

A NEW APPROACH FOR WATER QUALITY NETWORK MODELLING

A CASE STUDY OF A REGIONAL CHLORAMINATED DISTRIBUTION SYSTEM

S Moradi, C WK Chow, D Cook, M Drikas, P Hayde, R Amal

ABSTRACT

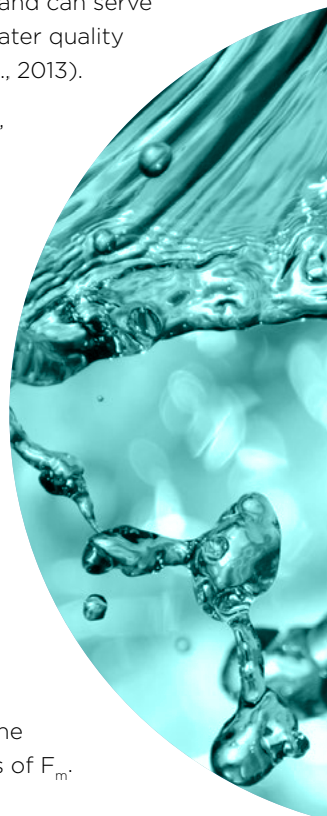
This study developed a new approach for water quality network modelling to enable estimation of monochloramine residual in real drinking water distribution systems using Bentley commercial hydraulic package (Water GEMS). The approach is based on using surrogate chemical and microbiological factors that affect chloramine decay rate. The model is based on an organic character (SUVA) as chemical factor, a laboratory measure of the microbiological decay of monochloramine (F_m) as microbiological factor, initial monochloramine concentration to the network, and hydraulic retention time (HRT) of the water samples through the distribution systems. The applicability of the proposed model for estimation of monochloramine residual was tested on a large regional chloraminated water distribution system in Australia through statistical test analysis between the experimental and estimated data. It was found that the developed model can recognise the nitrified locations in studied water distribution system, and therefore this modelling approach has the potential to be used by water treatment operators as a decision support tool in order to manage chloramine disinfection.

INTRODUCTION

Chloramine is commonly used as a disinfectant instead of chlorine to meet regulations regarding formation of disinfection by-products (DBPs) in drinking water, particularly in Australia and the USA (Krasner, 2009, Sarker et al., 2015, Sawade et al., 2016). The chloramine dose is crucial to ensure the water is safe to drink, but also needs to be considered based on taste and

odour problems arising from use of high chloramine doses. Maintaining a chloramine residual throughout the water distribution system is important in ensuring microbiologically safe water is supplied at the customer's tap (Fitzgerald et al., 2006). Modelling of disinfectant residual in treated water distribution systems is aimed at creating a better understanding of the effect of water quality on the disinfection consumption and can serve as a decision making tool for effective water quality control (Abdullah et al., 2009, Gnos et al., 2013).

In chloraminated drinking water systems, monochloramine decay occurs due to chemical and microbiological reactions (Sathasivan et al., 2005). To manage disinfection residuals in drinking water, it is important to discriminate between chemical and microbiological decay processes. Chemical factors affecting monochloramine decay include DOM measured as dissolved organic carbon (DOC) concentration, pH, nitrite, organic nitrogen compounds, chlorine to ammonia ratio and temperature (Zhang et al., 2010, Sathasivan et al., 2005, Cook, 2012). In addition, the presence of dead microbial cells and abiotic particles in water may also affect monochloramine decay. The impact of microbiological decay on monochloramine decay can be determined by the analysis of F_m .



This simple strategy involves comparing monochloramine decay rates in processed (0.2 μm membrane filtered) and unprocessed samples (Sathasivan et al., 2005). When considering the tools that operators might utilise to manage disinfection, models are potential options. Due to the complexity of the chloramine properties, surrogate parameters have been developed to predict its consumption and estimate its reactivity toward disinfection by products (DBPs) formation.

