} is the average VWS velocity; x (m) is the distance from the first chlorine injection point; and $\frac{d\mu}{dx}$ indicates the water velocity gradient ($\mu_2 - \mu_1$) per 1 km of the DWDS main pipe length. Then, $G_{dv}(s)$ equals $\frac{C(k_{\mu 2}) - C(k_{\mu 1})}{(\tau_{dv} s + 1)}$. Since the diurnal VWS affects $G_{dv}(s)$, it must also contain a dynamic model of VWS, $g_{dv}(s)$, which is established using the Matlab identification toolbox based on the VWS.

The MIMO system designed in Simulink Matlab software is shown in Fig. 3.

Model predictive control

MPC refers to a family of control algorithms that employ an explicit model to predict the future behaviour of the process over an extended prediction horizon.^[24] Linear MPC refers to a family of MPC schemes that use linear models to predict the process dynamics, even though the dynamics of the closed loop system is nonlinear due to the presence of constraints.^[25]

In this research, the CMPC control objective is to regulate the mass flow rates of gaseous chlorine as a new approach to control the FCR at monitored points within the constraints under the fluctuations of drinking water demand and volumetric water supply by multiple chlorine injection based on the diurnal VWS, the FCR concentration input of the VWS, the chlorine injection process, the temperature, and the circuiting flow in the main pipe as the disturbances. In order to ensure that the CVs along the pipe meets the required range, CVis and CVos, as the input and output of chlorine decay process, are constrained within the range of 0.2–0.6 ppm. The

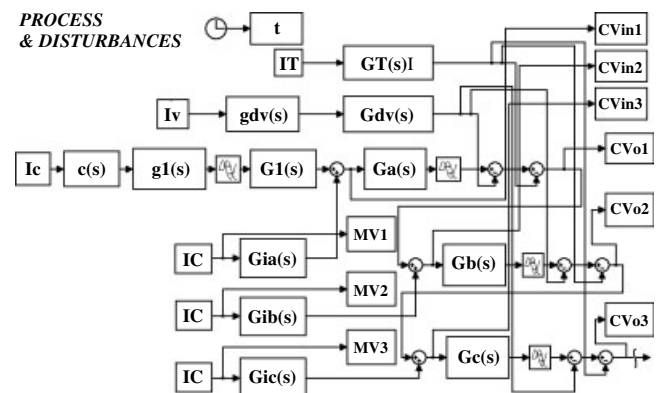


Figure 3. A MIMO system of the DWDS main pipe designed in Simulink Matlab software.

control action can also be computed subject to hard constraints on the MV and the controlled variables CVs. *MV* constraints:

$$u_{\min}(i) \leq u(j+i) \leq u_{\max}(i) \quad (13)$$

MV rate constraints:

$$|\Delta u(j+i)| \leq \Delta u_{\max}(i) \quad (14)$$

Output/*CV* constraints:

$$y_{\min}(i) \leq y(j+i|j) \leq y_{\max}(i) \quad (15)$$

The MPC 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 ($P = N + M$),^[21] output weight (*OW*), input weight (*IW*), rate weight (*RW*) and control interval (*CI*).^[26]

Figure 4 shows the block diagram of a CMPC designed using Matlab Simulink to deal with the MIMO system (only three chlorine boosters are shown) where $G_a(s)$, $G_b(s)$ and $G_c(s)$ represent the FCR decay transfer function within the 1st and 2nd boosters, the 2nd and 3rd boosters and the 3rd and 4th boosters, respectively; $G_{ia}(s)$, $G_{ib}(s)$ and $G_{ic}(s)$ represent the chlorine injection transfer function of the 1st, 2nd and 3rd boosters, respectively; Sp s are the setpoints for the controlled variables, *CV*o1, *CV*o2 and *CV*o3, respectively; *CV*in1, *CV*in2 and *CV*in3 are the FCR concentrations at just after the injection; and *MV*1, *MV*2 and *MV*3 denote the mass flow rate of pure gaseous chlorine as the *MVs* regulated by the CMPC.

$K_V(s)$, $K_{IP}(s)$, and $M(s)$ are the control elements^[21]; the control valve, transducer, and transmitter transfer function, respectively. A comparison of the CMPC and a decentralised PI (DPI) control performance is also presented in this study.

