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Model predictive control for chlorine dosing of drinking water treatment based on support vector machine model

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ABSTRACT

Chlorine is the most common disinfectant used in drinking water treatment. To meet the desired disinfection level and restrict the formation of harmful disinfectant by-products, the chlorine dosage should be adjusted in real time to cope with the varying influent water quality and to ensure that the free chlorine residual (FCR) of the clear-water reservoir outlet is within the prescribed limits. This control objective is difficult to achieve by the conventional proportional integral derivative (PID) feedback controls or manual control because of the complicated dynamics of the chlorination process. This study proposes a model predictive control (MPC) scheme for chlorine dosing, in which FCR can be predicted by the support vector machine (SVM) model. Both of the simulation and experimental results show that the proposed MPC scheme has better control performance than the conventional PID feedback control scheme because of the SVM predictions being accurate and the MPC outperforming the PID, and that it can effectively stabilize the quality of treated water.

Keywords: Chlorine dosing; Drinking water treatment; Model predictive control; Feedback control

1. Introduction

Disinfection is carried out to destroy pathogenic organisms and chlorine is the predominantly applied disinfectant in drinking water treatment because it is relatively inexpensive, effective, widely available, and easy to apply [1]. The correct chlorine dosage is crucial for the safety of drinking water [2]. Too little chlorine will not sufficiently disinfect the water, while an over-dosage is uneconomical and results in excessive, harmful disinfection by-products (DBPs), such as trichloromethane, tetrachloromethane, etc. However, these also require various DBP precursors to form [3]. Thus, an ideal chlorine dosage should be a trade-off between a sufficient disinfection effect and the minimization of the formation of DBPs. In China, drinking water treatment plants are required to comply with the Standards for Drinking Water Quality (GB5749-2006) [4], which is based on the World Health Organization (WHO) guidelines for water quality [5]. The free chlorine residual (FCR) of clear-water reservoir outlets is generally controlled to be within the regulated limits of 0.2–0.5 mg L^{-1}.

During drinking water treatment, chlorine undergoes complex reactions with numerous organic and inorganic micro-pollutants in the water. The reactions are not only governed by water quality characteristics and the environmental conditions but also affected by chlorine dosage and reaction time, amongst other factors [6,7]. A series of chlorine decay and consumption models have been developed in the literature to describe the chlorination process [8–10]. Most of these models are first-order, under the typical assumption of a constant influent water quality. However, the influent water quality of any clear-water reservoir changes frequently

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because of the varying raw water quality and the operational conditions of each link before the clear-water reservoir. More importantly, these models are only used for off-line decision support of manual control and cannot be used for real-time automatic control. Thus, the research of control-oriented modeling of chlorine dosing, which can cope with the varying influent water quality, is required.

Support vector machine (SVM) is a powerful machine-learning algorithm proposed by Vapnik [11,12]. Compared with traditional methods which minimize the empirical training error, SVM applies the structural risk minimization principle (SRM) [13]. The attractive properties of SVM are that it condenses training data information, and provides a sparse representation for small sample [14]. SVM has been widely used in dealing with the problems of classification, prediction, and signal processing [15–17]. However, the generalization performance of SVM is influenced by parameters such as penalty factor and kernel parameter, for example, δ in the Gaussian kernel [18]. Thus, it is important to obtain the optimal model parameters of SVM through effective methods. Traditional methods of SVM parameter selection such as grid search, gradient descent, and non-linear programming algorithms have the drawbacks of having a large computing cost and being easily trapped into local minima [19,20]. Particle swarm optimization (PSO) is a swarm intelligence-based global optimization method [21]. It carries on an intelligent search for the solution space through a 'cooperative' strategy of particles, compared with the 'competitive' strategy used by genetic algorithms (GAs). Suboptimal solutions in the PSO algorithm can, therefore, survive and contribute to the search process at later stages of iteration. PSO is applicable to the optimization of SVM model parameters and has been proved to have better parameter optimization performance than GA [22,23].

Generally, the control of chlorine dosing is achieved by conventional proportional integral derivative (PID) feedback control, or manual control based on operator's experience [24]. These two control methods adjust the chlorine dosage according to the deviation between the actual measurement value and the set value of FCR. Thus, the chlorine dosage cannot be adjusted in real time, and the FCR easily exceeds the regulatory limits when the influent water quality changes. Model predictive control (MPC) is considered an efficient method to deal with the control of process with non-linearity and large time-delay because of its prediction of future dynamic behavior [25–27]. The control action of MPC is based on the model-based prediction of the process output over an extended prediction horizon, under constraints [28–30]. Thus, the future process outputs can be driven 'closer' to the set value [31,32].

