Environmental Engineering Research

Environ. Eng. Res 2009 December,14(4) : 244-249

Research Paper

DOI:10.4491/eer.2009.14.4.244
pISSN 1225-1025 eISSN 2005-968X

Design Optimization of an Ozone Contactor Using Ozone Contactor Model (OCM) Software

Dooil Kim, Chaeyoung Lee[1], Woohyeun Joe[2], and Seockheon Lee[†3]

Environmental Project Management Group, Civil and Environmental Division, POSCO E&C, Seoul, Korea
[1] *Department of Civil Engineering, The University of Suwon, Hwaseong, Korea*
[2] *Seoul Waterworks Research Institute, Seoul, Korea*
[†3] *Center for Environmental Technology Research, Korea Institute of Science and Technology, Seoul, Korea*

Received July, 2009 ; Accepted November, 2009

Abstract

Designing an ozone contactor is complicated because the residual ozone, log *C. parvum* inactivation, and bromate formation should be optimized with fluctuating water quality. *OCM* software was developed to assist a plant designer or an operator to fulfill the sophisticated optimization required in the design or operation of a new or an existing plant. In this article, numerical simulations were carried out using the *OCM* software for the design of a new ozone contactor under diverse design factors (i.e., three pHs, three temperatures, low and high dispersion numbers, and four and ten cells with complete mixing) with kinetic parameters obtained from the sand-filter effluent of a water treatment plant treating water from the Paldang impoundment. The results of the simulation suggested that a high residual ozone concentration at low pH and low temperature would be challenging, and PFR-like hydrodynamics could lower the residual ozone concentration. The inactivation of *C. parvum* oocysts increased at a lower pH. A lower dispersion number and more cell division increased the inactivation efficiency. Bromate was instantaneously formed during the initial ozonation stage. The effluent concentration was much lower than the regulatory levels imposed by the USEPA because of the low bromide level in raw water.

Keywords : Ozone contactor design, Residual ozone, Bromate, *C. parvum* oocyst, Numerical simulation

1. Introduction

Ozone treatment is known to be more effective at inactivating *C. parvum* oocyst than chlorine[1, 2]but is also known to produce disinfection by-products, such as bromate. Higher *C. parvum* inactivation accompanies stronger ozonation, which is favored for greater bromate formation.(3) Therefore, balancing *C. parvum* inactivation and bromate formation should be carefully considered at the design stage.(4) The design factors that have to be considered for an ozone contactor are pH, temperature, hydraulic retention time, dispersion number (*d*) and the number of cells,[5, 6)] which need to be carefully determined during the design stage. Pilot studies have often been employed to determine key design and operational parameters for new ozone contactors as well as to upgrade and optimize existing ozone treatment facilities.(7) Pilot studies; however, are often time-consuming and labor and cost intensive. In addition, extrapolating the pilot-scale results to the design of full-scale treatment facilities has not always been straightforward. As an alternative to pilot-scale studies, mathematical modeling and numerical simulation have been suggested by several researchers.[8, 9)] Sophisticated steady-state or dynamic computer models could greatly simplify the tasks of understanding the physical, chemical, and biological processes involved in ozonation processes.(10) The mathematical modeling might further allow a prediction of the reactor performances under a wide spectrum of configuration and operational scenarios.

The ozone contactor model (*OCM*) software was developed by the Georgia Institute of Technology via cooperation with the University of Illinois at Urbana-Champaign and the US Environmental Protection Agency to carry out sophisticated simulations in the design and operation of bubble-diffuser ozone contactors.(6) The software runs on Microsoft Windows®, with graphical user-friendly interfaces. It can simultaneously predict the steady-state residual ozone concentration, *C. parvum* oocyst inactivation and bromate formation in multi-chambered ozone contactors with bubble diffusers.(6) The results of the simulation are given as the profiles over an entire ozone contactor. The applicability of the *OCM* has been verified in the US by full-scale experiments with two existing ozone contactors.[6, 11)]

The mathematical equations within the *OCM* software were composed of four coupled second order differential equations at steady state, which expressed dissolved ozone, fast ozone demand, *C. parvum* oocyst inactivation and bromate formation. Details of each expression are shown in the reference.(6) Each mathematical expression was composed of dispersion, convection, and chemical reaction terms. Ozone decay and bromate formation were assumed to be first order with respect to ozone. Ozone demand was assumed to be second order with respect to ozone

