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Review

Developments in computational fluid dynamics-based modeling for disinfection technologies over the last two decades: A review

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ABSTRACT

In the last two decades, Computational Fluid Dynamics (CFD) has shown great potential as a powerful and cost-efficient tool to troubleshoot existing disinfection contactors and improve future designs for water treatment industry. However, numerous challenges in the simulation of water disinfection processes still remain. This review summarizes past CFD studies of the hydraulic and associated disinfection efficiency of disinfection contactors. Hydraulic efficiency studies based on flow and tracer transport simulation were found to be the most common and successful. Challenges existing in flow and disinfection simulation are identified and discussed. These challenges can be overcome via advanced turbulent simulation approaches, such as Large Eddy Simulation and multi-phase resolving simulations. Although turbulence-chemistry interaction is found to be the most challenging problem for proper representation of the reaction system and inactivation kinetics, solutions to this challenge can be overshadowed unless errors induced by unresolved unsteady flow and multi-phase flow are reduced sufficiently.

1. Introduction

A wide range of models have been developed to understand complex phenomena in environmental flows, such as turbulent mixing in coastal waters (Yuan et al., 2007; Tejada-Martinez et al., 2011, 2012; Akan et al., 2013), wind flow around buildings (Stathopoulos and Baskaran, 1990; Tominaga et al., 1997; Blocken and Persoon, 2009; Blocken et al., 2012), and air pollution dispersion in urban areas (Fox, 1981; Leitl et al., 1997; Meroney et al., 1999; Canepa, 2004; Chu et al., 2005; Yang and Shao, 2008; Solazzo et al., 2009). Various modeling approaches have also been used to improve the hydraulics of flows in water and wastewater treatment facilities such as membrane filters (Ghidossi et al., 2006), flocculator (Bridgeman et al., 2010) and wastewater stabilization ponds (Verbyla et al., 2013). These models have been evaluated and improved aiming to predict flow and mass transport with a higher accuracy and resolution (Jakeman et al., 2006; Bennett et al., 2013). With rapid advances in computing technology, a powerful modeling tool-computational fluid dynamics (CFD) which has been prevalent in aerospace engineering and mechanical engineering flow applications has attracted much attention in environmental engineering due to its high accuracy and ability to provide comprehensive information. CFD has been applied to simulate water flows in various water treatment processes such as flocculation (Bridgeman et al., 2010), sedimentation (Goula et al., 2008; Ghawi and Kriš, 2012), desalination (Ghadiri et al., 2013), and disinfection (Cockx et al., 1999; Huang et al., 2004; Bartrand, 2006; Zhang et al., 2007; Bolaños et al., 2008; Wols et al., 2010a; Talvy et al., 2011; Zhang et al., 2014a). Among these applications, disinfection is a process that has been widely studied using CFD. This review focuses on CFD applications to disinfection of water.

The disinfection process is a critical safety step in water treatment that inactivates bacteria, viruses, and other pathogens. The most common disinfection approaches for water treatment include chlorine disinfection (including chlorination, chlorine dioxide, and chloramines), ozone disinfection, and ultraviolet (UV) disinfection. The history of chlorine disinfection can be traced back to the late 1800s (USEPA, 1986) and is still one of the most widely used technologies in the U.S. (Solomon et al., 1998). Ozone disinfection is becoming increasingly important because of its effective disinfection and odor control (Crittenden et al., 2005). Both chlorine disinfection and ozone disinfection inactivate pathogens primarily by oxidation. In UV disinfection, UV radiation penetrates the genetic material of pathogens and retards their ability to reproduce. Thus, it is a physical process rather than a chemical process, eliminating chemical residual issues associated with other disinfection approaches.

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The goal of optimizing contactor configuration to improve disinfection efficiency has driven engineers towards disinfection modeling in addition to physical experiments. The early models for disinfection, such as plug flow reactor (PFR) and completely mixed flow reactor (CMFR) were developed based on ideal flow conditions. Further details on the early models can be found in introductory textbooks on chemical reaction engineering (e.g. Hill, 1977; Levenspiel, 1998; Fogler, 1999). Successes have been reported on modeling ozone disinfection in column contactors using the axial dispersion reactor (ADR) model combined with reaction and inactivation kinetics (Chen, 1998; Kim et al., 2002, 2007). However, due to the lack of consideration of the effects of turbulence and complex flow conditions, such as dead zones and short-circuiting, it is impossible to apply this kind of model to a contactor with complex geometry.