The major contribution of this study is the development of a more effective real-time control method for the practical chlorine dosing process of drinking water treatment. First, a control-oriented model for the chlorine dosing process is established based on SVM. In addition to its use as the direct real-time control of chlorine dosing process, the novelty of the established model lies in the fact that it is based on a powerful non-linear modeling approach of SVM, which can cope with the very non-linear, and time-varying dynamics of the chlorine dosing process under varying influent water quality. Then, an MPC scheme, based on predictive model of SVM, is proposed to control the FCR of a clear-water reservoir outlet. To date, the proposed real-time control method for chlorine dosing in this manuscript has been simulated and an experiment has been successfully completed in the practical process control system of XY Water Works (XYWW) in Nanjing, China.

The rest of this paper is organized as follows. The process' features of drinking water treatment and chlorination are presented in Section 2. Chlorine dosing process modeling, based on SVM, is described in Section 3. After a brief description of the MPC scheme of the chlorine dosing process, simulations and experiments are conducted in Section 4. Finally, conclusions are given in Section 5.

2. Process description

2.1. Drinking water treatment process

The XYWW (capacity of 300,000 $m^3\ d^{-1}$) was originally put into service in 2001, and the raw water is captured from Yangtze River. The statistical analysis of the time series of daily values of raw water quality parameters during 2012–2017 is summarized in Table 1.

The overall drinking water treatment process of XYWW comprises pre-chlorination, coagulation, flocculation, sedimentation, sand filtration and post-chlorination, as shown schematically in Fig. 1.

Pre-chlorination is mainly utilized as a flocculation aid, as well being used to remove algae and organic matter. Coagulation is used primarily to hasten the agglomeration of fine particles. Coagulation, together with flocculation, constitutes a solid–liquid separation process for destabilizing dissolved and colloidal impurities, and producing large floc aggregates [33]. Sedimentation allows large floc-particle masses to settle [34]. Ultimately, physical removal

Table 1
Raw water quality of XYWW during 2012–2017

Parameter	Maximum	Minimum	Average	Standard deviation
pH	8.7	6.8	8.0	0.1
Temperature (°C)	27.6	2.1	13.8	5.1
Turbidity (NTU)	157.8	7.8	27.2	5.5
NH_4^+–N (mg L^{-1})	0.95	0.07	0.11	0.05
COD_{Mn} (mg L^{-1})	3.7	1.1	1.6	0.4
TOC (mg L^{-1})	3.77	0.82	1.35	0.25

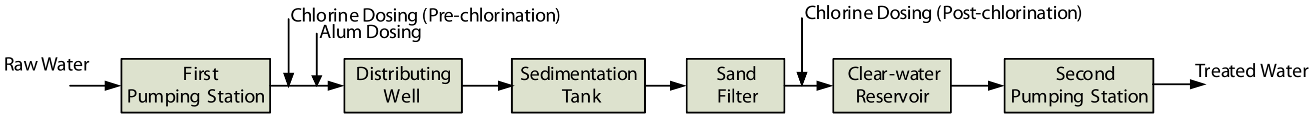

Fig. 1. Flow diagram of drinking water treatment process.

of turbidity and microorganisms is accomplished by sand filtration [35]. Post-chlorination is the main process of disinfection, oxidation of organic contamination and removal of pathogens, and directly affects the treated water quality [36]. Thus, the control of chlorine doses in the post-chlorination stage is developed in this work.

2.2. Chlorination process

Chlorine reacts with both inorganic and organic substances in water. As they are the most reactive with chlorine, inorganic substances in water such as iron, manganese, sulfide and ammonia lead to the rapid chlorine consumption, while reactions of organic substances with chlorine usually proceed relatively slow [37,38]. As a result of these reactions, the chlorine decay process is often characterized by a first-order model:

$$C_t = C_0 \exp\left(-k_{\mathrm{cl}} \times t\right) \tag{1}$$

where C_t is the chlorine concentration at time t (mg L^{-1}), C_0 is the chlorine concentration at time 0 (mg L^{-1}), and k_{cl} is the chlorine decay coefficient (1/h).