---

[†] Corresponding author
E-mail: seocklee@kist.re.kr
Tel: +82-2-958-5954 , Fax: +82-2-958-6831

and its demand. Inactivation of *C. parvum* oocyst was assumed to follow a delayed Chick-Watson model. Bromate formation was assumed to be zero order with respect to ozone concentration. These equations were solved for each chamber, assuming closed vessel boundary conditions at each boundary between adjacent chambers. While the original *OCM* software targeted an ozone contactor with fine bubble diffusers (FBD), it was modified to cope with an ozone contactor with side-stream venturi injectors (SVI). The term expressing ozone mass transfer from the gas into the liquid phase was removed, with the target initial ozone concentration assigned by the boundary conditions.

The objectives of this article were to: 1) estimate the design and operational parameters of a new ozone contactor by predicting the residual ozone concentration, *C. parvum* oocyst inactivation and bromate formation at three pHs and three temperatures for a new full-scale ozone contactor; 2) evaluate alternative design options, such as the number of cell division and hydrodynamic conditions expressed in the dispersion number.

2. Experimental Methods

2.1. A water treatment plant

The processes of the targeted water treatment plant were composed of coagulation/ flocculation/ sedimentation, sand filtration and secondary disinfection, as shown in Figure 1. New ozone contactors and biological activated carbon filters were added to the water treatment plant. The primary target of ozonation was to remove taste and odor rather than inactivate *C. parvum* oocyst. The water treatment plant would have two ozone contactors, both with a design volume of 1,914 m^3 (18.0 m W × 18.2 m L × 6.0 m H). The design flow rate of each ozone contactor was 183,751 m^3/d. The mean hydraulic retention time was 15.4 min. Ozone was injected using a side stream venturi injector at the inlet of the ozone contactors.

2.2. Numerical Simulations

For the entire simulation, the inlet ozone concentration was fixed as 1.0 mg/L, which was the target ozone concentration in the design phase and maintained by the injection of ozone using a side stream venturi just before the ozone contactor. Table 1 summarizes the simulation scenarios used in this study. The kinetic parameters at three pHs (i.e., 6.0, 7.0 and 8.0) and three temperatures (i.e., 5, 15 and 25^{o}C) were obtained from the literature,[12] with raw water was taken from sand filter effluents of a water treatment plant treating raw water from the Paldang impoundment in Korea. *C. parvum* oocyst inactivation kinetics was based on the following Chick-Watson model:

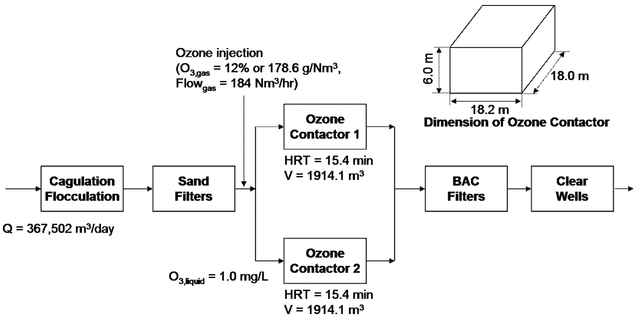

Figure. 1. A schematic diagram of the water treatment plant, with relevant dimensions and flow rates.

$$ln(N_t / N_0) = -KCt \qquad [1]$$

where N_t and N_0 are the numbers of viable *C. parvum* oocysts at times *t* and zero, respectively, and *C* the concentration of residual ozone. The second order mean inactivation kinetic constant, *K*, can be expressed by Equation [2] with respect to temperature, based on the information provided in the literature.[13]

$$K = 0.118 \times (1.10)^T \qquad [2]$$

This equation was proposed as the best fit to the experimental data, but did not include any safety factor. In contrast, the following equation used in this study estimated *K* within the 90 % confidence interval.[13]

$$K = 0.06 \times (1.10)^T \qquad [3]$$

The dispersion number (*d*) was varied from 0.1 and 10,000, which represent hydrodynamic conditions relatively close to PFR ($d = 0.1$) and CSTR (d = 10,000), respectively. The contactor was divided into either 4 or 10 cells to simulate the effect of cell division. The volumes of each cell division are shown in Table 2.

