A comparison of the Eulerian and particle tracking approaches for prediction of ozone contactor performance

Jianping Zhang, Peter M. Huck, Gordon D. Stubley and William B. Anderson

ABSTRACT

The Eulerian and particle tracking approaches, two commonly utilized numerical methods, were evaluated for modelling drinking water ozone disinfection systems. The Eulerian approach predicts disinfection performance by solving an advection-diffusion equation. Alternatively, the particle tracking (Lagrangian) approach calculates disinfection efficiency by numerically introducing particles into the flow and predicting their trajectories through a spatially varying field of ozone residuals. The two approaches were used for modelling two hypothetical ozone reactors and a full-scale operating ozone contactor. For ozone reactors with plug flow characteristics, the two approaches match well in evaluating disinfection efficiency (represented by the CT value). For reactors with non-ideal hydraulic performance, the particle tracking model predicted slightly lower CT values than did the Eulerian approach. This may be due to the trapping of particles in the dead zones of non-ideal reactors, and the limitation on the particle numbers that could be used for data processing. The results of a full-scale contactor study further confirmed these observations. The study also found that the effect of particle size (1–100 μm) used in this study on the particle tracking method was negligible. The Schmidt number has minor impacts on the Eulerian approach modelling results.

Key words | computational fluid dynamics, disinfection, Eulerian approach, ozone contactor, particle tracking approach

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INTRODUCTION

The use of an advanced modelling tool, computational fluid dynamics (CFD), has increasingly been applied for the simulation of various disinfection processes, including chlorination, UV irradiation, and ozonation (Do-Quang *et al*. 1999; Lyn & Chiu 1999; Greene 2002; Ta & Hague 2004; Templeton *et al*. 2006; Zhang *et al*. 2008). With a CFD modelling approach, the velocity field, residence time distribution (RTD), and disinfectant profiles can be obtained by numerical solution of the Reynolds-averaged Navier–Stokes and species transport equations (Zhang 2007).

CFD modelling has also been employed for directly predicting disinfection treatment efficiency (Do-Quang *et al*. 2002; Greene 2002; Mofidi *et al*. 2004; Ducoste *et al*. 2005). In general, two approaches have been used to model microbial inactivation processes: one is the Eulerian approach and the other is the particle tracking approach (also called the Lagrangian approach). In the Eulerian approach, the spatial distribution of viable microorganisms in a reactor is viewed as a continuous field, similar to that of a dissolved species. The concentration of microorganisms inside the reactor is expressed as a function of spatial coordinates and simulated by solving the species advection-diffusion transport equations with appropriate source terms (Do-Quang *et al*. 1999; Lyn & Chiu 1999). In a particle tracking approach, microorganisms are viewed as discrete particles and the motion of an individual microorganism is independent of others. The probable trajectory of each particle is calculated by solving the particle's equations of motion, assuming a

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known turbulent fluid velocity field. The inactivation efficiencies of microorganisms are then determined by incorporating microbial inactivation kinetics along each microorganism's trajectory through the reactor (Downey *et al.* 1998; Chiu *et al.* 1999).

Several studies had been done to evaluate the Eulerian and Lagrangian approaches in simulating UV drinking water disinfection systems (Chiu *et al.* 1999; Ducoste *et al.* 2005; Lyn & Blatchley 2005). Most of the results have shown that the two modelling approaches agree reasonably closely, although the Eulerian approach predicted slightly higher disinfection efficiency than the particle tracking method. However, to date, most of the previous ozone reactor modelling studies have been based on the Eulerian approach. The use of the particle tracking approach is very limited. There therefore is a need to thoroughly investigate the applicability of these two approaches.

In this study, both the particle tracking and Eulerian approaches were used to investigate different ozone reactors: two hypothetical reactors and one full-scale contactor. Specifically, the objective was to compare these two CFD approaches at different conditions for modelling the tracer RTD and characterizing ozone disinfection performance.

MATERIALS AND METHODS

Numerical methods

Flow equations

A two phase, three-dimensional (3D) CFD model has been developed by the authors to describe ozonation processes (Zhang *et al.* 2007). The hydrodynamics of ozone contactors were based on continuity and momentum balance equations for the two phases: water and gaseous ozone. The impact of turbulence on ozone contactor hydrodynamics was modelled in both phases. For the liquid phase, the standard k-ϵ model was used (Launder & Spalding 1974). The turbulence of the dispersed gas phase was modelled using a Dispersed Phase Zero Equation model and bubble-induced turbulence was taken into account as per Sato & Sekoguchi (1975).

To model ozone transport and associated reactions, ozone decomposition kinetics and mass transfer kinetics sub-models were included in the form of species transport equations. The general form of the transport equations is as below:

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha \varphi_\alpha) + \nabla \bullet (r_\alpha U_\alpha \rho_\alpha \varphi_\alpha) - \nabla \left(r_\alpha \left(\rho_\alpha D_\alpha^{(\varphi)} + \frac{\mu_{t\alpha}}{Sc_{t\alpha}}\right) \nabla \varphi_\alpha\right) = S_\alpha^{(\Phi)} \quad (1)$$

where φ_α is the concentration of the species per unit mass of phase α, r_α is the volume fraction of each phase, U_α is the flow velocity, ρ is the density of flow, $D_\alpha^{(\varphi)}$ is the kinematic diffusivity for the species in phase α, $Sc_{t\alpha}$ is the turbulent Schmidt number, $S_\alpha^{(\Phi)}$ is the source term for a species transport equation.

