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Nonlinear Model Predictive Control of Water Quality in Drinking Water Distribution Systems with DBPs Objectives

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***Abstract*—**The paper develops a Non-Linear Model Predictive Control (NMPC) of water quality in Drinking Water Distribution Systems (DWDS) based on the advanced non-linear quality dynamics model including disinfections by-products (DBPs). A special attention is paid to the analysis of an impact of the flow trajectories prescribed by an upper control level of the recently developed two-time scale architecture of an integrated quality and quantity control in DWDS. The new quality controller is to operate within this architecture in the fast time scale as the lower level quality controller. The controller performance is validated by a comprehensive simulation study based on an example case study DWDS.

***Keywords*—**Model predictive control, hierarchical control structure, genetic algorithm, water quality with DBPs objectives.

I. Introduction and Problem Statement

An increasing shortage of natural water resources around the world is observed, which is due to climate change, rising population and environment pollution [1], [2]. Hence, meeting demand on drinking water of required quality requires advanced control technology to operate DWDS which are typically large scale complex network systems [3], [4].

In the control of drinking water distribution systems (DWDS), quantity and quality are the two major aspects. The quantity control deals with the pipe flows and pressures at the water network junction nodes to produce optimized pump and valve control schedules so that the water demand at the consumption nodes is met and the associated electrical energy cost due to pumping is minimized [3], [5]. The main objective of the quality control is to maintain the free disinfectant concentration at the monitored nodes within the 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 health dangerous [6]. 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. Hence, the free chlorine concentration is often used for assessment of the water quality state [7]. In summary, the quality control aims at maintaining the free chlorine concentrations at the monitored nodes within the described lower-upper limits and minimizing the DBP concentrations at these nodes. Although the quality control has attracted great attention of the industrial and research communities worldwide, this paper proposes for the first time the quality control objectives with DBPs in place. The chlorine residuals are controlled directly by the treatment plant to ensure the water entering to the DWDS has required residual values. 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 safety of water may not be guaranteed particularly at remote consumption nodes. Hence, it is necessary to inject chlorine by using booster stations located at certain intermediate junction nodes of the DWDS. The chlorine injections are the quality control inputs while the booster stations are the corresponding quality actuators. The optimized allocation of booster station problem was presented in [8], [9]. The quality control inputs have no impact on the flows which are the hydraulic controlled outputs. However, the quality controlled outputs depend on the flows. Hence, the quality and quantity interaction exists although it is only one way interaction from quantity to quality. Therefore, the quality and quantity needs to be controlled in an integrated manner. However, due to different time scales in the internal dynamics of the hydraulic and quality, which is slow and fast respectively, a dimension complexity of the integrated MPC optimization task is large. This makes impossible direct application of MPC to integrated control of water quality and quantity even for small size DWDS [10]. Hence, the two time-scale hierarchical control structure was proposed in [11], [12] and illustrated in Fig. 1. The optimizing controller at the Upper Control Level (UCL) operates in the slow hydraulic time scale based on the accurate hydraulic model and simplified quality model with one hour time step applied in both models. The models are used to predict the quantity and quality controlled outputs over the quantity prediction horizon of 24 hours. At the beginning of a control period, the states of water quantity and quality are measured or estimated and then sent to the integrated quantity and quality optimizer. Moreover, the water demand prediction is also provided for the optimizer. Due to the one way interaction between the quantity and quality the hydraulic controls resulting from solving the MPC optimization task are truly optimal. The quality dynamic model in this optimization problem has the same time step as the quantity dynamic model.

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Although the problem dimension is decreased immensely, the quality modelling error is extremely increased. Hence, 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 [5], [10] and the growth dynamics of the DBPs [13], [14].

In order to achieve the operational objective of DWDS in a robustly feasible and cost effective way, information about the DWDS states, including quantity and quality, is required on-line. Monitoring the water quantity has been well developed in the previous research, while the quality monitoring is also presented in [14], [15]. Optimized placement of hard chlorine sensors achieving the required balance between the estimation accuracy and sensor maintenance and capital cost is presented in [16].