Many studies have illustrated that the k_{cl} is determined by water quality, temperature, alkalinity, etc. [39,40]. Since the influent water quality changes continuously and is full of uncertainty, the practical chlorination process is complicated.

3. Chlorine dosing process modeling

The practical chlorine dosing process exhibits complicated non-linear characteristics with a time-delay, which prevents an accurate mathematical model. In this paper, an SVM model is established to predict the process output (i.e., FCR), and a PSO algorithm is adopted to train the parameters of SVM model.

3.1. SVM model

SVM is an effective non-linear regression approach, based on the statistical learning theory and SRM principle. The basic strategy of SVM is to map the input vector into a high dimensional linear feature space through a non-linear transformation. Then the optimal decision function is constructed. The dot product operation in the higher dimensional feature space is replaced by the kernel function in original space, and the global optimal solution is obtained by the training of the sample.

The regression function for SVM is as follows:

$$f\left(X\right) = W \times \phi\left(X\right) + b \tag{2}$$

where W is the weight vector, $\phi(\cdot)$ is the non-linear mapping from the input space to the output space, and b is bias term.

The estimation function problem is transformed into function optimization problem by the SRM principle:

$$\min \frac{1}{2}\left\|W\right\|^2 + C\sum_{i=1}^{k}\varepsilon_i \tag{3}$$

where C is the penalty factor and ε_i is the relaxation factors.

The optimization problem is solved using a Lagrangian method. Then, the regression function of Eq. (2) can be formulated by the following form:

$$f\left(x\right) = \sum_{i=1}^{k} a_i \phi\left(X\right) \times \phi\left(X_i\right) + b \tag{4}$$

where a_i is the Lagrangian multiplier.
The kernel function is defined as:

$$K\left(X_i, X_j\right) = \phi\left(X_i\right) \times \phi\left(X_j\right) \tag{5}$$

Familiar kernel function for SVM has three forms that include Gaussian kernel, polynomial kernel and sigmoid kernel. Gaussian kernel is the most widely applied among them and is adopted in this work.

$$K\left(X_i, X_j\right) = \exp\left(\frac{-\left\|X - X_i\right\|^2}{2\delta^2}\right) \tag{6}$$

where δ is the Gaussian kernel parameter.

SVM is sensitive to the proper setting of model parameters. Within SVM, the penalty factor, C, and Gaussian kernel parameter, δ, are required to be specified. PSO is an evolutionary algorithm based on group intelligence, developed in recent years. Inspired by the social behavior of a flock of birds, it is used for finding the global optimum solution in a search space through the interactions of individuals in a swarm of particles. Each particle indicates a potential solution to the problem and it has its own feature of position, velocity and fitness. During each iteration, the velocity and position of the particle are adjusted dynamically to optimize the individual in the search space. The particle updates its velocity and position using the following equations:

$$v_i^{(k+1)} = h^{(k)} v_i^{(k)} + c_1 r_1 \left(p_i^{(k)} - x_i^{(k)}\right) + c_2 r_2 \left(p_g^{(k)} - x_i^{(k)}\right) \tag{7}$$

$$x_i^{(k+1)} = x_i^{(k)} + v_i^{(k)} \tag{8}$$

where i = 1,2,..., n, n is the number of particle, $v_i^{(k)}$ is the present velocity of particle i, $x_i^{(k)}$ is the present position of particle i, $p_i^{(k)}$ is the best position of particle i, $p_g^{(k)}$ is the best position of the swarm, k and k + 1 are the time index of current and next iterations, respectively, c_1 and c_2 are the acceleration constants, r_1 and r_2 are the random numbers selected between [0,1], $h^{(k)}$ is the inertia weight, which can be described as follows:

$$h^{(k)} = \frac{(h_1 - h_2)(k_{\max} - k)}{k_{\max}} + h_2 \tag{9}$$

where $k_{\max}$ is the max inertia number, h_1 and h_2 are the initial inertia weight and final inertia weight, respectively.

The fitness function of particle is shown in the following equation:

$$\text{Fitness} = \frac{1}{N}\sum_{i=1}^{N}(y_i - y_t)^2 \tag{10}$$

where N is the number of training samples, y_i is the ideal output, y_t is the actual output.