The species transport equations and the water quality-dependent source terms used for modelling ozone decomposition and ozone transfer have been described in detail by Zhang *et al.* (2007) and Zhang (2007).

CFD-based CT

A common approach for determining ozone disinfection efficiency involves the application of a C×T concept [C is the ozone residual concentration in the contactor at time (T)] (USEPA 1991). For a full-scale ozone contactor, C is usually defined as the ozone residual concentration at the outlet of a chamber and T is the residence time of microorganisms in the chamber. For T, the USEPA employs a conservative residence time T_{10} which is the residence time of the first 10% of the water (assumed to be the same as the first 10% of the microorganisms) to travel from the contactor inlet to outlet, to ensure a minimum exposure time for 90% of the water and microorganisms entering a disinfection contactor (USEPA 1991; Chen 1998). Because of the existence of dead zones and short circuiting in full-scale ozone contactors, microorganisms that enter the contactor at the same time may encounter significantly different pathways in the contactor. Therefore, using a single residence time T_{10} may result in the inaccurate prediction of contactor hydraulic performance. In addition, ozone residuals may also vary substantially in a contactor, suggesting that a single ozone residual value will not be able to characterize ozone distribution within a given contactor.

The subsequently developed integrated disinfection design framework (IDDF) is a more sophisticated approach for designing ozonation processes (Bellamy *et al.* 1998). The IDDF approach employs the tracer RTD together with a disinfectant decay kinetic model to predict disinfection efficiency in a chemical disinfection process. However, the use of the RTD ignores the complex 3D flow behaviour within a contactor. Additionally, the IDDF approach makes the assumption that fluids in the disinfection contactor are completely segregated. This assumption may over- or under-estimate disinfection efficiency (Greene 2002). Therefore, there is a need to develop a more accurate approach to contribute to the design and operation of ozone disinfection processes.

To accurately predict ozone disinfection efficiency, a CFD-based CT concept is introduced in the present study which is defined as the accumulated ozone exposure ($\int Cdt$) for all pathogens passing through an ozone reactor. This concept considers 3D variations of ozone profiles inside ozone contactors and the differences in residence time of the microorganisms. Such a CFD-based CT value can be modelled by the Eulerian or Lagrangian approaches.

Eulerian modelling approach

In the Eulerian modelling approach, the flow conservation equations were solved to steady state conditions. The steady state flow fields were then 'frozen' and the species transport equations for the dissolved ozone, chemical tracer, and CT were solved. The source term of the CT transport equation was derived as follows.

When a parcel of liquid fluid flows from the inlet to the outlet of a contactor, the cumulative ozone exposure as a function of time is defined as:

$$\mathrm{CT} \equiv \int_{t_{\mathrm{inlet}}}^{t_{\mathrm{outlet}}} C_{l,\mathrm{parcel}} dt \tag{2}$$

It then follows that

$$\frac{d(\mathrm{CT})}{dt} \equiv C_{\mathrm{l,parcel}} \tag{3}$$

At any instant in time of the parcel's travel from inlet to outlet, the total derivative $d(\mathrm{CT})/dt$ is defined as:

$$\frac{d(CT)}{dt} = \frac{\partial}{\partial t}\mathrm{CT} + u_i \frac{\partial}{\partial x_i}\mathrm{CT} \tag{4}$$

Combining the above two equations, and multiplying the result by the liquid phase volume fraction, r_l, gives the transport equation for ozone exposure (CT). As with other additional variable equations, the effects of turbulent diffusion should also be included, thus the final form of the CT transport equation is given as:

$$\frac{\partial}{\partial t}(r_l\mathrm{CT}) + \nabla \bullet (r_l U_l \mathrm{CT}) - \nabla\left(r_l\left(\frac{\mu_{tl}}{\rho_l \mathrm{Sc}}\right)\nabla \mathrm{CT}\right) = r_l C_l \tag{5}$$

As such, the source term for CT was defined as:

$$S_{\mathrm{CT}} = r_l C_l \tag{6}$$

where r_l is the volume fraction of water. In most cases, r_l is close to 1, therefore:

$$S_{\mathrm{CT}} = C_l \tag{7}$$

For a continuous flow system, the mass flow rate weighted average CT value at the outlet of a contactor was determined by:

$$\overline{CT}_{\mathrm{outlet}} = \frac{\int \mathrm{CT}dm}{\int dm} \tag{8}$$

where m is the local mass flow at the outlet of the contactor.

Particle tracking modelling approach

In the particle tracking approach, the flow conservation equations and chemical species transport equations were solved first to obtain steady state solutions. The microorganisms were then treated as discrete particles where their trajectories were tracked simultaneously in 3D space and with time by solving Newton's law of motion, with drag and added mass forces being accounted for in the simulations.

Newton's second law:

$$m_p \frac{dv_p}{dt} = F_{\mathrm{All}} = F_D + F_B + F_{\mathrm{VM}} \tag{9}$$

where m_p is the particle mass, v_p is the particle velocity, F_{All} is the sum of forces acting on a particle, F_D is the drag force acting on the particle, F_B is the buoyancy force due to gravity, and F_{VM} is the virtual (or added) mass force. This is the force to accelerate the virtual mass of the fluid in the volume occupied by the particle.