Early work has proven the applicability of CFD to disinfection processes (Falconer and Ismail, 1997; Do-Quang and Laine, 1997; Janex et al., 1998). CFD has been applied in not only evaluating the hydraulic efficiency (excluding reaction and inactivation) of existing reactors (including contactors for disinfection), but also in optimizing future reactor designs (Cockx et al., 1999; Evans et al., 2003; Stamou, 2002, 2008; Wols et al., 2008b; Kim et al., 2010; Tafilaku, 2010; Amini et al., 2011). However, it is still a great challenge to conduct a complete CFD simulation of disinfection processes involving flow, reaction, and inactivation.

The primary goal of this review is to identify the challenges in disinfection process simulation. In this review, the steps of a complete disinfection process simulation are first outlined. Then, the state of current research is reviewed by categorizing it into three groups: development of simulation method or framework for disinfection process, the impact of operation, configuration, and modeling parameters on disinfection efficiency, and optimization of contactor configuration. Then, the challenges in a CFD simulation of flow, tracer transport, reaction and inactivation are examined. Potential solutions to overcome these challenges are discussed.

2. Stages of CFD applied to disinfection process

CFD technology has been used to model the flow in water treatment since the late 1990s (Falconer and Ismail, 1997; Do-Quang and Laine, 1997; Wang and Falconer, 1998a, b; Janex et al., 1998), including water intake infrastructures, flocculation tanks, sedimentation basins, and disinfection reactors (Craig et al., 2002; Kamimura et al., 2002). The early success of CFD in water treatment flow simulation led to an increased interest in applying CFD to disinfection processes as shown by the increase in related publications in Fig. 1.

The increasing interest in CFD applied to disinfection process is partly due to the rapid advancement of computer technology making intensive computing affordable; and partly due to the demand for modeling of the disinfection process. The primary goals in the modeling of disinfection processes are to increase disinfection efficiency and reduce cost, or to optimize reactor design to comply with regulations or both.

Modeling of disinfection process can be divided into four stages: flow simulation, tracer transport simulation, reaction process simulation, and inactivation simulation. The latter three stages are heavily dependent on the first one, flow simulation. Thus, the accuracy of flow simulation is the most important one among the four. Note that, inactivation simulation also needs important input from the reaction process simulation.

2.1. Flow simulation

The most basic governing equations of incompressible fluid flow are the continuity equation and momentum equations (or Navier–Stokes equations). The continuity equation is

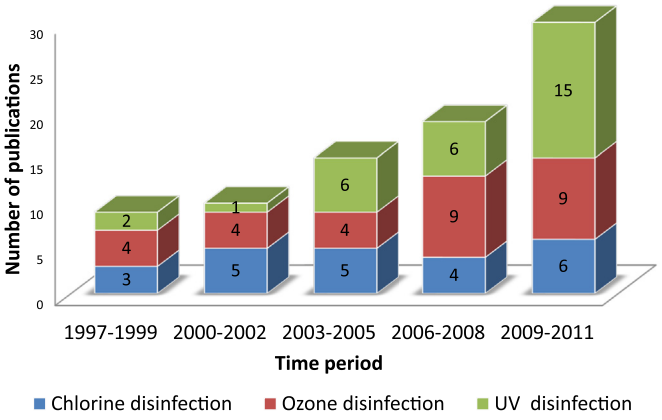

Fig. 1. Statistics of publications on CFD applied to disinfection (searched with Engineering Village and Web of Knowledge).

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

where u_i and x_i are velocity and position in the i-th direction.

The momentum equations are derived from Newton's second law. A general form of the momentum equations is

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i \tag{2}$$

where t is time, ρ is fluid density, p is pressure, ν is the kinematic viscosity, and f_i represents a body force (the force per unit of mass) in the i-th direction.

An important issue in flow simulation is how to model turbulence. Turbulent flows contain a wide range of spatial scales, the size of the larger scales being comparable to the size of the flow domain. The range of motions in a turbulent flow grows with the Reynolds number (Re) and thus the size of the smaller scales can become less than millimeters.

Three primary strategies for turbulent flow simulation are well known (Pope, 2000): Reynolds-Averaged Navier–Stokes simulation (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS).

DNS resolves the governing Navier–Stokes equations numerically over the entire range of turbulent scales. However, the requirements on mesh resolution and time-step put high demands on computational resources, rendering it unsuitable for most engineering applications. More specifically, the grid for DNS should contain approximately $Re^{9/4}$ points. Typical Reynolds numbers are $O(1 \times 10^6)$ giving rise to the need for large numbers of grid points that make DNS computationally prohibitive.