3.2. Modeling results

The structure of the SVM model as shown in Fig. 2 is selected in this study, and d is the time delay.

In this study, a k-fold cross validation (k = 10) is used to randomly divide the original sample of 3,000 data set groups into 10 sub-samples. Then, a single sub-sample is picked up as the validation data for testing the model, and the remaining nine sub-samples are regarded as training data for the model. These procedures are repeated 10 times and each of the 10 sub-samples is used only once as the validation data. A single estimation can then be produced by averaging the 10 results from the folds.

Besides the PSO algorithm, GA and GD are also adopted to train the SVM model for comparison. Fig. 3 shows the SVM modeling results of the chlorine dosing process.

The Theil's inequality coefficient (TIC) is adopted here to evaluate the model accuracy:

$$\text{TIC} = \frac{\sqrt{\sum_i (y_i - y_{m,i})^2}}{N \times \sqrt{\sum_i y_i^2} + \sqrt{\sum_i y_{m,i}^2}} \tag{11}$$

where y_i is the actual value, $y_{m,i}$ is the model predictive value.

The TICs for modeling results of the SVM are trained by PSO, GA, and GD are 0.032, 0.045, and 0.056, respectively; the TICs are all lower than 0.3, indicating a good agreement [41]. Furthermore, the SVM model trained by the PSO algorithm has a better modeling accuracy than that trained by the GA and GD algorithms, and, therefore, it is applied to the predictive model of MPC for the chlorine dosing process.

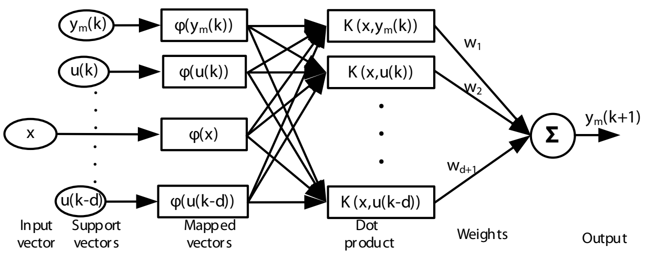

Fig. 2. Schematic structure of SVM.

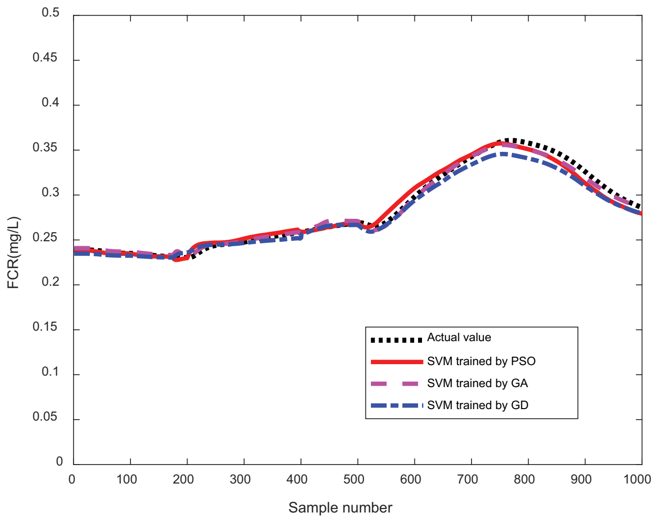

Fig. 3. Modeling results of the chlorine dosing process.

4. MPC for the chlorine dosing process

In this section, the MPC scheme, based on the aforementioned SVM model, is proposed for the chlorine dosing process. The real-time control objective is to regulate the chlorine dosage to maintain the FCR of a clear-water reservoir outlet at the desired constant value under varying influent water quality. In order to ensure the safety of disinfection, chlorine dosage – as the input of chlorine dosing process –- is constrained within the range of 0.3–1.2 mg L^{-1}.

4.1. MPC control algorithms

MPC refers to a class of control algorithms that employ an explicit model to predict the future behavior of the process over an extended prediction horizon [42]. The MPC scheme of this work, shown in Fig. 4, uses an SVM model to predict the process dynamics.