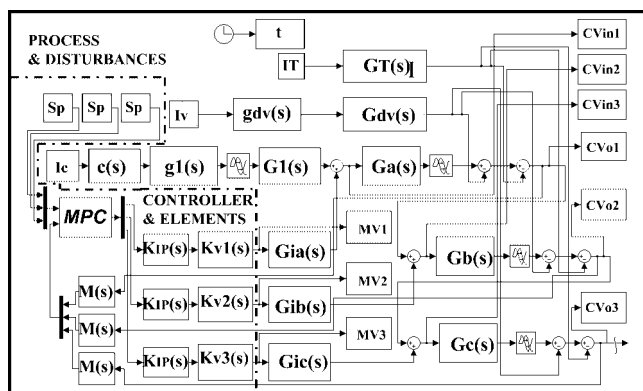


Figure 4. A centralised model predictive control (CMPC) in the MIMO system.

RESULTS AND DISCUSSION

Parameters for simulation

Process parameters need to be assumed in order to simulate simultaneous chlorine dosing and decay in a main pipe of the simulated drinking water distribution system (SDWDS). Thus, the SDWDS is assumed to have a main pipe of 12-in. diameter with the maximum and minimum volumetric *VWS* of 2.457 and 0.4915 km/h respectively, which is 1.25 times the maximum water flow rate in the main pipe of water distribution network of the New Haven.^[27] This assumed maximum *VWS* velocity can meet the increase in New Haven average residential users demand from 1.77 million l/day in 2004^[23] to 2.2125 million l/day with the maximum *VWS* of about 4.27789 million l/day. The *VWS* is assumed to follow the trend of water usage in summer,^[28] which is more dynamic compared to the winter time. Then, the *VWS* and *VWS* velocity are shown in Fig. 5.

The water velocity is decreased from the upstream (the *VWS* velocity) to downstream due to increasing water consumption along the main pipe. Here, total decreased velocity of 0.0218/km is assumed with chlorine overall decay rate constant, k , which is taken from Rossman^[5], related to the pipe diameter size of 12-in. and the bulk chlorine decay rate constant of 0.55 m/day. It is also assumed that the water plant of the SDWDS has filtration process with rapid sand filter, since a 0.5-log reduction of *Giardia* cysts is required from the chlorine disinfection. On the basis of the average *VWS* velocity over 24 h (Fig. 5), which is 0.8863 km/h, an assumption of the first consumer located at 0.83 km with FCR concentration of 0.6 ppm. Therefore, the SDWDS does not require a reservoir and the CDR and CDSC can be neglected in the MIMO system.

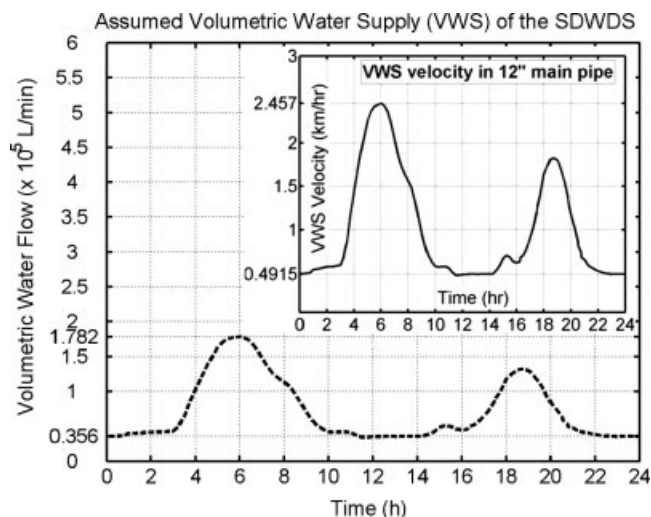


Figure 5. Assumed volumetric water supply and velocity over 24 h in 12-in. main pipe of the SDWDS.

With regard to the effects of temperature, $G_T(s)$ in the MIMO system, the FCR deviation is about 0.0220 ppm 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 10 to 30 °C (in summer) each 1440 min (per day). This result gives $G_T(s) = 0.000000007384/(180s + 1)$ with the assumed time constant being 180 min, where the process gain of temperature changes is equal to $0.0220 \times 10^{-6}/30$ kg FCR/(kg chlorine solution °C). Since the temperature changes from 00:00 to 24:00 is 20 °C per 24-h cycle, the repeating sequence input with time value of [024] and output of [0 20], is used for the simulation.