RANS is a statistical approach for the simulation of turbulent flow. RANS involves the application of Reynolds averaging to decompose Navier–Stokes equation solution variables into their means and the turbulent fluctuations about these means. The Reynolds-averaged equations are solved for the mean component of the flow without explicit computation of the turbulent scales. Instead, the Reynolds-averaged equations contain a Reynolds stress term accounting for the effect of the unresolved turbulent scales on the explicitly computed mean component of the flow. Often, the Reynolds stress is modeled following the eddy viscosity hypothesis (Pope, 2000). The primary advantage of RANS is the relative low requirement on computer resource given that it only resolves the mean flow. Therefore, RANS has been applied to simulation of high

Reynolds number flows, such as flow simulation around a full-scale airplane. However, RANS has two main drawbacks: 1) it only resolves the mean flow and all of the unresolved turbulent scales must be modeled, thus rendering the turbulence model crucial for the accurate representation of the mean flow; 2) no universal RANS turbulence model exists, thus a specific model may be needed for the particular flow problem.

LES aims to reduce the requirements on mesh resolution imposed by DNS. The idea of LES is to use a spatial filter to separate the turbulent flow field into two components. The larger scale, more energetic structures that can be resolved by the numerical method on a given mesh are referred to as the resolved scales. The smaller structures that cannot be captured by the mesh are called sub-grid scales. The influence of sub-grid scales on resolved scales must be modeled. Often the sub-grid-scale (SGS) model is based on an eddy viscosity hypothesis. The principle of LES lies on the fact that the small (unresolved) scales of the turbulence are homogeneous and isotropic and therefore easier to model relative to the larger scales. Furthermore, these small (unresolved) scales are universal and thus the SGS model could be applicable to different flow problems. Results of LES would be closer to those of DNS under mesh refinement as the size of scales that require modeling become smaller and less energetic. LES is in between DNS and RANS in terms of accuracy and computational cost. Due to the physics of turbulence in the vicinity of an impermeable no-slip wall boundary being considerably different from the other parts of flow, typical eddy viscosity hypothesis-based SGS models such as the Smagorinsky model (Smagorinsky, 1963) are not suitable for representing near-wall sub-grid scales. A common solution is to refine the mesh near the wall to the resolution of DNS. Thus, LES still has a high computational cost that cannot be afforded for engineering applications. LES is sometimes performed with a near-wall model in order to avoid DNS-like resolution of the near-wall region (Pope, 2000).

2.2. Tracer transport simulation

Non-reactive tracer transport is often incorporated into a flow simulation in order to investigate hydraulic efficiency of the water treatment system, for example, in terms of mean residence time and other quantities of interest derived from residence time distributions. The tracer is a conservative element, typically a dye or salt. In CFD simulation, the tracer is usually treated as a passive scalar which has no impact on hydraulic characteristics. The basic technique used to conduct a tracer study is to introduce the tracer at the reactor inlet and measure the response at the outlet in order to obtain residence time statistics.

Two main approaches for the simulation of tracer transport are based on Lagrangian particle motion modeling (particle tracking) and solving a transport equation for tracer concentration, respectively. Particle tracking modeling has been applied successfully (Thyn et al., 1998; Stropky et al., 2007; Wols et al., 2008a). However, the Lagrangian-based approach is less popular than solving a transport equation for tracer concentration because common CFD codes are based on an Eulerian system.

For simulation of the tracer transport in fluid flow, an advection–diffusion equation is used:

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} - \frac{\partial}{\partial x_j}\left(D \frac{\partial C}{\partial x_j}\right) = 0 \tag{3}$$

where u_i is the flow velocity, C is the tracer concentration, and D is the molecular diffusivity for the scalar.

Solution of the above advection–diffusion equation needs the input of the flow velocity field. Note that the passive tracer transport does not affect the flow hydraulics. There are two strategies to input the velocity field, namely frozen flow and dynamical flow:

1. Frozen flow: Based on the assumption of steady mean flow, the mean flow is solved first. The advection–diffusion equation for scalar concentration in (3) is then solved using the frozen velocity field.
2. Dynamical flow: This strategy consists of solving the flow equations and the advection–diffusion equation for tracer concentration simultaneously at each time step.