At every sampling instant, the set of future control moves is planned in such a way that the predictive out is as close to the reference trajectory as possible. The future control action is computed by real-time optimization of a cost function, written as follows:

$$J = \sum_{j=1}^{N_y} q\left[y^*(k+j) - y_m(k+j)^2\right] + \sum_{j=1}^{N_u} \lambda\left[\Delta u(k+j)\right]^2 \tag{12}$$

subject to

$$y_{\min} \le y_m(k+j) \le y_{\max} \quad \text{for} \quad 1 \le j \le N_y \tag{13}$$

$$u_{\min} \le u_m(k+j) \le u_{\max} \quad \text{for} \quad 1 \le j \le N_u \tag{14}$$

$$\left|\Delta u(k+j)\right| \le \Delta u_{\max} \quad \text{for} \quad 1 \le j \le N_u \tag{15}$$

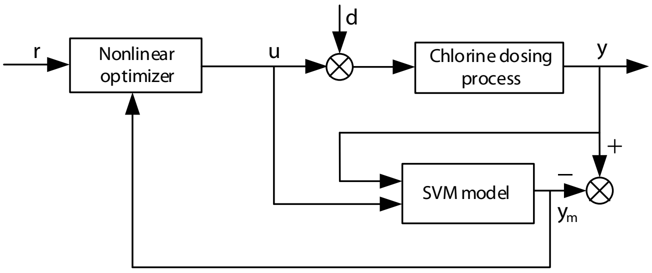

Fig. 4. MPC scheme based on SVM model.

where N_y is the prediction horizon, N_u is the control horizon, q is the output tracking weights, λ is the input weights, $\Delta u(k)$ is the change of manipulated variable, $y_m(k)$ is the prediction output of SVM model proposed in Fig. 2, $y^*(k)$ is the output set-point trajectory, written as follows:

$$y^*(k+j) = y_r(k+j) - \alpha\left[y_r(k) - y(k)\right] \tag{16}$$

where $y_r(k)$ is the output set point, α is the softening factor of set point, $y(k)$ is the actual output value.

The selection of prediction horizon N_y depends on the sampling interval. Longer prediction horizon N_y can retrieve more future information and promote the stability of control system. However, overlarge prediction horizon N_y brings computational burden and is difficult to further improve the closed-loop system performance. Control horizon N_u is chosen from 1 to 6 generally and overlarge control horizon N_u is difficult to further promote the dynamic performance of closed-loop system. In this application, the control horizon N_u is chosen as 1, and the prediction horizon N_y is chosen through comparing the control results under different prediction horizons with the SVM model. The output tracking weights q and input weights λ in (Eq. (12)) and softening factor of set point α in (Eq. (13)) has great influence on the dynamic properties of system. We chose these parameters through trail and error in the simulation and experiments.

At time step k, the non-linear optimizer computes both the present- and future-manipulated variable moves, such that the predictive output follows the output reference trajectory through minimizing the cost function. The range of optimal value of manipulated variable is known. And the optimization problem is solved using the golden section search method. The sampling time of solving the non-convex MPC problem is smaller than the sampling time of system. Only the first move of manipulated variable is applied to the process, and this step is repeated for next time step.

4.2. Simulation results

The simulation of the proposed MPC scheme based on the SVM model is performed on MATLAB 2017 with Intel Core i5 CPU 2.3 GHz and the time range is 0–500 min. As in the above analysis, the chlorine dosing process exhibits a first-order and time-delay characteristic, in which parameters change with the varying water quality. Thus, two first-order plus time-delay (FOPTD) model (Eqs. (17) and (18)) under certain different conditions of water quality are considered here as the chlorine dosing process for simulation, within the time range of 0–250 min and 251–500 min, respectively.

$$G_p(S) = \frac{0.18}{32s+1}e^{-18s} \tag{17}$$

$$G_p(S) = \frac{0.2}{36s+1}e^{-22s} \tag{18}$$

The simulation of the MPC scheme based on the SVM model is conducted to maintain FCR a set-point trajectory that smoothly varies to the required set-point. The MPC scheme based on FOPTD model and PID scheme are also conducted for comparison purposes. The control effect, under varying water quality, is studied in the nominal case, as well as the model mismatch case. To further verify the disturbance rejection performance of the proposed MPC scheme, an external disturbance of 0.1 mg L^{-1}, which is shown in Fig. 4 d, is applied at the 400th min of the simulation. Through the comparison results with different horizons as shown in Fig. 5, we select the prediction horizon $N_y = 6$, the control horizon $N_u = 1$.