Table 1. Numerical simulation scenarios for a new ozone contactor.

Run ID	pH	Temperature (^{o}C)	Dispersion No. (d)	No. of cells
1	8.0	5, 15, 25	0.1	10
2	7.0	5, 15, 25	0.1	10
3	6.0	5, 15, 25	0.1	10
4	8.0	5, 15, 25	10,000	10
5	7.0	5, 15, 25	10,000	10
6	6.0	5, 15, 25	10,000	10
7	8.0	5, 15, 25	10,000	4
8	7.0	5, 15, 25	10,000	4
9	6.0	5, 15, 25	10,000	4

Table 2. The volumes of 10 cells (Run 1-6) and 4 cells (Run 7-9)

	10 cell	4 cell
	V (m^3)	V (m^3)
1	87	87
2	87	87
3	224	1570
4	224	87
5	224	-
6	224	-
7	224	-
8	224	-
9	224	-
10	87	-

3. Results and Discussions

Numerical simulations were carried out with the *OCM* software to estimate the performance of a new ozone contactor under nine scenarios, as shown in Table 1. Figures 2, 3 and 4 show representative simulation results for Runs 1, 4 and 7, respectively. Table 3 summarizes the overall simulation results for residual ozone, *C. parvum* oocyst and bromate formtion. Of particular concerns were the residual ozone and *C. parvum* oocyst inactivation, while the formation of bromate received less attention because the bromide concentration in the raw water was relatively low (i.e., *circa* 9.46 μg/l for the experiments of kinetics).[12)]

3.1. Residual Ozone Concentration

Controlling the residual ozone concentration is critical for successful contactor operation because residual ozone within the effluent may negatively influence subsequent unit processes. For example, residual ozone could cause irritant odor, corrosion and oxidation of activated carbon in the biological activated carbon filters. Especially, ozone contactors designed for the controls of taste and odor have a shorter residence time than those targeting the inactivation of *C. parvum* oocyst. Hence, these types of ozone contactor might not provide enough time to completely consume residual ozone, especially at low temperature and pH.

3.1.1. pH effect

The residual ozone concentration was strongly affected by pH, with the highest and lowest values at pH 6.0 and 8.0, respectively, among three pHs investigated, as shown in Figure 5. The simulation results suggested that an initial ozone concentration of 1 mg/L might result in a significantly high residual ozone concentration under most simulation conditions, except pH 8.0 and 25°C, which could be a challenge for the plant operation due to the aforementioned reasons. Increasing the pH would be preferred for low ozone concentrations within the effluent.

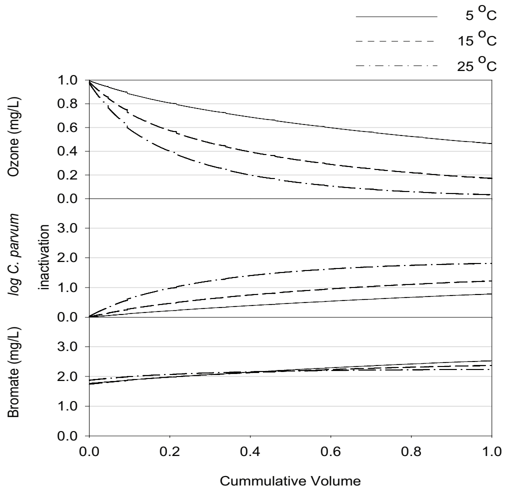

Figure. 2. Representative simulation results (pH 8.0, *d* = 0.1, 10 cells).

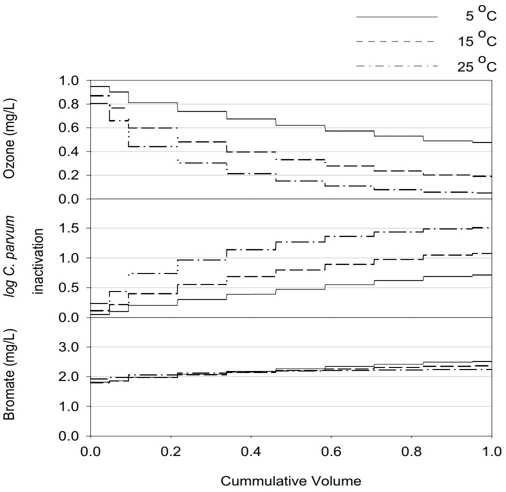

Figure. 3. Representative simulation results (pH 8.0, *d* = 10,000, 10 cells).