The buoyancy force and the virtual mass force are less important for this study because the density of the pathogen particles is close to that of water and the particle sizes are very small (1–100 μm). The drag force between flow and particles is the major force being considered and is modelled as:

$$F_D = \frac{1}{2}\rho C_D A_F |U_s| U_s \tag{10}$$

where ρ is the density in the continuum, A_F is the effective particle cross section area, U_s is the slip velocity between the particle and the surrounding fluid and C_D is a drag coefficient. In the present study, C_D is given by the Schiller-Naumann Drag model (Ansys 2005).

In fluids, the random motion of fluid elements (eddies) imparts a continuous random motion to suspended particles. Repeated eddy interactions cause the particles to disperse over time. In the present study, the effect of turbulent dispersion is included within the particle transport model using the classical stochastic approach of Gosman & Ioannides (1983). It is assumed that a particle is always within a single turbulent eddy before entering another eddy. The characteristic fluctuating velocity v_f', the eddy lifetime τ_e and the eddy length l_e are calculated based on the following equations (Ducoste *et al.* 2005):

$$v_f' = \Gamma \left(\frac{2k}{3}\right)^{0.5} \tag{11}$$

$$l_e = \frac{C_\mu^{3/4} k^{3/2}}{\varepsilon} \tag{12}$$

$$\tau_e = \frac{l_e}{(2k/3)^{1/2}} \tag{13}$$

where k and ε are the local turbulent kinetic energy and dissipation, and C_μ is a turbulence constant. The variable Γ is a normally distributed random number which accounts for the randomness of turbulence about a mean value.

It should be noted that the turbulence time and length scales in Equations (12) and (13) are of the same order of magnitude as the corresponding turbulent scales used for describing turbulent diffusion in the Eulerian modelling approach (Zhang 2007). Therefore, the two approaches are consistent in theory, although they are not identical in describing the impacts of turbulence on particle behaviour in a fluid (Gosman & Ioannides 1983; Lyn & Blatchley 2005). The k and ε values used in both approaches are obtained by solving the liquid phase turbulent model (i.e. k-ε model in this study), thus the turbulent model affects the above two approaches in the same way.

The sizes of the neutrally discrete particles used in this study were between 1 and 100 μm, which encompass the size range of pathogenic protozoa in water (MWH 2005). For each particle size, the particles were uniformly injected into the contactor from the inlet in a very short period of time (i.e. 0.1 s). The particle trajectories were obtained through a transient particle tracking solution.

Since the particles were injected simultaneously at the contactor inlet but exited the contactor at different times and at different particle number rates, the average CT was used to represent ozone contactor disinfection performance. First, the CT for each particle trajectory was calculated by the integration of ozone concentration and particle tracking times along the particle trajectory. Then, the average CT value at the outlet of a contactor was determined by the following equation:

$$\overline{CT}_{\mathrm{outlet}} = \frac{\sum (CT)_i E_{pi} \Delta t}{\sum E_{pi} \Delta t} \tag{14}$$

where $(CT)_i$ is the accumulated CT along the ith particle trajectory, E_{pi} is the number rate of the particles that receive the ozone dose $(CT)_i$, Δt is the time period over which these particles exit the contactor outlet.

The procedures for calculating CT via the Eulerian and Particle tracking approaches are summarized in Figure 1.