Simulation on the circuiting flow effect using the analytical solution gives the FCR deviation of 0.02609 ppm for the assumed velocity change of 14% per 1-km length. With the assumption that every 1.24 km of the main pipe with closed loop gives the FCR deviation of 0.02609 ppm in 25 min, so $G_{dv}(s) = 0.000000495/(25s + 1)$, where the process gain of the velocity change is equal to $0.02609 \times 10^{-6} \times 5.8/1.24 \times (100 - 14)/100$ -kg FCR/(kg chlorine solution km). Since the diurnal VWS velocity affects the change in the FCR as a result of the change in k , simulation data using the diurnal VWS velocity (Fig. 5) and the FCR concentration based on Eqn (5) over 24 h, gives $g_{dv}(s) = 1.606e^{-1800s}/(102.4737s + 1)$, which is established using the Matlab identification toolbox. It could be accepted that the change in the water velocity along the main pipe is random. Subsequently, the input of $G_{dv}(s)$ could be a uniform random number with the assumed minimum and maximum numbers of 0 and 0.8 (0 denotes no circuiting flow when the water consumption is zero and 0.8 denotes maximum circuiting flow based on the average VWS velocity of about 0.8 km/h).

For the feedback control elements (Figs 1 and 3), I/P transducer (*current-to-pressure transducer*) is assumed to act as a linear device with negligible dynamics. 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.^[20] Thus, the transducer transfer function should be $K_{IP}(s) = 18.5625$.^[21]

The behaviour of control valve is assumed to be a first-order transfer function with a time constant of 0.08333 min. In order to produce the change in the pure gaseous chlorine feed for the 3–300 psi change in the input signal changes to the control valve, the control valve steady-state gain is assumed to be $3.758 \text{ kg min}^{-1} \text{ psi}^{-1}$, based on the average diurnal maximum mass flow rate of chlorine. Then, the transfer function should be $K_V(s) = 3.758/(0.0833s + 1)$. The zero and span of each composition transmitter is assumed to be 0–6 ppm (the FCR mass fraction, $0-6 \times 10^{-6}$ kg FCR/kg chlorine solution) with the output range assumed to be 4–20 mA, and the time delay associated with each measurement assumed to be the

same, which is 0.5 min. Thus, the transmitter steady-state gain is $K_t = 0.26$, and the transmitter transfer function based on the Padé approximation method^[21] is $M(s) = (-0.65s + 2.6)/(0.65s + 2.6)$.

The uncontrolled FCR concentration of FCR decay process output

Simulation results of the uncontrolled FCR concentration at the points of 1.8, 3.8 and 5.8 km (0.03 km before the 2nd, 3rd and 4th boosters) are shown in Fig. 6. The curves a2, b2 and c2 show CVo1, CVo2 and CVo3 (outputs of Ga(s), Gb(s) and Gc(s)), respectively, without the disturbances of temperature and circuiting flows, over a period of 3 days with the flow rate of pure gaseous chlorine of 0.0003 kg/min injected by the 1st booster at the point of 0 km.

The results show that the FCR concentration at the point of 1.8 km almost meets the required limit as shown by the curve a1 in Fig. 6. However, the FCR concentrations at the points of 3.8 and 5.8 km are approximately 0.08 ppm, which are 0.12 ppm less than the required lower limit of 0.2 ppm (the curves b1 and c1 in Fig. 6).

Both temperature and circuiting flows cause the FCR profile to be more dynamic and decay faster over time. This may be due to the FCR decay following the moderate temperature fluctuation from 00:00 to 24:00 every day. The circuiting flows could result in unstable water velocity over time leading to the time-varying k . Since the FCR concentration depends on the value of k , a faster decay is created as shown by solid curves in Fig. 6. In addition, because the diurnal VWS affects