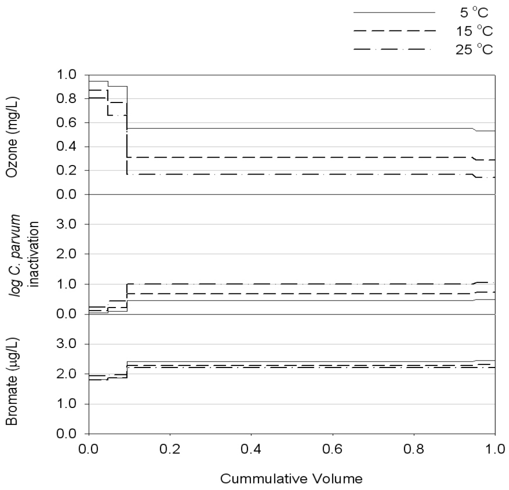

Figure. 4. Representative simulation results (pH 8.0, *d* = 10,000, 4 cells).

Figure 5 shows that the hydrodynamic conditions (i.e., degree of dispersion in ozone contactor) can affect the residual ozone concentration. When Runs 1-3 and 4-5, with a low and high dispersion numbers, respectively (i.e., d = 0.1, close to PFR and d = 10000, close to CSTR) were compared, the hydrodynamic conditions closer to PFR would result in a lower residual ozone concentration for all pHs and temperatures, although the difference was relatively minor compared to the effects of pH and temperature.

3.1.2. Number of Cells

Simulations were performed with ten (Runs 4-6) and four cells (Runs 7-9). Runs 4-9 were performed with the same dispersion number of 10,000. The simulation results suggested the effluent ozone concentration for Runs 4-6 (i.e., 10 cells) would be much lower than those for Runs 7-9 (i.e., 4 cells) especially at high temperature. The difference was smallest at 5°C and highest at 25°C. These results suggested that dividing the ozone contactor into a larger number of cells would be beneficial for lowering the residual ozone concentration within the effluent. Note: a greater number of cells results in overall contactor hydrodynamic conditions closer to PFR.

3.1.3. Summary

Residual ozone would be more problematic at low temperature and low pH. Hydrodynamic conditions might also play important role, especially with respect to division of the contactor using baffle walls. Decreasing dispersion number and increasing number of cell divisions could be beneficial for lowering the effluent residual ozone concentration, although there could be limited solution for low temperature seasons. Given a 1 mg/L ozone concentration in the influent to the ozone contactor, the simulation results suggested that it might be a challenge to control the residual ozone within the contactor effluent unless the addition of quenching agents, such as hydrogen peroxide, was considered. An alternative ozonation point (i.e., shift from post filtration to pre-filtration or pre-coagulation) could be considered. More natural organic matter before filtration process could promote ozone decay by promoting both hydroxyl radical chain reactions and direct oxidation. Additionally, better removals of both taste and odor could be expected due to the presence of abundant hydroxyl radicals.[3] However, ozonation before pre-filtration could be accompanied by excessive bubble formation in the sedimentation tanks or filters, which would be a trade-off.

3.2 *C. parvum* oocyst Inactivation

C. parvum oocyst inactivation is one of the primary objectives of the ozonation process in many water treatment utilities. pH, temperature, dispersion number and cell division within an ozone contactor can affect the *C. parvum* oocyst inactivation efficiency; therefore, the effects were analyzed using the *OCM* software in this article.