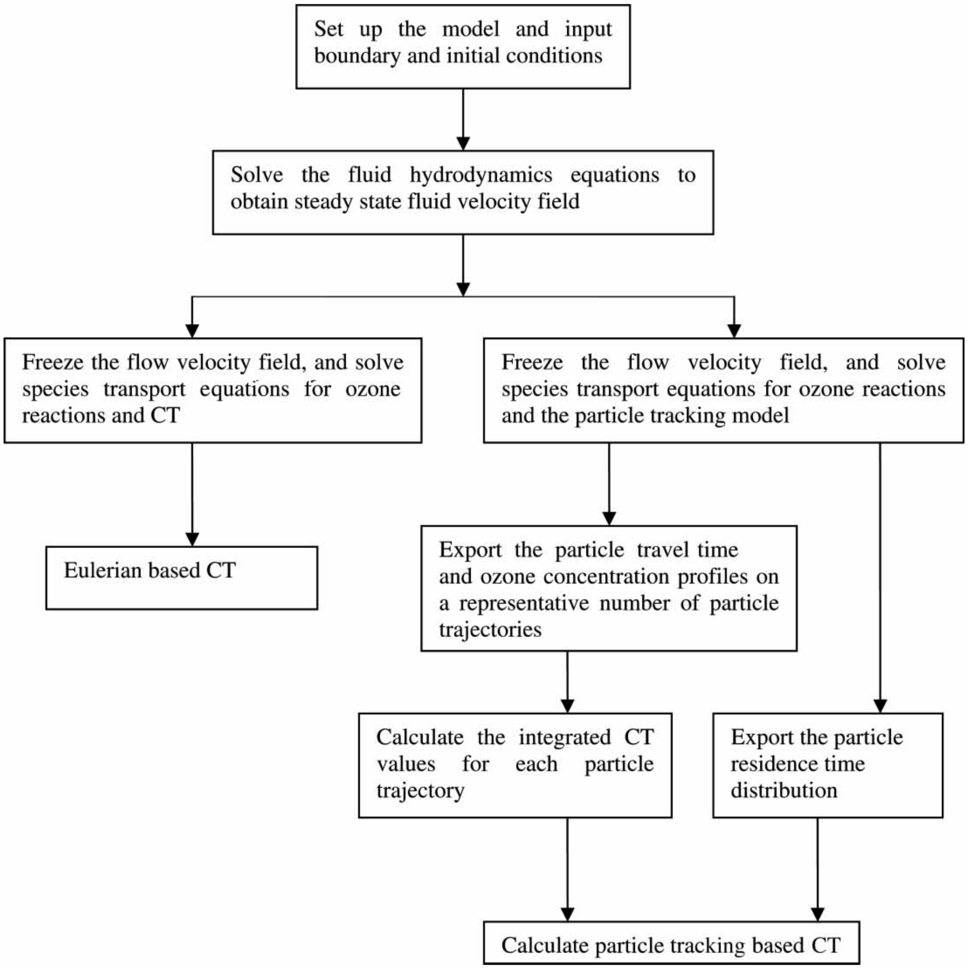

Figure 1 | Procedures for predicting CT through the Eulerian and particle tracking approaches.

Description of case studies

Verification case study

Two hypothetical ozone reactor configurations were used to examine the difference between the Eulerian and particle tracking approaches, and to study the impact of flow patterns on the CT distributions. Figure 2 presents the geometries. Both reactor geometries are two-dimensional and neither geometry represents a particular type of ozone reactor. Both geometries were meshed with a hybrid triangular-quadrilateral mesh. The numbers of the mesh elements for the two reactors were 10,564 and 19,376 respectively. To simplify the analysis, both systems were assumed to be single phase reactors. Both dissolved ozone and influent water were assumed to enter the systems from the reactor inlets. The inlet velocity of the water was set to be 0.186 m/s and the influent dissolved ozone was assumed to be 2 mg/L. The instantaneous ozone demand of influent water and ozone decay kinetics constant were set as 0 mg/L and 0.05 min^{-1}.

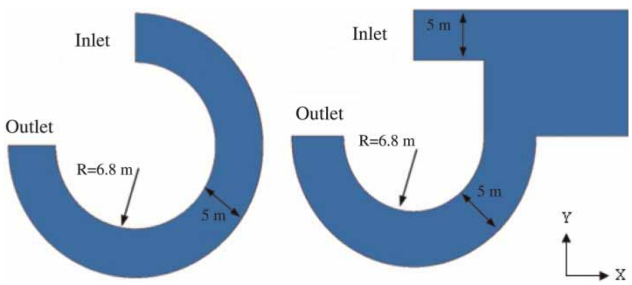

Figure 2 | Geometries of two hypothetical ozone reactors.

These are reasonable values for ozone systems, and the overall conclusions would not be expected to be sensitive to the values chosen.

In all the simulations, second-order discretisation of the governing equations was applied and the simulations were considered to be converged when the root mean square normalised residuals for all the equations were less than 10^{-4} and the global conservation imbalance of each species was less than 0.1%.

In the particle tracking model, three different sizes of particles (1, 10 and 100 μm) were injected individually at the reactor inlets over a period of 0.1 s. The number of each type of injected particles was set as 5,000 to provide sufficient modelling accuracy even though injecting lower numbers of particles (3,000) generates almost identical modelling results in terms of CT and particle RTD prediction. CT values were calculated from the particle trajectory histories as summarized in Figure 1.

Full-scale ozone contactor study

A full-scale case study was performed for ozone contactors located at the DesBaillets Water Treatment Plant (WTP) in Montreal, Canada, which has a capacity of 1,200 million litres per day. The St. Lawrence River is used as source water. The raw water is treated by filtration and ozonation, followed by chlorination before entering the distribution system. The DesBaillets WTP has six parallel ozone contactors each with 2 cells and ozone gas is fed in the first cell of each contactor through 126 porous fine bubble diffusers. The total length, width, and height of each contactor is 23.8, 5.50 and 7.16 m, respectively. Figure 3 shows the geometry of a DesBaillets ozone contactor. A 3D CFD model was developed; unstructured tetrahedral grids were generated and were refined in regions close to the gas diffusers and baffles. The total element number was about 420,000.

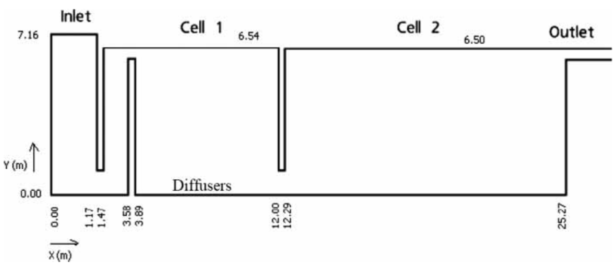

Figure 3 | Geometry of a DesBaillets WTP ozone contactor.

The system was modelled as a multiphase reactor. Based on the common range of ozone system operational parameters in the DesBaillets WTP, the inlet velocity of the water and the velocity of the gas at the diffuser surfaces were set at 0.186 and 0.022 m/s, respectively. The concentration of ozone in the gas was 1.4% by weight. For both the Eulerian and Particle Tracking approaches, the ozone contactor was modelled using the same procedures as for modelling the hypothetical ozone reactors. For Particle Tracking modelling, three different sizes of particles (1, 10 and 100 μm) were injected individually at the ozone contactor inlets over a period of 0.1 s. By trial and error, the number of each type of injected particles was determined to be 5,000, which is small enough to reduce computational time but is sufficient to provide accurate modelling results. For instance, the average residence times predicted by using 5,000 and 10,000 particles differ less than 1%.