The tracking weights $q = 1$, the input weights $\lambda = 0.02$, the input constraints $\Delta u_{max} = 0.5$ mg L^{-1}, $u_{min} = 0$ mg L^{-1}, $u_{max} = 2.5$ mg L^{-1}. The computational time of each step is 0.05735 s ($N_y = 6$, $N_u = 1$). The overshoot, settling time and integral of absolute error (IAE) – as shown in Eq. (19) – are chosen as the quantitative indices to evaluate the performance of the control system.

$$\text{IAE}(t) = \frac{1}{N}\sum_{t=1}^{N}\left|y^*(t) - y(t)\right| \tag{19}$$

where $y^*(t)$ is the reference signal and $y(t)$ is the actual process output.

4.2.1. Nominal case

When the established SVM model is matched with the actual chlorine dosing process, namely $G_m(s) = G_p(s)$, the simulation results are shown in Fig. 6, and performance

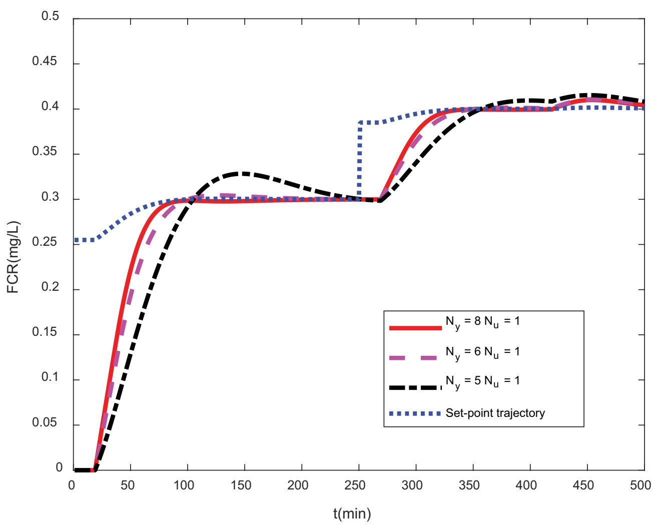

Fig. 5. Comparison results with different horizons.

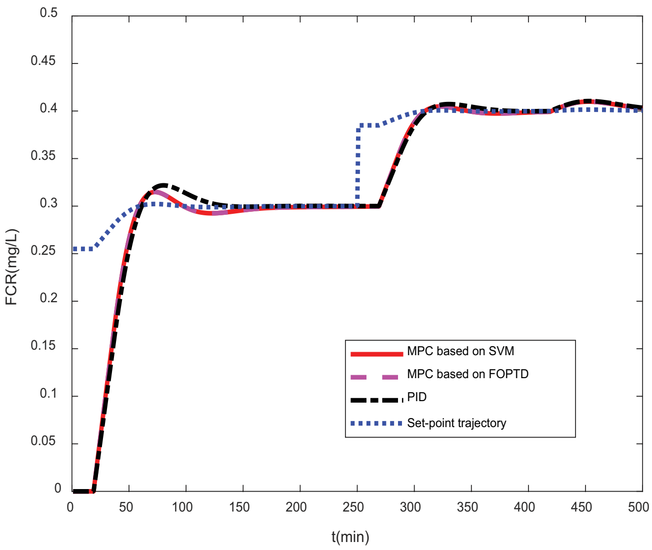

Fig. 6. Simulation results of output response of FCR in the nominal case.

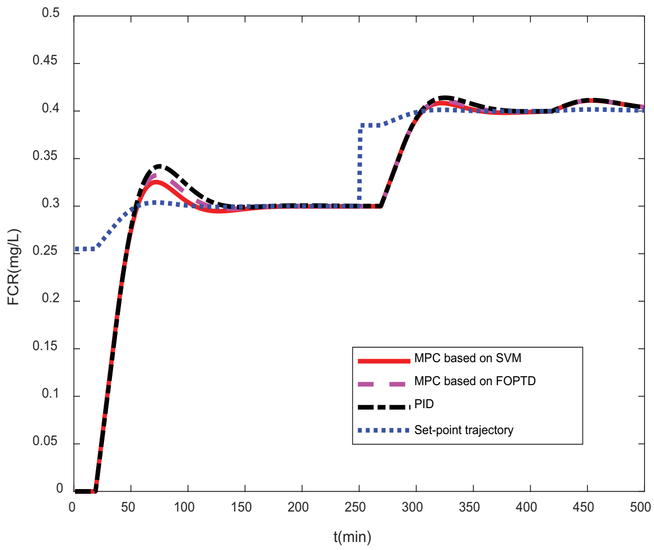

Fig. 7. Simulation results of output response of FCR in the model mismatch case.

indices are shown in Table 2. It shows that the proposed MPC scheme based on SVM model and MPC scheme based on FOPTD model produce the same control performance because the SVM model is matched with the FOPTD mode. Compared with the PID scheme, both of them provide faster convergence speed and smaller amplitudes of fluctuations.