3.2.1. pH effect

The predicted *C. parvum* oocyst log inactivation increased at the lower pH, as shown in Figure 6. Since the kinetics of *C. parvum* oocyst inactivation are known to be almost independent on pH, a higher residual ozone concentration at lower pH would be preferred to enhance the efficiency. Note: the level of *C. parvum* oocyst inactivation is determined only by the degree of exposure to residual ozone, often expressed in terms of *CT* (ozone

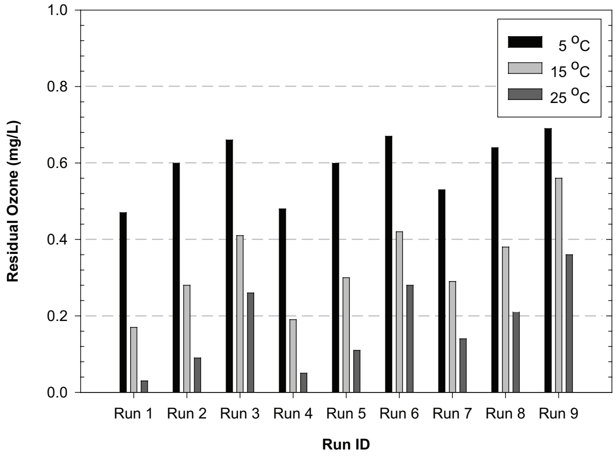

Figure. 5. Predicted residual ozone concentrations in the contactor effluent

Table 3. Simulated results of ozone, C. parvum oocyst inactivation and bromate for the final effluent of the ozone contactor.

		Residual Ozone (mg/l)	Log. C. parvum inactivation	Bromate (μg/L)
Run 1	5 °C	0.47	0.78	2.53
	15 °C	0.17	1.22	2.37
	25 °C	0.03	1.81	2.24
Run 2	5 °C	0.60	0.89	2.30
	15 °C	0.28	1.53	2.14
	25 °C	0.09	2.41	1.83
Run 3	5 °C	0.66	0.92	1.94
	15 °C	0.41	1.78	1.74
	25 °C	0.26	3.58	1.81
Run 4	5 °C	0.48	0.71	2.51
	15 °C	0.19	1.07	2.36
	25 °C	0.05	1.51	2.24
Run 5	5 °C	0.60	0.81	2.29
	15 °C	0.30	1.32	2.13
	25 °C	0.11	1.92	1.83
Run 6	5 °C	0.67	0.83	1.94
	15 °C	0.42	1.51	1.74
	25 °C	0.28	2.68	1.81
Run 7	5 °C	0.53	0.49	2.43
	15 °C	0.29	0.72	2.30
	25 °C	0.14	1.05	2.21
Run 8	5 °C	0.64	0.54	2.22
	15 °C	0.38	0.82	2.05
	25 °C	0.21	1.21	1.79
Run 9	5 °C	0.69	0.56	1.93
	15 °C	0.56	0.97	1.75
	25 °C	0.36	1.46	1.80

concentration × contact time).

3.2.2. Temperature effect

The kinetics of *C. parvum* oocyst inactivation was strongly affected by temperature. Accordingly, as the temperature decreased, the predicted inactivation efficiency dramatically decreased during all Runs. It is noteworthy that the level of inactivation at 5°C was quite low, which might raise an issue in relation to the effectiveness of ozone disinfection during winter. Increasing the initial ozone concentration could be an appropriate solution for enhancing the inactivation, but could also induce the problem of elevated residual ozone within the effluent. These were caused because this contactor was targeting not *C. parvum* oocyst, but taste and odor (i.e., shorter HRT). In case where higher inactivation is the aim, it seems inevitable that an extended ozonation time longer than 15.4 minutes should be considered at the design flow rate used.

3.2.3. Dispersion Effect

Figure 6 shows that the effect of the hydrodynamic conditions on *C. parvum* oocyst inactivation was more apparent than that of the residual ozone concentration. Simulation Runs 1-3 and Runs 4-5 were performed with dispersion numbers of 0.1 and 10,000, respectively. The simulation results showed that a hydrodynamic condition close to PFR ($d = 0.1$) resulted in much higher levels of inactivation at all pHs and temperatures than the condition close to CSTR ($d = 10{,}000$). These results were consistent with previous observations found in the literature,[6)] suggesting that designing a contactor hydrodynamic condition close to plug flow (i.e. smaller dispersion number) was favorable to achieve higher inactivation efficiency of *C. parvum* oocyst for the same amount of ozone input.