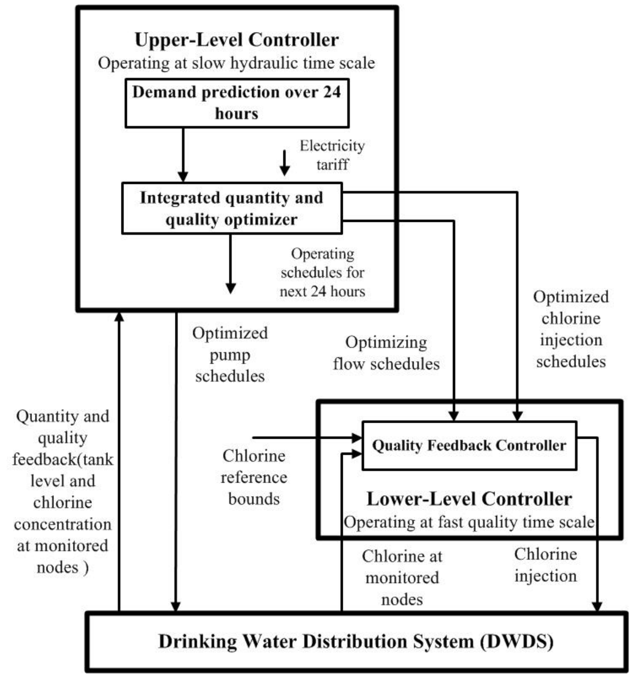

Fig. 1 Hierarchical two-level structure for optimizing control of integrated quantity and quality

Till now the quality control considered only the bacterium objective [17], [18]. In this paper for the first time both the bacterium and DBPs objectives are jointly considered and the MPC is applied to synthesize the Lower Level Controller (LLC) at LCL of the structure in Fig. 1. The paper is organized as follows. In Section II, the quality model dynamics is presented as to be used for the quality output prediction within MPC. The optimizing MPC controller is designed in Section III and it is applied to an example case study DWDS in Section IV. The conclusions and future research are presented in Section V.

II. The Quality Model Dynamics with DBPs

The recently derived model of the quality state [13] is too complex for the MPC applications. The model was simplified in [14] and applied for robust monitoring the quality with DBPs and it is utilised in this paper. As opposed to the previously used models for the quality control limited to the free disinfectant objective only, this model is highly non-linear due to the non-linear dynamics of chlorine decay and DBPs build up reactions.

A. A Dynamics of the Quality Kinetics

The chemical reactions generating the chlorine and DBPs are presented in [14], [19]. Based on the chemical reactions, the quality kinetics can be derived as [14]:

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

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], $k_{Cl}, k_{DBP1}, k_{DBP2}$ 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:

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

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

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

B. The Quality Model Dynamics at DWDS

The following assumptions are made [14]:

- DWDS is composed of water sources, pressure pipes, nodes and tanks.
- The flow directions are constant over considered modelling time horizon.
- The flow rate and flow velocities are known.
- Concentration of free chlorine and DBP at external water sources are known.
- Mixing at the nodes, pipes and tanks is instantaneous and complete and in addition it is free of storage at the nodes.
- 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 (3) the quality advection transport along a pipe $p \in NP$ with length L_p can be described as [14], [20]:

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

Equation (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 $m = 1,..., NS_p$, (4) can be approximated in space as [14], [15]:

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

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 (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; $c_{in,n}^1(t)$ denotes the free chlorine dosing into the node n by flow paced booster quality controlling devices[5]. The pipe junction nodes with the dosing are the quality control nodes. For the very practical reasons a set of these nodes $CNPJ$ is limited to only achieving controllability of the quality [21]. The quality control inputs are $c_{in,n}^1(t)$, where $n \in CNPJ \subset NPJ$. The resulting quality output $c_n(t)$ at the junction node n can be expressed as[14]:

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

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

Furthermore, consider the quality dynamics in the tank. As similar 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 [14], [15]:

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

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 (6) is the output equations in the quality state-space model.

It is now clear that the quality state-space model described above is the non-linear time-varying dynamical system under 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.

III. Optimizing Model Predictive Controller for Water Quality with DBP Objectives

Due to the non-linear dynamic described in the quality model and the multivariable constrained control problems, the Model Predictive Control (MPC) is selected to implement the quality control with DBP objectives at DWDS. The basic MPC control loop in Fig. 2 is made up of three core modules: plant model, output predictor/state estimator and solver of the MPC model based optimization problem (MBOP).