4.2.2. Model mismatch case

During drinking water treatment, the influent water quality of chlorine dosing process is time varying. This sometimes results in a mismatch between the established model and the actual process. To verify the robustness of the proposed MPC scheme, a 20% decrease of the parameters in Eqs. (17) and (18) is simulated for the model mismatch case. The corresponding simulation results are shown in Fig. 7 and the performance indices are shown in Table 3. It can be observed that the proposed MPC scheme based on SVM model also provides a faster convergence speed and smaller amplitudes of fluctuations than the MPC scheme based on FOPTD model and PID scheme. This means that the underlying model accuracy of SVM and the excellent control of MPC scheme make the proposed control scheme achieve a better control performance, even in the case of severe model mismatches.

4.3. Experimental results

To test the practical application effects of the proposed MPC scheme based on SVM model, experiments of the proposed MPC scheme based on FOPTD model, together with the PID scheme, are also conducted with similar water quality conditions. The control algorithms are coded on the commercial SCADA software of XYWW. All the online signals from, or to the chlorine dosing process control system are interconnected through the distributed control system as shown in Fig. 8. Process data are saved in a database on a PC server, and the control schemes are programmed on a PC and executed through a programmable logic controller.

During the practical chlorine dosing process, the chlorine dosing point locates the inlet pipeline of clear-water reservoir. The contact time of chlorine and water is an important factor to ensure the disinfection effect. The chlorine and water should be fully mixed in the clear-water reservoir, and the contact time should be longer than 30 min. After chlorine dosing, chlorine and impurities in the filtered water fully react in the clear-water reservoir, then through the second pumping room into the water supply system. The control block diagram of chlorine dosing system is shown in Fig. 9.

Influenced by the varying raw water quality and the processes before chlorination, the cases of model mismatch and external disturbance are common in the actual

Table 2
Performance indices of output response of FCR for the simulation results in the nominal case

Method	0–250 min			251–500 min		
	Overshoot (%)	Settling time (min)	IAE (mg L^{-1})	Overshoot (%)	Settling time (min)	IAE (mg L^{-1})
MPC based on SVM	4.6	152	0.009	3.7	119	0.005
MPC based on FOPTD	4.6	152	0.009	3.7	119	0.005
PID	6.5	156	0.012	5.1	127	0.007

Table 3
Performance indices of output response of FCR for the simulation results in the model mismatch case

Method	0–250 min			251–500 min		
	Overshoot (%)	Settling time (min)	IAE (mg L⁻¹)	Overshoot (%)	Settling time (min)	IAE (mg L⁻¹)
MPC based on SVM	11.6	156	0.013	7.1	107	0.006
MPC based on FOPTD	12.5	160	0.017	8.7	117	0.007
PID	13.8	166	0.020	9.2	126	0.009

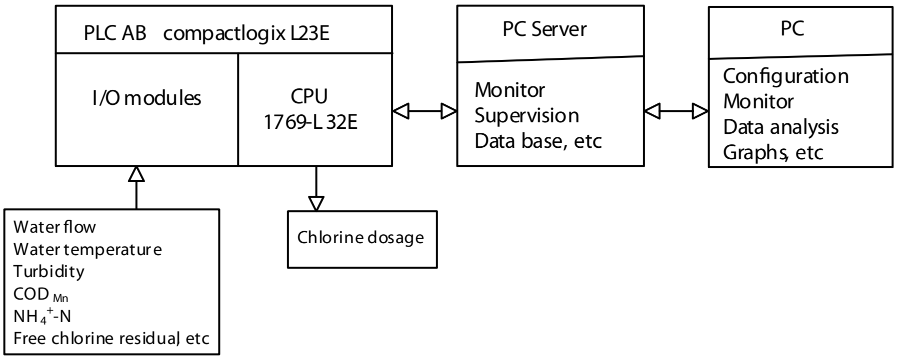

Fig. 8. Distributed control system for the chlorine dosing process.