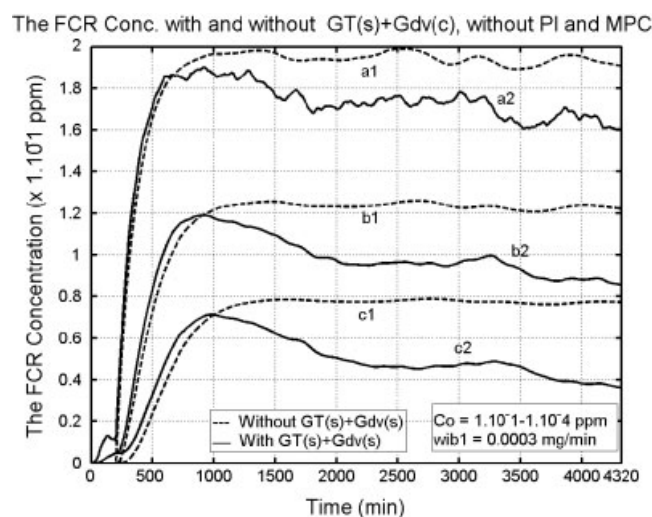


Figure 6. The FCR concentration in the MIMO system with only one booster operated without any PI and MPC with the initial chlorine concentration of 0.1–0.0001 ppm and w_{i1} of 0.0003 kg/min (a, b and c denote the FCR at the points 1.8, 3.8 and 5.8 km).

the velocity in the circulating flows, the overall pattern of the fluctuated FCR profile follows the diurnal VWS as shown by the mounting overall response of curve a1 for the first 1440 min.

The CMPC setpoint tracking and CVo constraint performances based on the better tuning parameters

Simulating the CMPC with different tuning parameters yields the best performance parameters in tracking the setpoint and settling time, as shown in Fig. 7. As concluded in Fig. 7, the CMPC with the new tuning parameter value is better in tracking the setpoint compared to the previous CMPC, although the response is more aggressive and dynamic. This is the compensation for increasing the RW value. However, the oscillation is still acceptable because the decay ratios are greater than 1/4. The settling time of $CVo1$, $CVo2$ and $CVo3$ are about 300, 504 and 712 min, respectively (the zoomed graphs in Fig. 7). Interestingly, increasing RW by 82.22% from 0.45 to 0.82 is able to reach the response faster where settling time is reduced by about 25.37, 22.69 and 20.44% for $CVo1$, $CVo2$ and $CVo3$, respectively. Therefore, the CMPC based on the tuning parameters is more able to track the setpoint and control CVo within the constraint of 0.2–0.6 ppm.

A COMPARISON OF THE CMPC AND PI CONTROL PERFORMANCES

In order to compare the CMPC performance, PI control is chosen for the comparison, because it is generally

accepted in the industry and over 90% of control loops use PI control.^[21] To begin with, PI's on-line controller tuning setting of Ziegler-Nichols (ZN) is used to fine-tune the settings, because the loops in the MIMO have third-order transfer functions.

However, as shown in Fig. 8, the PI control with ZN method causes a certain level of overshoot on $CVo1$, $CVo2$ and $CVo3$. Moreover, $CVin1$ is approximately 0.6–0.807 ppm during 217–650 min, $CVin2$ is approximately 0.6–0.861 ppm during 310–825 min, and $CVin3$ is approximately 0.6–0.83 ppm during 310–890 min (Fig. 9). So, the $CVins$ at these time

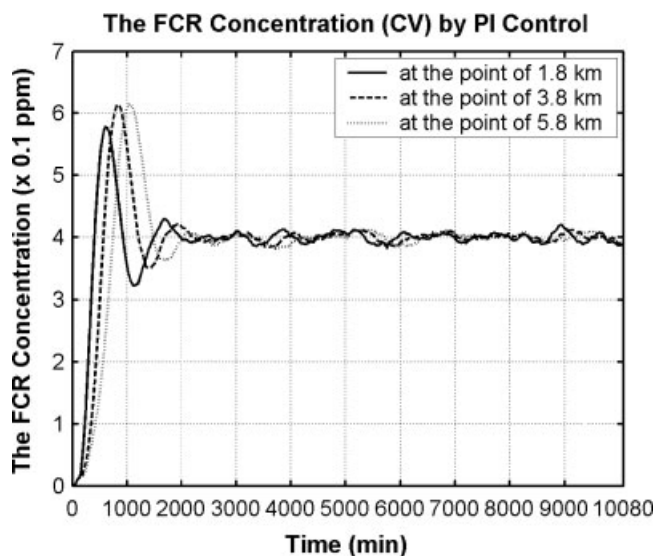


Figure 8. $CVo1$, $CVo2$ and $CVo3$ by PI control (ZN method); $K_{C1,2,3} = 0.009$, $\tau_{i1} = 0.11$, $\tau_{i2} = 0.028$, $\tau_{i3} = 0.019$, $S_p = 0.4$ ppm.