In order to simulate how chloramine behaves when it moves through the distribution system, Water Quality Network Models (WQNM) can be applied (Rossman, 1999). WQNM for water distribution systems use information such as flow and velocity provided by hydraulic models (Alexander and Boccelli, 2010, Propato and Uber, 2004). EPANET introduced a great enhancement in water quality modelling in the 1990s which extended water quality modelling applications for real and commercial distribution systems that can even be used nowadays (Rossman, 1999). To develop a hydraulic model, information such as the length, the diameter, and the roughness factors of the pipes in the system, the demand, as well as other specific information regarding tanks, valves and the pumps are required. After the model is constructed, it is necessary to calibrate the model correctly such that it closely reproduces the observed behaviour in the real system (Jiang et al., 2012, Shen and McBean, 2011, Walski et al., 2004). Modelling of disinfectant residual in treated water distribution systems is aimed at creating a better understanding of the effect of water quality on the disinfection consumption and can serve as a decision-making tool for effective water quality control.

The aim of this study was to develop a new WQNM for estimation of monochloramine residual based on chemical and microbiological factors that affect chloramine decay rate via nonlinear regression analysis method. The model is based on organic character and content as determined by specific UV absorbance (SUVA) which is the ratio of UV absorbance at 254nm to Dissolved Organic Carbon (DOC) concentration, microbiological decay factor (F_m) determined from laboratory chloramine decay test, initial monochloramine concentration to the network, and hydraulic retention time (HRT) of the water samples through the distribution systems. The applicability of the proposed model for estimation of chloramine residual was tested on a full scale water distribution system (Tailem Bend to Keith (TBK) water distribution system (WDS)) in Australia through statistical test analysis between the experimental and estimated data. This numerical approach for monochloramine residual estimation based on the water quality and dosing conditions can be considered as a pre-warning method to control disinfection dosing process in drinking water system. This modelling approach has the potential to be used by water treatment operators as a decision support tool in order to maintain and manage chloramine disinfection.

EXPERIMENTAL AND SIMULATION METHODS

Sampling locations

Water samples were collected at twelve different locations from the TBK WDS, Australia. TBK WDS is a long distribution system where the water is transferred up to several hundred kilometres, mostly in above ground pipes, to reach customers. Distribution system sampling sites focused on major tanks located at varying distances in the distribution system. The TBK water supply system is located approximately 80 km South East of Adelaide, Australia and extends from Tailem Bend to Keith, with branches to the Lower Lakes, Meningie and Karoonda. The water source for the TBK water supply system is the River Murray. Water drawn from the River Murray is treated at the Tailem Bend Water Treatment Plant. The TBK source water is treated by conventional treatment (coagulation / flocculation / sedimentation / filtration) followed by disinfection by UV and chloramination (Moradi et al., 2016). The treated water is stored in a Treated Water Tank before being pumped into the system. The description of sampling sites and their abbreviations are described in Table 1.



Table 1. The description of sampling sites, the averaged hydraulic retention times and averaged measured monochloramine residuals for two water supply patterns in sampling sites of TBK WDS.

site	Description	Abbreviation	Water supply pattern			
			Peak		Averaged	
			HRT (days)	Monochloramine residual (mg/L)	HRT (days)	Monochloramine residual (mg/L)
1	Water treatment plant	W.T.P	0.0	4.50	0.0	4.50
2	1.5km after chloramination	A.C	1.0	3.34	2.7	3.55
3	Coomandook Tank	C.T	2.5	3.00	5.6	3.28
4	Binnies Lookout Tank	B.L.T	4.0	2.71	8.5	3.12
5	Seymour Tank outlet	S.T	5.2	2.65	8.7	3.10
6	Meningie Tank	M.T	7.7	2.48	9.5	2.92
7	Wynarka Tank 1	W.T.1	8.0	2.45	12.7	2.88
8	Wynarka Tank 2	W.T.2	9.0	2.35	17.5	2.31
9	Sugarloaf Hill	S.H	11.2	1.94	18.0	2.10
10	Wingamin Tank	W.T	12.0	1.80	18.5	2.00
11	Keith customer tap	Ke.C.T	12.5	1.77	24.0	1.85
12	Karoonda customer tap	Ka.C.T	13.0	1.70	27.5	1.80

Model development

Electronic Geographic Information Systems (GIS) data was used to develop the hydraulic water network model of the TBK WDS in Bentley commercial hydraulic package (Water GEMS) (Figure 1). The tanks were incorporated into the model, and their locations were defined using the GIS information.

The Hydraulic Retention Time (HRTs) of water in a distribution system at different sampling locations (Table 1) can be determined from the hydraulic model.