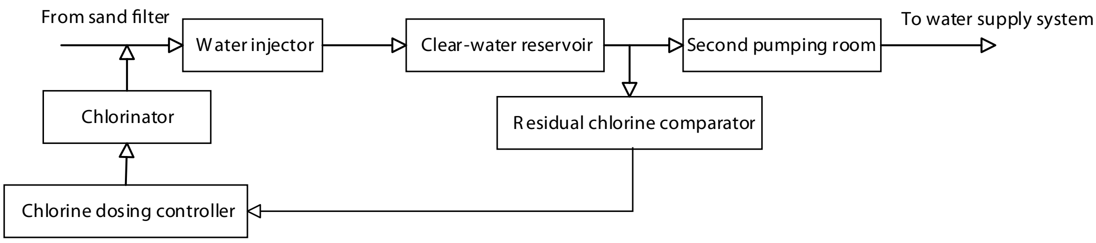

Fig. 9. Control block diagram of chlorine dosing system.

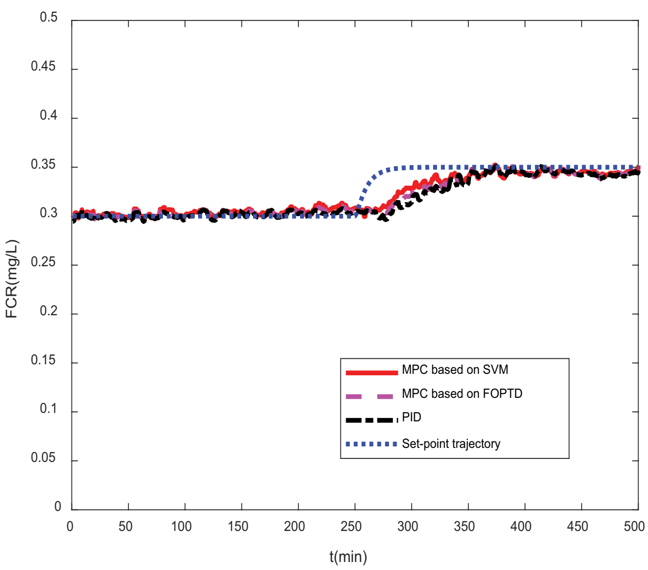

Fig. 10. Experimental results of output response of FCR.

Table 4
Performance indices of output response of FCR for the experimental results

Method	Overshoot (%)	Settling time (min)	IAE (mg L⁻¹)
MPC based on SVM	0.8	116	0.030
MPC based on FOPTD	1.0	125	0.032
PID	1.3	137	0.038

chlorination. It can be seen from the experimental results in Fig. 10 and Table 4 that the proposed MPC scheme based on SVM model behaves more robustly against the variation of water quality than the MPC scheme based on FOPTD model and PID scheme. This is basically consistent with the previous analysis of the simulation results in the model mismatch case. In addition, the overshoot and settling time of the experimental results are smaller than those of the simulation results. This is because the actual variation amplitude of the influent water quality is smaller during the experimental periods. Thus, the degree of model mismatch is smaller. On the other hand, the IAE of the experimental results is larger than that of the simulation results. This is because the actual influent water quality is time-varying and, therefore, the actual FCR is changing continuously.

Through analysis of open-loop step response experiments, the practical chlorine dosing process is open-loop stable. The variation of water quality is slow and not frequent. Thus the stability of the closed-loop can be guaranteed within a finite region. The detailed discussion can be found in the studies by Quevedo et al. [43] and Aguilera and Quevedo [44].

5. Conclusions

MPC has been employed to handle the complicated, non-linear control of the chlorine dosing process of drinking water treatment. An accurate predictive model of the chlorine dosing process has been developed based on SVM. Compared with MPC scheme based on FOPTD model and PID scheme, the simulation and experimental results of the proposed MPC scheme based on SVM model have demonstrated significant performance improvements because of the SVM predictions being accurate and the MPC outperforming the PID. For realizing more reliable real-time automatic control of the chlorine dosing process, the proposed control scheme should be investigated in a longer experiment, and further stability evaluations should be conducted.

Acknowledgment

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