RESULTS AND DISCUSSION

All results were obtained with the commercial available finite volume CFD code Ansys CFX©.

Results of verification case study

Figure 4 displays the simulated velocity fields inside the two hypothetical ozone reactors. As expected, flow in reactor 1 was essentially uniform throughout the whole domain, while significant short-circuiting existed in reactor 2. A substantial stagnation zone or dead zone could be observed in the rectangular segment of reactor 2, where the flow field has a very low velocity, indicating that microorganisms may become trapped or may experience a relatively long residence time if they enter this rectangular segment.

Similar phenomena were displayed by the particle tracking results shown in Figure 5. For reactor 1, particles passed smoothly from inlet to outlet without recirculation and short-circuiting. For reactor 2, a small portion of the particles was trapped in the 'dead zone' and most particles passed through a short 'passageway' next to the dead

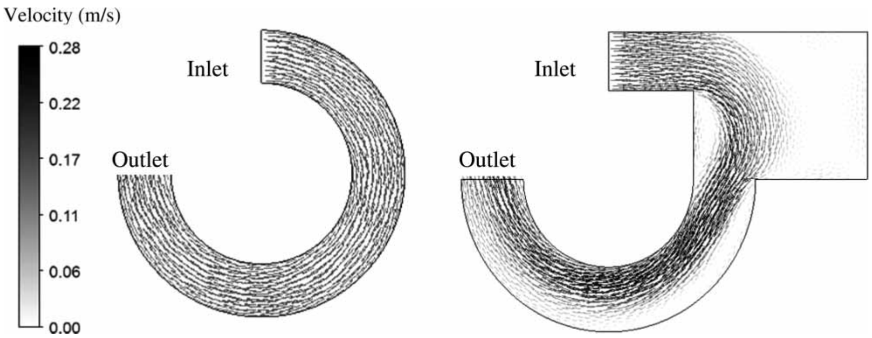

Figure 4 | Flow velocity fields in reactor 1 (left) and reactor 2 (right).

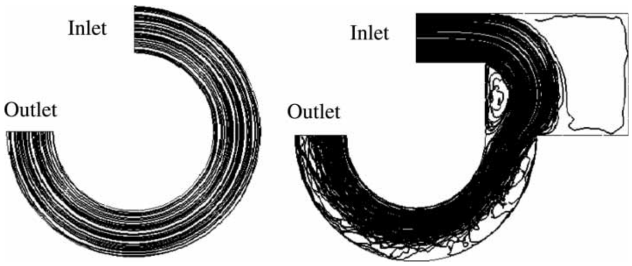

Figure 5 | Particle trajectories in reactor 1 (left) and reactor 2 (right).

zone, as shown in the figure. Thus, reactor 1 was considered to be close to an ideal plug flow system, and reactor 2 represented a non-ideal system in which flow mixing was more complex as found in most full-scale ozone contactors.

Using the methodologies described in Figure 1, the CT value can be obtained either by solving a species transport equation (Eulerian approach) directly or by calculating it from particle tracking modelling results. Figure 6 shows the CFD-simulated CT value distributions based on the Eulerian approach at a default Schmidt number of 0.9. Obviously, the flow field significantly affects the CT distribution. In reactor 1, CT increased smoothly from inlet to outlet. However, in reactor 2, much higher CT values were observed in the dead zone compared with those in the short-circuiting zone due to the substantially higher residence time in the dead zone.

Figure 7 shows the velocity and Eulerian-based CT value profiles along the outlets of reactors 1 and 2. It can be observed that both the velocity and CT values were more uniformly distributed at the outlet of reactor 1. However, they varied greatly from one to the other side at the outlet of reactor 2 due to the existence of strong short-circuiting inside the reactor.

Table 1 compares the CFD-simulated CT values at the outlets of the reactors determined using the Eulerian and particle tracking approaches. It can be observed that the effects of the particle size (1, 10 and 100 μm) on CT prediction were negligible for both approaches. Since the size of the primary target pathogens (*Cryptosporidium* oocysts

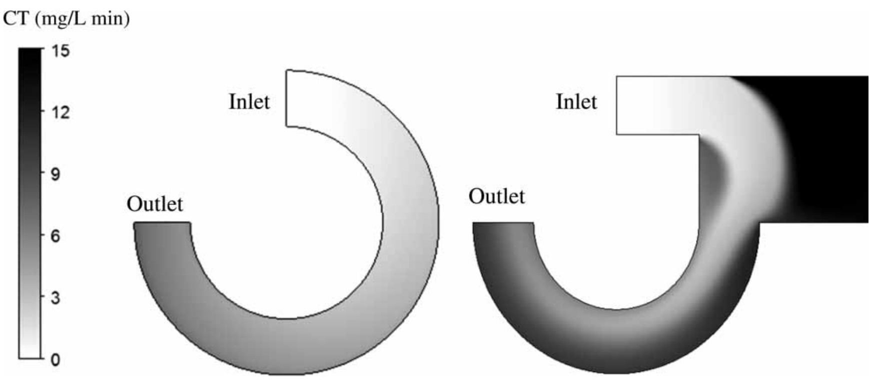

Figure 6 | Eulerian CT distribution in reactor 1 (left) and reactor 2 (right).