To develop a WQNM into EPANET-MSX (Multi-Species Extension) which is a software tool recently added in Water GEMS, one approach can be based on complex decomposition reactions proposed by Vikesland et al. (2001) and Duirk et al. (2005). In this approach, all the reaction rates and equilibrium constants are at constant temperature of T=25°C. To develop a new approach for WQNM, the chloramine decay equations have to be applied in EPANET-MSX. Since a significant loss of chloramine happens in the first few minutes of contact time with NOM, chloramine decay was assumed to be described by the sum of two first-order equations, in which

the first part describes a rapid decay and the second simulates a slower decay.

$$(1) \frac{\partial C}{\partial t} = -k_1 \cdot x \cdot C - k_2 \cdot (1 - x) \cdot C$$



Figure 1. Taillem Bend to Keith Distribution System in Water GEMS

In this equation, k_1 and k_2 are rate constants for the fast and slow reactions, respectively. It is known that increasing the SUVA and F_m as chemical and microbiological effects may result in a greater monochloramine decay rate (Hua et al., 2015, Sathasivan et al., 2005). Therefore, it was assumed that the monochloramine demand after two days for water samples from TB WDS can be expressed by chemical (SUVA) and microbiological (F_m) parameters (Moradi et al., 2017). It is also assumed that the chemical and microbiological factors are increased with a constant rate over the time.

$$(2) \quad t \rightarrow 2 \Rightarrow C_{t=2\text{days}} = a \cdot F_m + b \cdot \text{SUVA} + c \cdot F_m \cdot \text{SUVA}$$

$$(3) \quad \frac{\partial[F_m]}{\partial t} = k$$

$$(4) \quad k_1 = -\frac{1}{2} \ln\left(\frac{a \cdot F_m + b \cdot \text{SUVA} + c \cdot F_m \cdot \text{SUVA}}{C_0}\right) - \frac{1}{2} \ln\left(\frac{1-x}{x}\right) - k_2$$

$$(5) \quad k_2 = -\frac{1}{\text{HRT}_{\max}} \ln\left(\frac{C_{\text{HRT}_{\max}}}{C_0}\right)$$

After calibrating the model parameters based on 70% of water samples from TBK WDS, all the aforementioned equations (Equations 1 to 5) were solved via a fifth order Runge-Kutta method with automatic time step control to estimate monochloramine residual through different sampling locations in the distribution system.

RESULTS AND DISCUSSION

The values of initial monochloramine residual, chemical, and microbiological parameters at some sampling locations were required to run the model. Table 2 presents the averaged value of water quality parameters for raw and treated (before disinfection) water samples from TBK water treatment plant.

A multi-response regression determinant criterion method was programmed in MATLAB 8.5 to calibrate the WQNM with optimal parameters that best matched simulations with the 70% of experimental data based on minimisation of the sum of the square of differences between the experimental data and the estimated values. The model parameters determined via nonlinear regression analysis based on 70% of water samples from TBK WDS that is sourced from Murray River are shown in Table 3.

Table 2. The averaged value of water quality parameters for raw and treated (before disinfection) water samples from TBK water treatment plant.

Variable	Unit	TBK water treatment plant	
		Raw water samples	Treated water samples before disinfection
Turbidity	NTU	120 ± 5	0.150 ± 0.1
Conductivity	µS/cm	480 ± 20	526 ± 20
Color	HU	55 ± 5	5 ± 1
UVA254	cm-1	0.477 ± 0.05	0.095 ± 0.03
DOC	mg/L	11.8 ± 0.2	5.25 ± 0.1
Fm	-	4.8 ± 0.2	0.67 ± 0.1

Table 3. Coefficients of the proposed water quality network model for monochloramine residual estimation for water samples from TBK WDS.

Model parameter	a	b	c	x	k
Tailem Bend WDS	1.62	0.40	-0.48	0.85	0.01

In order to check whether calculated model parameters (presented in Table 3) can estimate monochloramine residual in the network based on surrogate chemical and microbiological parameters for water samples from TBK WDS that were not included in parameter optimisation, the experimentally measured and estimated monochloramine residual at different HRTs, collected at summer 2014, from TBK WDS are compared (as shown in Figure 2).