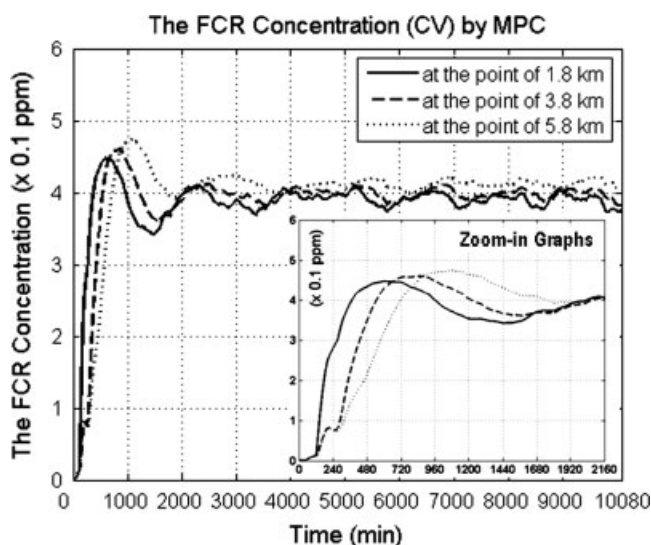


Figure 7. $CVo1$, $CVo2$ and $CVo3$ by the CMPC with $CI = 8$, $M = 20$, $P = 28$, $RW = 0.82$, $IW = 0.1$, $OW = 1$, $S_p = 0.4$ ppm, CVo constraint of 0.2–0.6 ppm.

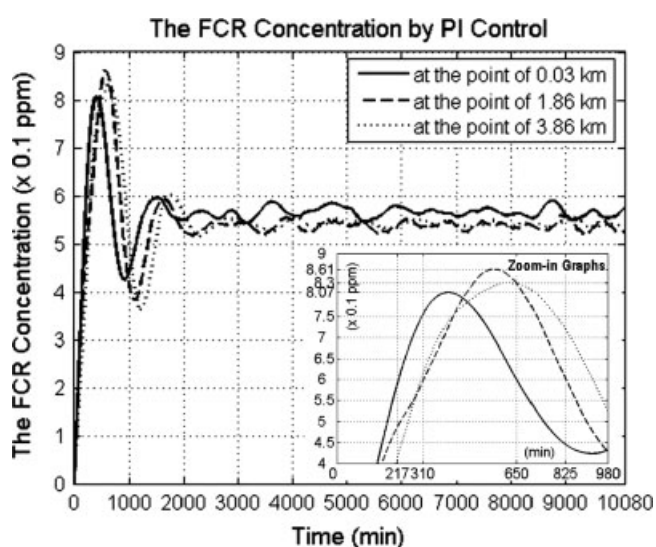


Figure 9. $CVin1$, $CVin2$ and $CVin3$ by PI control (ZN method); $K_{C1,2,3} = 0.009$, $\tau_{i1} = 0.11$, $\tau_{i2} = 0.028$, $\tau_{i3} = 0.019$ with $S_p = 0.4$ ppm.

ranges cannot meet the required upper level of FCR concentration (0.6 ppm).

For a fair comparison, the integral time absolute error (ITAE) was also used to tune the PI control because it usually results in the most conservative controller setting. As shown in Fig. 10, CV_{o1} , CV_{o2} and CV_{o3} by the ITAE-based PI control are much more stable than the ones by both CMPC (Fig. 7) and ZN-based PI control.

However, the settling time of CV_{o1} , CV_{o2} and CV_{o3} are about 836, 1070 and 1218 min, respectively (Fig. 10), which are almost double the settling times in CMPC.

Since CV_{o1} , CV_{o2} and CV_{o3} ($Sp = 0.4$ ppm) depend on w_i regulated by the control valve, it is necessary to know the value of w_{i1} , w_{i2} and w_{i3} as the MV for both CMPC and PI control. Figure 11 shows w_{i1} , w_{i2} and w_{i3} by the ITAE-based PI control in Fig. 11(a) and by CMPC in Fig. 11(b).

As shown in Fig. 11, w_{i1} , w_{i2} and w_{i3} regulated by the CMPC is faster leading to the faster responses in controlling the CV s (Fig. 7) and the CV ins (Fig. 12(b)). These are more aggressive at the beginning (200 min) compared to the PI ones. As a result, it seems that w_{i1} , w_{i2} and w_{i3} of about 0.00059, 0.0002 and 0.00019 kg/min are required to be regulated by both control valves in tracking the setpoint.