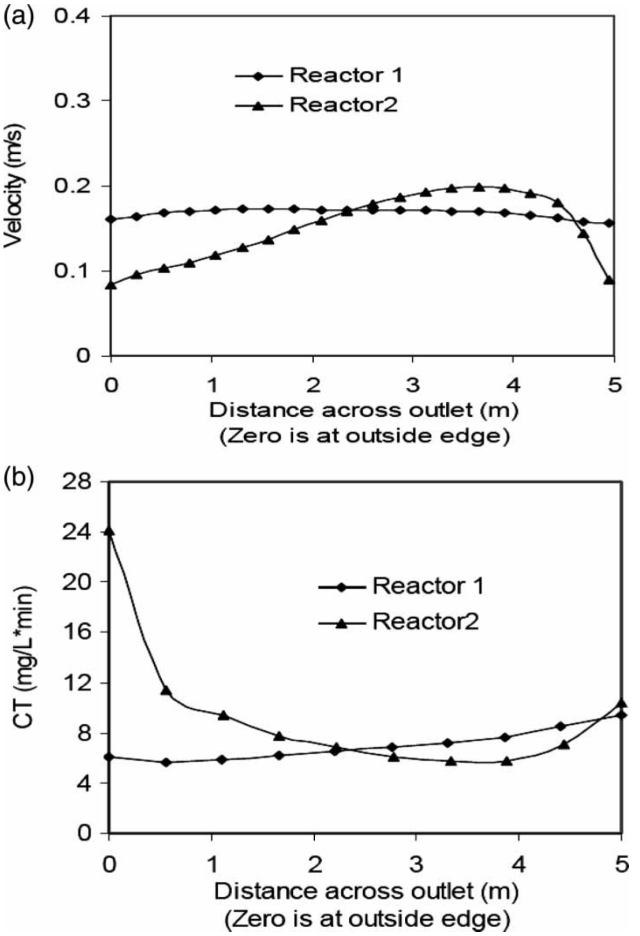

Figure 7 | Distribution of (a) velocity and (b) Eulerian-based CT at the outlet of reactors 1 and 2.

and *Giardia* cysts) for ozone disinfection treatment falls within the simulated range (MWH 2005), the above result suggests that an arbitrary particle size in the range of 1–100 μm could be chosen when the particle tracking model is used to simulate ozone disinfection performance.

The most important finding from the results in Table 1 is that the CT values predicted by the two different approaches were very close for reactor 1 but differed slightly for reactor 2. The negligible difference for reactor 1 was due to the fact that reactor 1 exhibited more ideal plug flow behaviour and there were no short-circuiting or dead zones within the system. Therefore, the corresponding residence time (T) and ozone profiles (C) on particle trajectories can better represent those values in the main flow. Both approaches are equally capable of characterizing the performance of this reactor.

Table 1 | Comparison of CT values: Eulerian versus particle tracking

Case study	Particle diameter (μm)	CT at outlet simulated by particle tracking (mg/L min)	CT at outlet simulated by Eulerian approach (mg/L min) Sc* = 0.9	Sc = 1,000
Reactor 1	1	6.50		
	10	6.48		
	100	6.48	6.52	6.50
Reactor 2	1	6.98		
	10	6.96		
	100	6.95	7.74	7.68

*Sc: Schmidt number.

For reactor 2, the particle tracking-based CT was slightly lower than the Eulerian approach-based ozone exposure CT. The reason for this might be that a small portion of the particles were trapped in the dead zone as shown in Figure 5. The particles which enter into this low velocity recirculation area take a very long time to pass through it. Even though a very long tracking time was set for the particle tracking modelling, still about 2–5% of particles were not able to escape from this dead zone after five times the hydraulic retention time. These particles, however, should be considered to be disinfected, as they have sufficient time to contact with ozone residual during their very long stay in the fluid domain.

The effect of the Turbulent Schmidt number (Sc) on the Eulerian approach was studied. The Schmidt number is a measure of the relative strength of the turbulent viscosity and turbulent diffusion (Launder & Spalding 1974). In most environmental flow situations, both turbulent viscosity and turbulent diffusion are important, and the Schmidt number is usually close to 1 (Lakehal 2002). As shown in Equation (5), when the Schmidt number is much lower than 1, turbulent diffusion may be dominant for the transport process. When the Schmidt number is much higher than 1, it means that turbulent diffusion is relatively unimportant.

Figure 8 shows a comparison of the CT value distributions in reactor 2 at two different Schmidt number conditions: one was the Ansys© CFX default value 0.9 and the other was 1,000. The purpose of modelling CT at a high Schmidt number (1,000) was to 'turn off' the turbulent diffusion term and thereby investigate the effect of turbulent

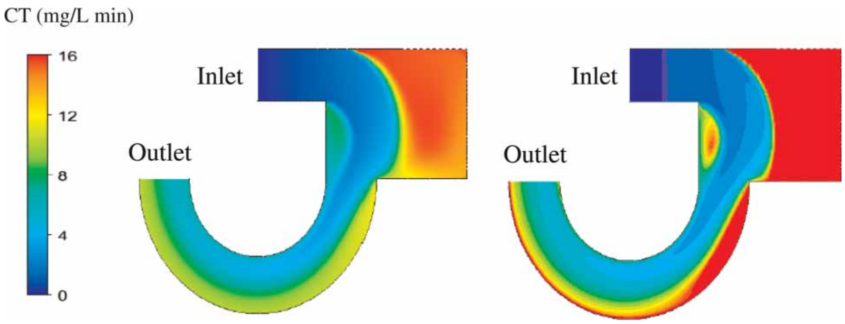

Figure 8 | CT distribution in reactor 2 at different Schmidt number conditions (left: Sc = 0.9; right: Sc = 1,000).

diffusion on the CT value prediction. It was observed that the CT distributions were similar in the main flow stream for the two Schmidt number conditions, but they differed inside the dead zone areas. Higher CT could be observed in these dead zones for a high Schmidt number (1,000) due to reduced turbulent diffusion, which also led to a thin stream of flow with high CT values along the outside wall. However, the velocity of this sidewall flow was substantially lower than in the main flow stream (as shown in Figure 4). As such, it is expected that the contribution of this high CT sidewall flow on the mass flow averaged CT at the outlet location is limited.