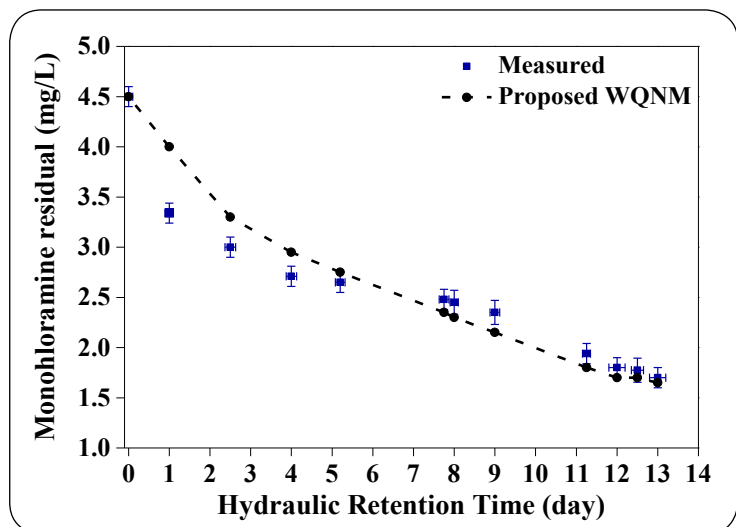


Figure 2. The measured, and the predicted chloramine residual according to developed new WQNM at different HRTs in Tailem Bend WDS in summer 2014.

As figure 2 shows, the new WQNM can estimate monochloramine residual at different sampling locations (with different HRTs) through the water distribution system, and the difference between measured and estimated monochloramine residuals is lower at sites with longer residence times. However, the WQNM which is based on monochloramine decomposition reactions can also estimate the monochloramine residual at different sampling locations within TBK WDS when the temperature would be around 25°C. It should be noted that in the new WQNM approach, the temperature effects have been taken into account indirectly via F_m value. In other words, the F_m value can reflect the effects of temperature in monochloramine residual estimation because its value would be higher during summer seasons (with higher temperature) than winter seasons due to the increased microbiological activities.

The main advantage for the proposed WQNM in comparison with the WQNM which is based on

monochloramine decomposition reactions are presented in Figure 3. Figure 3 represents how these two different approaches would estimate the monochloramine residual in a sampling location that experienced nitrification (Raukkan customer tap) in TB WDS during different months of the year with two different water supply patterns.

As it can be seen from Figure 3, since the microbiological effects have not been considered in the WQNM which is based on monochloramine decomposition reactions, the estimated monochloramine residual in nitrified locations would be higher compared to measured monochloramine residual in those sampling locations. On the contrary, the estimated monochloramine residuals in this sampling location via the new WQNM approach that considers the microbiological effects (F_m) are quite closer to the measured values. Therefore, it seems this approach can be helpful in recognition of nitrified locations within the water distribution systems.