One of the key features of CMPC is that we can conveniently put a constraint on MV when designing the CMPC to optimally adjust MV s. In this case, $MV1$ and $MV2$ are limited within the constraint of $6.98E-5$ – $2.09E-4$ kg/min, and $MV3$ is limited at the constraint of $4.88E-4$ – $6.28E-4$ kg/min, as shown in Fig. 11(b). As shown in Fig. 12(b), these CMPC-based MV s also results in more acceptable CV in2 and CV in3, which are

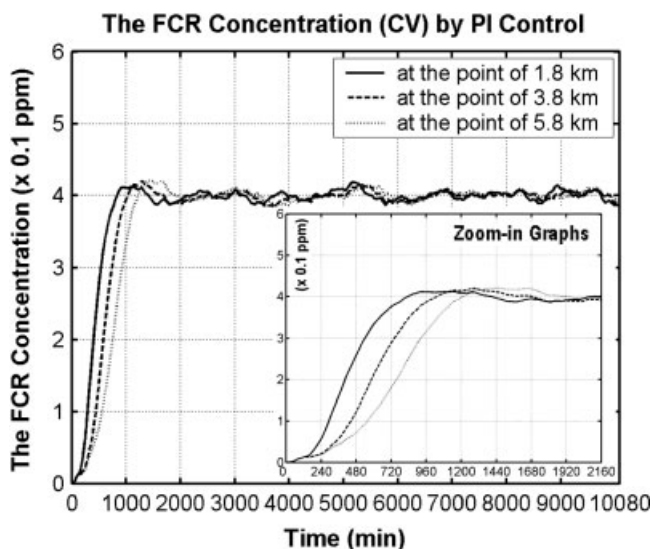


Figure 10. CV_{o1} , CV_{o2} and CV_{o3} by PI control (ITAE method); $K_{C1} = 0.047$, $\tau_{i1} = 0.05$, $K_{C2} = 0.048$, $\tau_{i2} = 0.011$, $K_{C3} = 0.051$, $\tau_{i3} = 0.009$, $Sp = 0.4$ ppm.

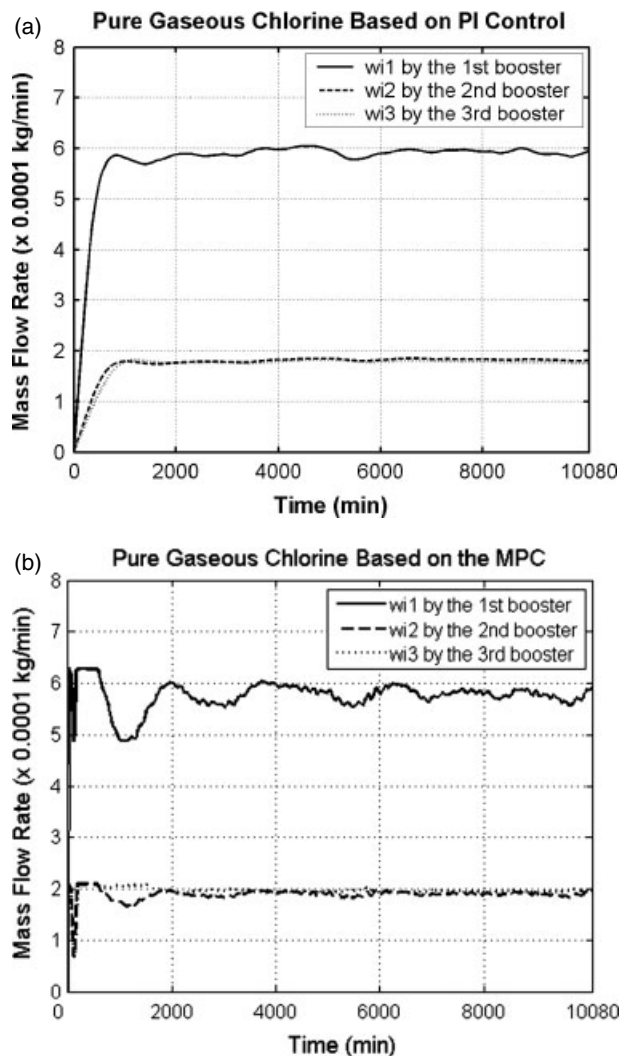


Figure 11. A comparison between w_{i1} , w_{i2} and w_{i3} by PI control (ITAE method); $K_{C1,2,3} = 0.0093$, $\tau_{i1} = 0.11$, $\tau_{i2} = 0.028$, $\tau_{i3} = 0.019$ and the CMPC ($Cl = 8$, $M = 20$, $P = 28$, $RW = 0.82$, $IW = 0.1$, $OW = 1$).

approximately 0.642 and 0.660 ppm at 380–800 and 540–1240 min, respectively, compared to the ones by ZN-based PI control (Fig. 9).