Table 1 shows the Eulerian approach-based CT values at the outlets of reactors 1 and 2 for the two different Schmidt numbers. The Schmidt number had a negligible effect on reactor 1 performance but did affect CT predictions for reactor 2 to a somewhat greater extent, although the impact was less than 2% over the range simulated. For reactor 2, even with a very high Schmidt number (1,000), the Eulerian-based CT values were still slightly larger than the particle tracking-based CT values. This is consistent with the results of Grimm (2003) in investigating other scalar transport problems. Grimm investigated the effect of spatial variations in the value of the turbulent Schmidt number and showed that in both natural environmental flows and engineered structures, predictions of solute transport were insensitive to changes in the Schmidt number.

Full-scale ozone contactor study

The two CFD modelling approaches were also applied to simulate the hydraulics of and determine CT for the ozone contactor in the DesBaillets Water Treatment Plant.

Figure 9 displays typical particle trajectories inside the contactor. It was observed that large recirculation zones existed in the two cells, causing short-circuiting and dead zones. The existence of these might reduce the overall contacting opportunities between ozone and pathogens and make disinfection efficiency significantly less than it otherwise could be. These non-ideal flow behaviours may be responsible for the difference in modelling results obtained using the two approaches, as discussed below.

Figure 10 presents a comparison of the tracer RTD curves simulated by the Eulerian and particle tracking approaches and those measured by tracer tests. The tracer

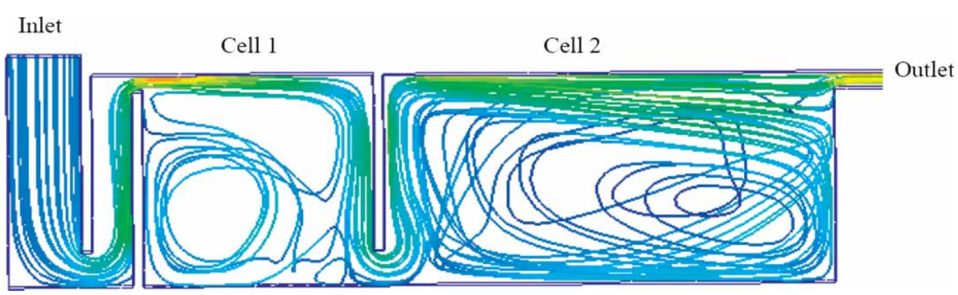

Figure 9 | Particle trajectories in the DesBaillets ozone contactor.

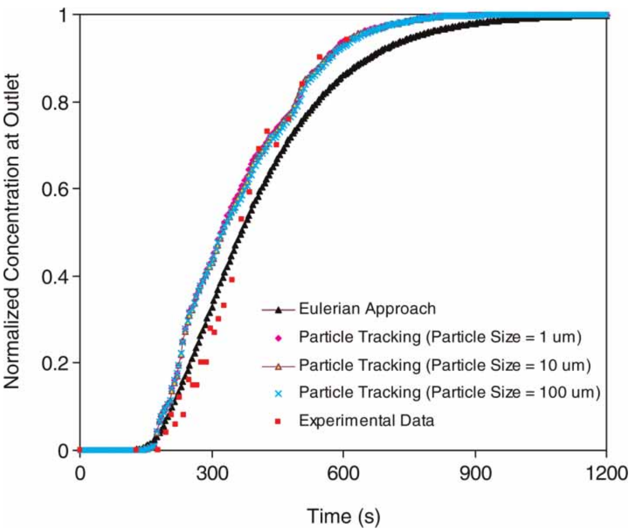

Figure 10 | Comparison of tracer curves: particle tracking versus Eulerian approaches.

tests were performed using a step injection of hydrofluorosilic acid. A distribution pipe was installed on the inlet surface to provide uniform injection of the tracer across the width of the contactor and tracer samples were collected at the contactor outlet. All analyses were performed by École Polytechnique de Montréal researchers (see El Baz 2002 for details). The RTD results of both approaches fitted the measured residence time data reasonably well, although minor differences between the two modelling approaches can be observed. Such minor differences are not surprising given the fact that the two modelling approaches are different in nature even though they tend to predict particle turbulent diffusion in similar orders of magnitude. The particle tracking-based RTD curve appears to slightly under-predict actual experimental results, indicating that the particle tracking approach may predict less particle dispersion than actually occurs. As such modelled particles may escape from the short-circuiting passages faster, resulting in a premature RTD curve. On the other hand, the Eulerian approach may slightly over-predict species diffusion, resulting in a delayed RTD curve. In addition, the deviation between the experimental and the modelling results may also be influenced by possible experimental errors, including those associated with field sampling, uneven tracer injection at the inlet, and impact of tracer sampling locations.