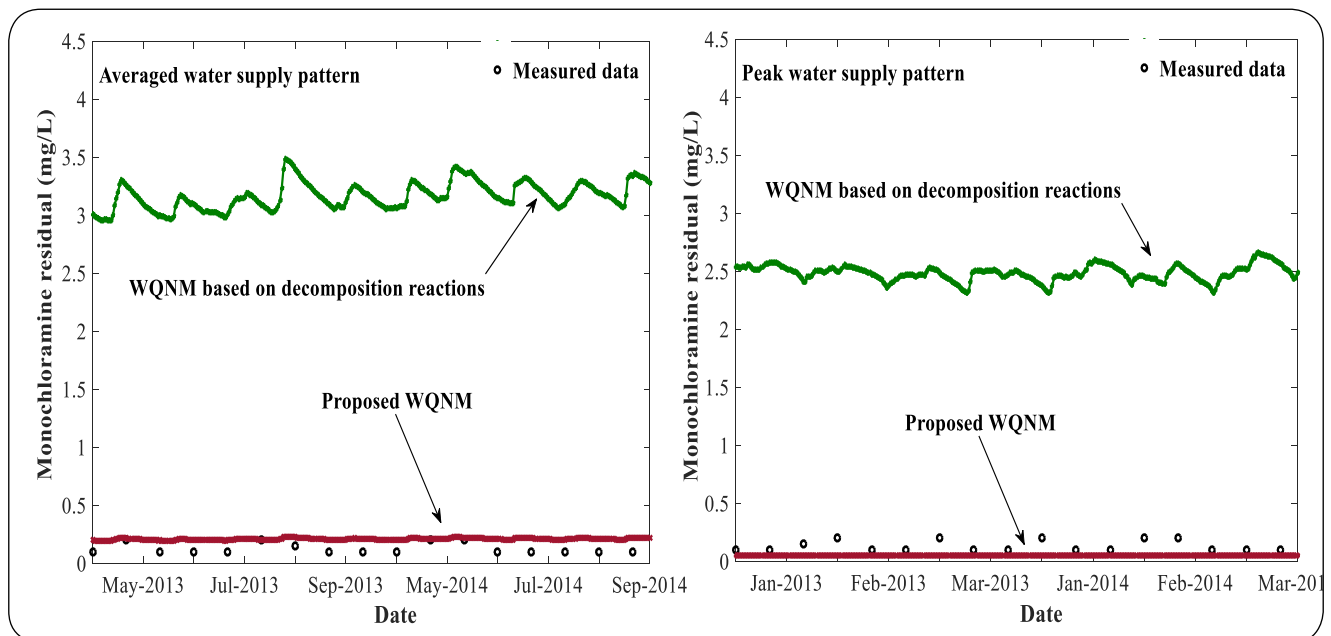


Figure 3. The measured, and the estimated monochloramine residual according to both proposed WQNM, and WQNM based on decomposition reactions for two different water supply patterns in 2013 and 2014 at Raukkan customer tap in Taillem Bend WDS.

CONCLUSION

This study was conducted to derive a new WQNM to estimate monochloramine residual using chemical and microbiological parameters that impact on chloramine decay rate. To test the validity and applicability of this model, new sets of data from TBK WDS in South Australia were analysed and compared to the estimated values. Validation results showed that there were no significant differences and the errors of prediction were low between the observed and the estimated data (Figures 2, and 3). In addition, the model could be used as a guide in decision making to choose the appropriate strategies to reduce monochloramine consumption and improve the disinfection process particularly to avoid nitrification. The proposed water quality network model has been implemented in one case study of a real operational water distribution system, Tailem Bend WDS in South Australia. Additional studies from other water distribution systems are warranted to confirm the applicability of the proposed model and model approach for other water samples.

ACKNOWLEDGMENTS

This research was supported under the Australian Research Council's Linkage Projects funding scheme (LP110100459). We gratefully acknowledge the provision of in-kind and financial support from the Australian Water Quality Centre (SA Water) for supplying water samples.

THE AUTHORS



Sina Moradi (email: s.moradi@unsw.edu.au) is a Postdoctoral Research Associate in the School of Chemical Engineering, Faculty of Engineering, University of New South Wales, Sydney, Australia. His research focus is on assessment and modeling of chloramine residual decay in drinking water distribution systems, and as part of his Ph.D. project, he derived a new water quality model to predict chloramine residual using chemical and microbiological parameters that affect chloramine decay rate. Sina received Best Presentation Award in 18th International Conference on Water Pollution and Treatment in London, UK on May 2016. He has been awarded the Hodgson Student award on November 2016 by the Australian Water Association.



Christopher W.K. Chow (email: christopher.chow@unisa.edu.au) is the Professor of Water Science and Engineering, School of Natural and Built Environments, University of South Australia. Chris obtained his M.App.Sc in environmental monitoring and PhD in analytical chemistry from UniSA in 1995 and worked as an industry researcher for over 20 years with SA Water. He has been involved in a number of major water treatment and distribution system related research projects. More recently he is working on data visualisation and data analytics using online monitoring systems to improve treatment plant performance.



David Cook (email: David.Cook@sawater.com.au) David is a Senior Scientist in the Water Science Team at SA Water Corporation. In his role, David has been investigating water quality issues associated drinking water treatment processes and distribution systems since 1997.



Mary Drikas is the Manager of the Water Science Team at SA Water Corporation. Mary has been leading research in water treatment processes for over 30 years.

Patrick Hayde (email: patrick.hayde@sawater.com.au) is manager for water in the Treatment and Network Planning team at SA Water. Patrick has more than 20 years of experience in water modelling, design and infrastructure planning.



Patrick Hayde (email: patrick.hayde@sawater.com.au) is manager for water in the Treatment and Network Planning team at SA Water. Patrick has more than 20 years of experience in water modelling, design and infrastructure planning.



Rose Amal (email: r.amal@unsw.edu.au) is an ARC laureate fellow and Scientia professor in the School of Chemical Engineering, University of New South Wales, Sydney, Australia.