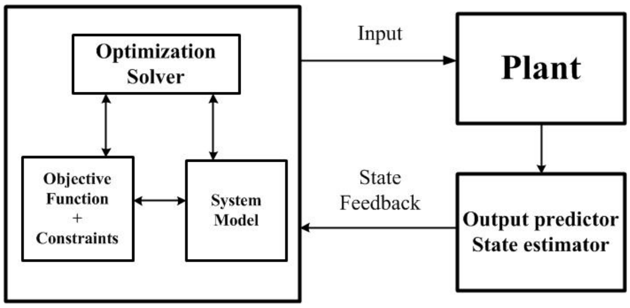

Fig. 2 The Basic MPC control loop

A. Formulation of MBOP

Denote $u_i(t)$ and $y_j(t)$ 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:

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

where $u_i^{\min}(t), u_i^{\max}(t), y_j^{1\min}(t), y_j^{1\max}(t)$ 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:

$$f(t) = \min \sum_{t \in H_P} \left(\sum_{j \in MNPJ} y_j^2(t) \right) \quad (9)$$

where H_P presents the prediction horizon.

B. 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[14] is applied to produce the robust state estimates on-line. The free chlorine and DBP concentrations along pipes, tank heads and free chlorine and DBP concentrations in tanks are DWDS state variables. Denoting the state vector at time instant *t* as[12]:

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

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

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

1) The DWDS state *X(kT)* is measured or estimated and the demand and DWDS quality boundary conditions are predicted.
2) The MPC optimization problem (9) is solved.
3) Only the first optimized control action is used and applied to DWDS.
4) Set $k = k + 1$ and return to 1).

C. Solver of MBOP

The optimizer is designed as performing the search in the space of the control inputs. This is supported by employing fast and reliable simulator of the quality at DWDS. Hence, the Genetic Algorithm (GA) is applied to solve the optimization problem as faster non-linear optimization algorithms such as SQP are hardly applicable to the chosen structure of the optimization search (the gradients and second derivatives are not analytically available). The initial quality states are provided by the state estimator. GA begins with random population of individuals and/or 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 [22].

D. Model Simulator: EPANET and EPANET-MSX

EPANET is an open source software package published by the National Risk Management Research Laboratory of United State Environment Protection Agency in 2000 and is used in simulation and design of hydraulic behavior with pressurized pipe networks. Constructing the distribution network, calibrating and tuning the coefficients of the network can be modeled using EPANET. Moreover, EPANET can generate the EPANET input file which stores the simulation data in 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 optimization functions. In addition, the quality reaction dynamics presented in this paper are involved in multiple species DBPs, EPANET has its limitation on tracking the transport and fate of multiple species. Therefore, the EPANET-MSX software package is required to solve these mentioned problems. EPANET-MSX allows the original EPANET to model any system of multiple, interacting chemical species, and this capability has been incorporated into both a stand-alone executable program as well as a toolkit library of functions that programmers can use to build custom applications, where MSX stands for Multi-Species Extension [23]. In this paper, both of the EPANET and EPANET-MSX simulators are used to generate the simulation results data of water network, including node pressure, pipe flow, and quality concentration and so on.

IV. Application to Example Case Study DWDS and Simulation Results

A. Example Network

The topology of the case-study network is illustrated in Fig. 3. There are 8 consumption nodes: *n11, n12, n13, n21, n22, n23, n3* and *n32*. Node 9 represents the reservoir, and node 2 stands for a switching tank. Link between node 9 and node 10 is the pump which is the only energy-consumed 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 limit on inputs is from the requirement of health regulations. A value of 4(*mg/L*) is defined by US EPA. In practice, the DWDS operates at lower value than this since the usage of chlorine booster stations. Hence, for the purpose of simulation study, the upper limit on chlorine injection is taken as $u_i^{\max}(t) = 1(mg/L)$ because of the simulation is implemented on a small network. Furthermore, the lower limit on chlorine injection is set as $u_i^{\min}(t) = 0(mg/L)$. 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 water head in the tank which determines the tank operating status. The whole modeling horizon is 24 hours includes filling cycle and draining cycle due to the operation of the tank. Filling cycle operates in the first 13 hours, and then, the example DWDS switches to draining cycle which sustains 11 hours. In terms of quality control which has fast dynamics, the control horizon is set as 6 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.