The effects of particle size on the prediction of flow hydraulics, represented by particle RTDs, were studied for three particle sizes (1, 10 and 100 μm). Figure 10 clearly shows that the effect of particle size with respect to particle RTD prediction was negligible.

Table 2 shows the average CT value at the DesBaillets WTP ozone contactor outlet calculated by the Eulerian and particle tracking approaches. Again it can be seen that particle size had a negligible effect on the particle tracking-based CT.

The results also showed that, for the DesBaillets WTP ozone contactor, the difference of the CT values predicted by the two modelling approaches was less than 12%, with the Eulerian approach-based CT being higher than the particle tracking-based CT. This was consistent with the observations of the verification case studies. As suggested by the verification study results, such a difference is mainly due to the existence of the short-circuiting and dead zones in the ozone contactor.

Table 2 also shows that the Eulerian-based CT value simulated at two different Schmidt numbers (0.9 and 1,000) was approximately 5% smaller at the higher Schmidt number. However, even when the Schmidt number was set at an unreasonably high value of 1,000 (when turbulent diffusion is negligible), the Eulerian-based CT value was still larger than particle tracking-based CT values, although the difference was less. This is consistent with the modelling results for hypothetical reactor 2, as discussed above.

With reference to UV reactors, Ducoste *et al.* (2005) observed that 'turning off' the diffusion term by setting a high Schmidt number may make the Eulerian approach fit better with the Lagrangian approach. This may be because UV reactors are usually designed to have high hydraulic efficiency. By visual inspection of the velocity fields predicted

Table 2 | Comparison of Eulerian versus particle tracking approaches for prediction of CT values for the DesBaillets WTP ozone contactor

Particle diameter (μm)	CT at contactor outlet simulated by particle tracking (mg/L min)	CT at contactor outlet simulated by the Eulerian approach (mg/L min)	
		Sc* = 0.9	Sc = 1,000
1	0.94		
10	0.98		
100	0.95	1.07	1.02

*Sc: Schmidt number.

by many researchers (Chiu *et al*. 1999; Lyn & Blatchley 2005; Ducoste & Linden 2006), UV reactors typically have much smaller recirculation zones than those in the ozone contactors investigated in the present study. For ozone contactors which can be expected to have at least some short-circuiting and/or dead zones, it appears to be inappropriate to completely shut off the diffusion term in the Eulerian approach. In addition, it is also questionable to turn off the diffusion term in the Eulerian approach but use the dispersion model in the Lagrangian approach.

The results of this study suggest that the differences in the predicted values between the Eulerian and particle tracking models may be caused by the discrete nature of the particle tracking method and the limited number of particles used in the data processing procedures.

Table 3 presents predicted CT values using the exported data with different numbers of particle trajectories. The maximum number of particle trajectories used for the data processing was 100. Since the particles are modelled as passive particles and do not influence the hydrodynamics or turbulent dispersion it is only necessary to have sufficient particles to cover the range of possible paths through the flow domain and to provide sufficient samples for quantifying the impact of turbulence on the mean particle trajectories. It becomes very time and computer memory consuming to export and post-process data for particle trajectory numbers over 100 because each particle trajectory is comprised of very large numbers of points and each data point contains multiple parameters. The results in Table 3 suggest that CT predictions based on particle tracking modelling results may fit better with the Eulerian approach if the data processing method could be improved to allow a sufficiently large number of particles to be exported and used for CT predictions.

Table 3 | Effect of particle trajectory numbers on CT prediction (particle diameter = 10 μm)

Particle trajectory numbers	CT at contactor outlet simulated by particle tracking (mg/L min)
20	0.96
40	0.95
60	0.98
100	1.02

CONCLUSIONS

The disinfection performance of two hypothetical ozone reactors and a full-scale operating ozone contactor for the treatment of drinking water has been simulated using a CFD model. The Eulerian and particle tracking approaches, two commonly utilized methods for the study of ozone disinfection processes, have been compared. Several important conclusions can be drawn from the cases considered here:

- For ozone reactors with plug flow characteristics, the Eulerian and particle tracking approaches fit well in predicting contactor disinfection efficiency (CT value).
- For reactors with non-ideal hydraulic performance, the particle tracking model predicted slightly lower CTs than did the Eulerian approach. The difference in CT was about 12%. This difference was mainly due to the discrete nature of the particle tracking method and complex particle trajectories in the non-ideal reactors. It is expected that, to obtain more accurate particle tracking modelling results, more powerful computers and specifically designed post-processing programs could be employed to process a larger number of particles.
- The effect of particle size (1–100 μm) on the particle tracking method was negligible.
- The Schmidt number has only a very limited impact on the Eulerian approach modelling results.

The implications of this work are that both the Eulerian approach and particle tracking approach are useful tools for understanding the complex performance of multiphase ozonation systems. The Eulerian approach may be a more practical method for the simulation of ozone disinfection performance since it is much more computationally economical than the particle tracking approach. However, the particle tracking method more closely reflects the actual physical behaviour of the microorganisms (as particles) and has been successfully applied in UV reactor design and optimization. Further investigation should be conducted to study the effects of model inputs on the two modelling approaches and to evaluate the accuracy of the two approaches based on bioassay validation studies on pilot or full-scale ozone disinfection systems. In the meantime, it might be appropriate to slightly reduce, for design purposes, CT values obtained using the Eulerian approach. For the real contactor investigated here, a reduction of approximately 10% would be appropriate.

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