REFERENCES

- ABDULLAH, M. P., YEE, L. F., ATA, S., ABDULLAH, A., ISHAK, B. & ABIDIN, K. N. Z. 2009. The study of interrelationship between raw water quality parameters, chlorine demand and the formation of disinfection by-products. *Physics and Chemistry of the Earth, Parts A/B/C*, 34, 806-811.
- ALEXANDER, M. T. & BOCCELLI, D. L. 2010. Field Verification of an Integrated Hydraulic and Multi-Species Water Quality Model. *Water Distribution Systems Analysis*.
- COOK, D. M., JIM AND MOBIUS, WERNER. 2012. Water treatment plant generation of rapid monochloramine decay. WDSA 2012: 14th Water Distribution Systems Analysis Conference. Adelaide, South Australia.
- DUIRK, S. E., GOMBERT, B., CROUE, J. P. & VALENTINE, R. L. 2005. Modeling monochloramine loss in the presence of natural organic matter. *Water Res.* 39, 3418-31.
- FITZGERALD, F., CHOW, C. & HOLMES, M. 2006. Disinfectant demand prediction using surrogate parameters—a tool to improve disinfection control. *Journal of Water Supply: Research and Technology—Aqua*, 55, 391-400.
- GNOS, G., CRUVEILLER, L., CHOW, C. W. K., FABRIS, R., HENDERSON, R. & MULCAHY, D. 2013. Kinetic modelling approach as a decision support tool for chloraminated distribution systems. *Journal of Water Supply: Research & Technology-AQUA*, 62, 255-267.
- HUA, G., RECKHOW, D. A. & ABUSALLOUT, I. 2015. Correlation between SUVA and DBP formation during chlorination and chloramination of NOM fractions from different sources. *Chemosphere*, 130, 82-89.
- JIANG, B., ZHANG, F., GAO, J. & ZHAO, H. 2012. Building a Water Distribution Network Hydraulic Model by Using WaterGEMS. ICPTT 2012. American Society of Civil Engineers.
- KRASNER, S. W. 2009. The formation and control of emerging disinfection by-products of health concern. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 367, 4077.
- MORADI, S., LIU, S., CHOW, C. W. K., LEEUWEN, J. V., COOK, D., DRIKAS, M. & AMAL, R. 2016. Developing a Chloramine Decay Index to understand nitrification: A case study of two chloraminated drinking water distribution systems. *Journal of Environmental Sciences*.
- PROPATO, M. & UBER, J. G. 2004. Vulnerability of Water Distribution Systems to Pathogen Intrusion: How Effective Is a Disinfectant Residual? *Environmental Science & Technology*, 38, 3713-3722.
- ROSSMAN, L. A. 1999. The EPANET Programmer's Toolkit for Analysis of Water Distribution Systems. WRPMD'99.
- SARKER, D. C., SATHASIVAN, A. & RITTMANN, B. E. 2015. Modelling combined effect of chloramine and copper on ammonia-oxidizing microbial activity using a biostability approach. *Water Research*, 84, 190-197.
- SATHASIVAN, A., FISHER, I. & KASTL, G. 2005. Simple Method for Quantifying Microbiologically Assisted Chloramine Decay in Drinking Water. *Environmental Science & Technology*, 39, 5407-5413.
- SAWADE, E., MONIS, P., COOK, D. & DRIKAS, M. 2016. Is nitrification the only cause of microbiologically induced chloramine decay? *Water Research*, 88, 904-911.
- SHEN, H. & MCBEAN, E. 2011. Hydraulic Calibration for a Small Water Distribution Network. *Water Distribution Systems Analysis 2010*. American Society of Civil Engineers.
- VIKESLAND, P. J., OZEKIN, K. & VALENTINE, R. L. 2001. Monochloramine Decay in Model and Distribution System Waters. *Water Research*, 35, 1766-1776.
- WALSKI, T. M., WU, Z. Y., ARNIELLA, E. F. & GIANELLA, E. 2004. Modeling for hydraulic capacity. *Journal / American Water Works Association*, 96, 104-106.
- ZHANG, Y.-J., ZHOU, L.-L., ZENG, G., SONG, Z.-G. & LI, G.-B. 2010. Factors affecting the formation of trihalomethanes in the presence of bromide during chloramination. *Journal of Zhejiang University SCIENCE A*, 11, 606-612.