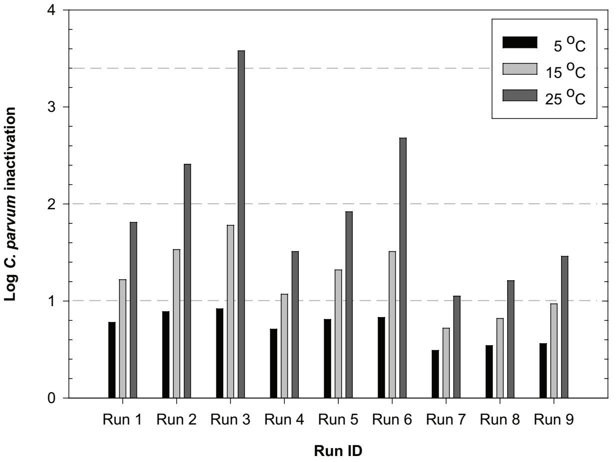

Figure 6. Predicted log *C. parvum* oocyst inactivation in the contactor effluent

3.2.4. Number of Cells

As described previously, simulation Runs 4-6 were performed with ten cells and Runs 7-9 with four. All the simulations were performed assuming the same dispersion number of 10,000. The predicted inactivation efficiencies were much higher for Runs 7-9 than Runs 4-6, which was ascribed to the lower dispersion number with more cells. The estimated dispersion numbers (d) were 0.048 and 0.111 for ten and four cells, respectively, assuming that all cells are CSTRs. These results suggested that designing the overall contactor with an increased cell division might be beneficial for enhancing the inactivation efficiency.

3.2.5. Summary

Increasing the number of cells in the ozone contactor, or lowering the dispersion number (d) in each cell, have been recommended to increase the efficiency of *C. parvum* oocyst inactivation. Low pH was favored for achieving higher inactivation efficiency due to increases in the residual ozone concentration. However, higher inactivation efficiency and higher residual ozone issues with the effluent could be a trade-off. Achieving an adequate level of *C. parvum* oocyst inactivation at lower temperatures might be challenging for this specific ozone contactor because this plant was primarily designed for controlling taste and odor and; therefore, has a short HRT.

3.3. Bromate Formation

The simulation results shown in Figures 2, 3 and 4 suggest that bromate might be rapidly formed during the initial stage of ozonation for all the scenarios investigated, which was consistent with the observation at the batch tests.[12)] The predicted overall effluent bromate concentrations were less than 3 μg/L, as shown in Figure 7, which were much lower than the current maximum contamination level (MCL) of 10 μg/L imposed by the USEPA. These results suggested that bromate formation during ozonation might not be a concern for the new ozone contactor.

More bromate was produced at the lower temperature in these simulations, although the conversion kinetics was faster at the higher temperature.[12)] This was ascribed to some of the bromate being formed from direct reaction with bromide and ozone molecules. Note: the residual ozone concentration was higher at low temperature. More bromate was produced at higher pH because more OH radicals and hypobromite (OBr^-) were formed, with the latter being a key intermediate of bromate formation. A lower dispersion number and larger number of cells negligibly contributed to bromate formation. These suggested that efforts to decrease the dispersion number or increase the number of cell could be beneficial for *C. parvum* inactivation and reducing the residual ozone, with negligible increase in the bromate concentration.