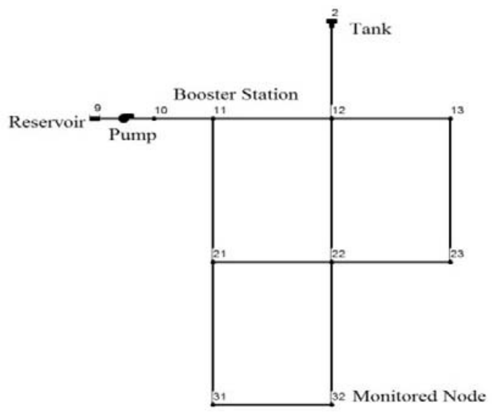

Fig. 3 The example DWDS network

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*.

B. Software Implementation

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

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

C. Simulation Results

As shown in Fig. 4, the trajectory of chlorine concentration at monitored node is maintained within the limits. Fig. 5 illustrates the trajectory of minimized DBP concentration at the monitored node. As shown in Fig. 5, the concentration of DBPs during most of the draining cycle period is at its saturation level showing on poor controllability over this period.

As the tank stores the DBPs produced there during filling cycle, the high quantity of DBPs from tank is transferred into the monitored node during the draining cycle. This makes the DBPs concentration at monitored node high during the draining cycle. As duration of these two cycles is determined by the network hydraulic operation, a significant impact of the hydraulics on the quality is demonstrated supporting a relevance of the UCL in Fig. 1. Figs. 6-9 illustrate the performance of quality control with different lengths of draining cycle (sum of the two cycles' duration is 24 hours).

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 Figs. 10 and 11. Clearly, the chlorine constraints are met but the chlorine profiles are different as shown in Figs. 4 and 10. Table I presents the total and average amount of DBP concentration at monitored node under different scenarios of controller and flow generated by UCL. According to the results listed in Table I, the performance of quality controller without considering DBPs is worse than that considering DBPs since its high average amount of DBP concentration along the modeling horizon. Hence, an advantage of the proposed controller can be clearly seen.

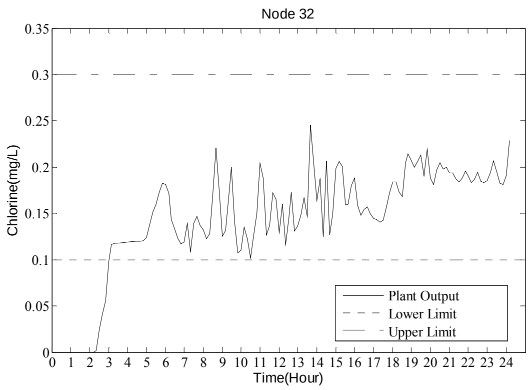

Fig. 4 The chlorine concentrations at monitored node under 11 hours of draining cycle

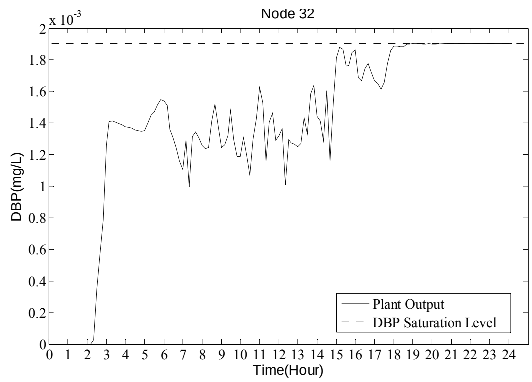

Fig. 5 DBP concentrations at monitored node under 11 hours of draining cycle

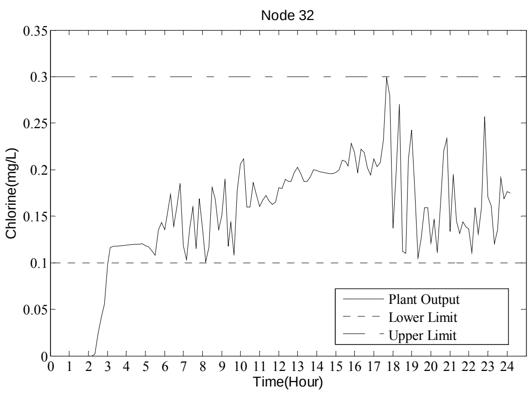

Fig. 6 The chlorine concentrations at monitored node under 6.8 hours of draining cycle