Although the CMPC strategy appears more aggressive compared to ITAE tuned PI controller in controlling CV ins (Fig. 12(a) and (b)), the gain is in its fast response, short settling time while remaining sufficiently stable in the required quality range, which is highly desirable in DWDS for the sake of public health.

CONCLUSIONS

A MIMO system in Simulink Matlab software has been developed and used to design booster locations and distribution along a main pipe of the DWDS, and to monitor and control the FCR concentration as CV within the required range of 0.2–0.6 ppm.

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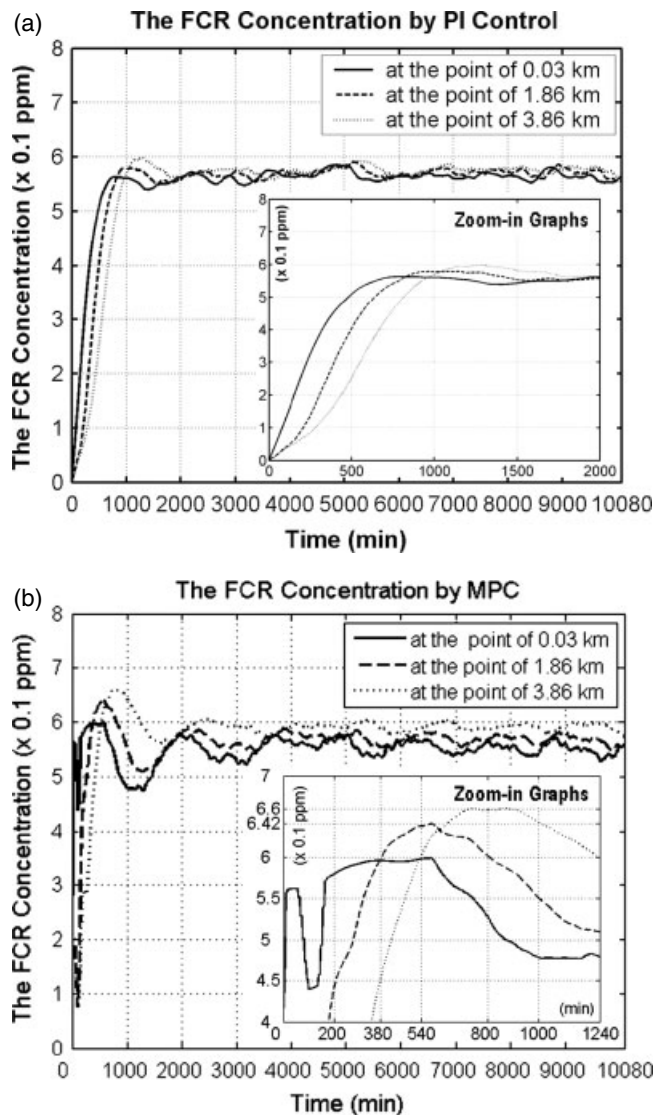


Figure 12. CVin1, CVin2 and CVin3 by (a) the ITAE-based PI control and by (b) CMPC where they are located at the points of 0.03, 1.86 and 3.86 km, respectively.

This study proposed a CMPC to regulate the optimal MVs in order to optimally control CVs. The simulation results over a period of 7 days using CMPC show that the CMPC can optimally control CVs in the main pipe of 12-in. diameter size of the simulated DWDS with the assumed wall and bulk decay constants of 0.45 and 0.55 m/day, respectively. A comparison of the performance between the ITAE-based PI control and the CMPC shows that the CMPC performance in controlling the MIMO system is in the same range as the ITAE-based PI control performance, while CMPC responses much faster. The overall performance of CMPC is superior in FCR control in DWDS, where swiftness and stability of a control system are equally important.

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