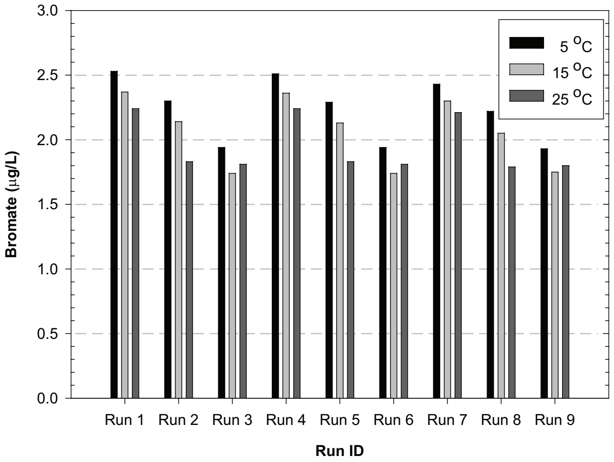

Figure. 7. Predicted bromate concentration in the contactor effluent

4. Conclusions

The residual ozone concentrations within the effluent were influenced by pH, temperature, dispersion number and the number of cells. Minimizing the effluent ozone concentration to less than the allowed level was challenging in most simulations. Hence, decreasing the initial ozone concentration, using a quenching agent and by shifting the ozonation point should be considered in the design. The efficiency of *C. parvum* oocyst inactivation would be strongly affected by pH and temperature. The adequate control of *C. parvum* oocyst might become significantly challenging, especially during low temperature periods. Design of the overall reactor hydrodynamic conditions closer to PFR, by dividing the contactor into more cells or reducing the dispersion number of the cells, might be advantageous for achieving higher inactivation efficiency. The predicted bromate concentration in the contactor effluent was negligible. Therefore, as long as the bromide level in the raw water does not significantly increase, the formation of bromate might not provoke any regulatory issues for the new ozone contactor.

5.References

1. Rennecker, J. L., Kim, J. H., Corona-Vasquez, B., Mariñas, B. J., "Role of disinfectant concentration and pH in the inactivation kinetics of Cryptosporidium parvum oocysts with ozone and monochloramine," *Environmental Science & Technology*, **35**, 2752-2757 (2001).
2. Gürek, L. L., Finch, G. R., Belosevic, M., "Modeling chlorine inactivation requirements of Cryptosporidium parvum oocysts," *Journal of Environmental Engineering-ASCE*, **123** (9), 865-875 (1997).
3. von Gunten, U., Hoigné, J., "Bromate formation during ozonation of bromide-containing waters - Interaction of ozone and hydroxyl radical reactions," *Environmental Science & Technology*, **28** (7), 1234-1242 (1994).
4. Kim, J. H., von Gunten, U., Mariñas, B. J., "Simultaneous prediction of Cryptosporidium parvum oocyst inactivation and bromate formation during ozonation of synthetic waters," *Environmental Science & Technology*, **38** (7), 2232-2241 (2004).
5. Finch, G. R., Haas, C. N., Oppenheimer, J. A., Gordon, G., Trussell, R. R., "Design criteria for inactivation of Cryptosporidium by ozone in drinking water," *Ozone-Science & Engineering*, **23** (4), 259-284 (2001).
6. Kim, D. I., Hasan, S., Tang, G., Mariñas, B. J., Couillard, L., Shijkairy, H., Kim, J. H., "Simultaneous simulation of pathogen inactivation and bromate formation in full-scale ozone contactors by computer software", *Journal American Water Works Association*, **99** (8), 77-91 (2007).
7. Huang, T., Brouckaert, C. J., Docrat, M., Pryor, M., "A computational fluid dynamic and experimental study of an ozone contactor," *Water Science and Technology*, **46** (9), 87-93 (2002).
8. Kim, J. H., Elovitz, M. S., von Gunten, U., Shukairy, H. M., Mariñas, B. J., "Modeling Cryptosporidium parvum oocyst inactivation and bromate in a flow-through ozone contactor treating natural water," *Water Research*, **41** (2), 467-475 (2007).
9. Huang, T. H., Brouckaert, C. J., Pryor, M., Buckley, C. A., "Application of computational fluid dynamics modelling to an ozone contactor," *Water SA*, **30** (1), 51-56 (2004).
10. Do-Quang, Z., Roustan, M., Duguet, J. P., "Mathematical modeling of theoretical Cryptosporidium inactivation in full-scale ozonation reactors," *Ozone-Science & Engineering*, **22** (1), 99-111 (2000).
11. Tang, G., Adu-Sarkodie, K., Kim, D., Kim, J. H., Teefy, S., Shukairy, H. M., Mariñas, B. J., "Modeling Cryptosporidium parvum oocyst inactivation and bromate formation in a full-scale ozone contactor," *Environmental Science & Technology*, 39 (23), 9343-9350 (2005).
12. Kim, D. I., "Development and application of integrated ozone contactor design and optimization tools," Ph.D. Thesis, Atlanta, Georgia Institute of Technology (2007).
13. Clark, R. M., Sivagenesan, M., Rice, E. W., Chen, J., "Development of a CT equation for the inactivation of Cryptosporidium oocysts with ozone," *Water Research*, 36 (12), 3141-3149 (2002).