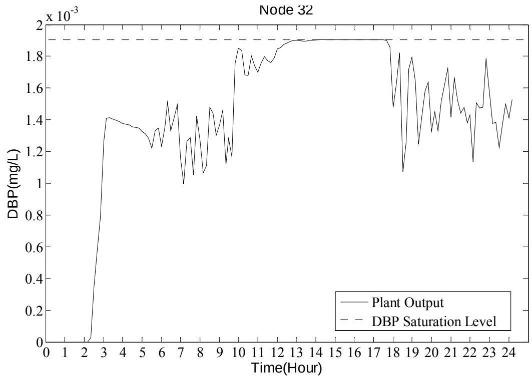

Fig. 7 DBP concentrations at monitored node under 6.8 hours of draining cycle

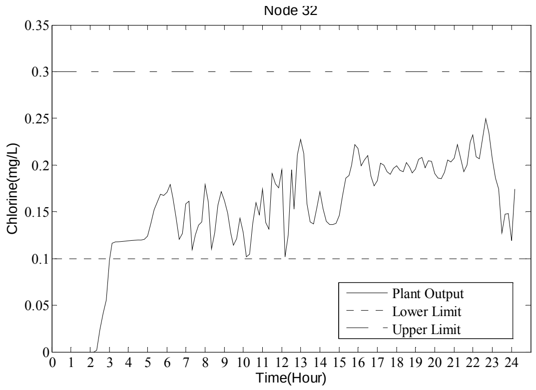

Fig. 8 The chlorine concentrations at monitored node under 9.5 hours of draining cycle

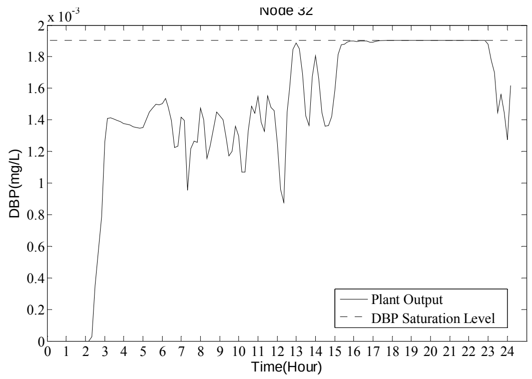

Fig. 9 DBP concentrations at monitored node under 9.5 hours of draining cycle

V. Conclusion and Future Work

The paper has developed the NMPC control of water quality in DWDS based on the advanced non-linear water quality dynamics model including DBPs objectives. The results illustrate a good and sustainable performance at LCL with the fast quality feedback. Moreover, an importance of the hydraulic support as the quality control input is demonstrated. Further development of the MPC controller with the DBP objectives is under current research to achieve its recursive robust feasibility.

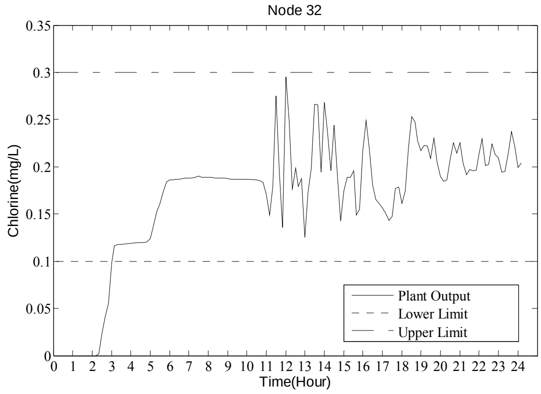

Fig. 10 The chlorine concentrations at monitored node obtained by MPC controller without considering DBP objective under 11 hours of draining cycle

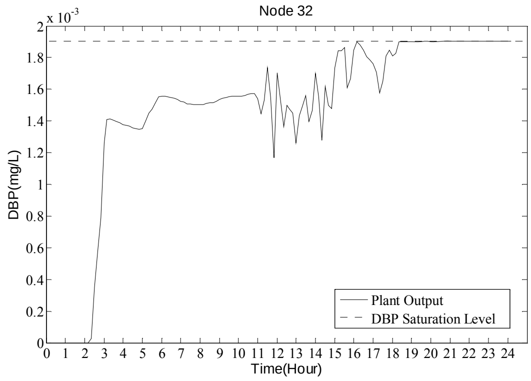

Fig. 11 DBP concentrations at monitored node obtained by MPC controller without considering DBP objective under 11 hours of draining cycle

TABLE I
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)

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