The first strategy fits within the RANS methodology described earlier and has been commonly used due to its relatively low computational cost (Huang et al., 2004; Khan et al., 2006; Hofman et al., 2007a; Kim et al., 2010). Note that LES is only compatible with the second strategy of tracer transport simulation because LES resolves smaller scales of the flow which are inherently unsteady.

Typically, in LES and RANS involving solution of Equation (3), the effect of the unresolved scales is modeled following the eddy viscosity hypothesis mentioned earlier for the momentum equations. In LES involving (3), an SGS eddy diffusivity for the non-reacting (conservative) scalar is added equal to the SGS eddy viscosity for momentum divided by the molecular Schmidt number. For example, Kim et al. (2009) chose to take the SGS diffusivity as the SGS eddy viscosity divided by 1000 in order to maintain the same ratio of molecular viscosity of water to molecular diffusivity of Rhodamine 6G, the passive tracer being simulated (thereby retaining the same molecular Schmidt number). Meanwhile, in RANS, the eddy diffusivity is set equal to the eddy viscosity divided by the turbulent Schmidt number (Sc_t) with Sc_t set to 0.7 (Launder, 1978). Furthermore, typically, the resulting eddy diffusivities in both RANS and LES are much bigger than the molecular diffusivity, thus the molecular diffusion is discarded from the scalar advection–diffusion equation.

2.3. Reaction process simulation

The main goal of reaction process simulation is to predict disinfectant dose distribution, requiring solutions of a series of chemical reactions. For example, in ozone disinfection, commonly considered chemical reactions include: reaction between ozone and natural organic matter (NOM) or total organic carbon (TOC); self-decomposition of dissolved ozone; formation of by-products, such as bromate (Crittenden et al., 2005). Similar reactions and by-products occur in chlorine disinfection.

To model the transport of chemical species in a fluid flow, a general advection–diffusion equation similar to Equation (3) is used:

$$\frac{\partial C_i}{\partial t} + u_j \frac{\partial C_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left(D_i \frac{\partial C_i}{\partial x_j}\right) = S_i \tag{4}$$

where u_i is the flow velocity, C_i is the species concentration, D_i is the molecular diffusivity for the chemical species, and S_i is the external volumetric source term including generation, consumption and transfer to another phase. Typical species are listed in Table 1. In RANS or LES, the molecular diffusivity D_i is replaced with the eddy diffusivity calculated for the tracer transport equation in (3), as described earlier. Note that this eddy diffusivity is independent of chemical species.

The external volumetric source term, S_i, on the right side of Equation (6), makes the simulation of a reaction process much more

Table 1
Commonly used source terms of transport equations for modeling ozone disinfection process.

Species	Source terms for transport equations	References
Dissolved ozone, C_l	$S_{C_l} = -k_d C_l$	Sotelo et al. (1987), Beltrán (1995), Muroyama et al. (1999), Huang et al. (2004)
NOM	$S_{[NOM]} = -k_{NOM}[NOM]C_l$	Lev and Regli (1992), Chen (1998), Kim et al. (2002)
Bromate, C_B	$S_{C_B} = k_B C_l$	von Gunten and Hoigné (1994), Kim et al. (2002), Tang et al. (2005)
Tracer	$S_{tracer} = 0$	Zhang (2006), Zhang et al. (2007)
CT (Concentration-Contact time)	$S_{CT} = C_l$	Zhang (2006), Zhang et al. (2014a)
UV dose	$S_{UV\ dose} = G$	Wright and Hargreaves (2001), Elyasi and Taghipour (2006)

complicated than tracer transport in (3). For example, the commonly used source terms for ozone disinfection are listed in Table 1. In this table, k_d is the ozone decay constant, C_l is the concentration of dissolved ozone, k_{NOM} is the reaction rate constant for the reaction between dissolved ozone and *NOM*, [*NOM*] is the concentration of *NOM*, and k_B is the bromate formation rate constant. For dissolved ozone, the source term is usually set to be the rate of dissolved ozone decay which corresponds to a first-order reaction. Similar to ozone decay, bromate formation is taken as a first-order reaction. In Table 1, the source term in the transport equation for [*NOM*] is written as a second-order reaction as was taken in the reduced order models of Lev and Regli (1992), Chen (1998), and Kim et al. (2002). Zhang (2006) used second-order representation of the source term for the *NOM* transport equation in CFD simulations. Zhang et al. (2014a) used second-order representations of the source terms for the *NOM* and bromate transport equations in CFD simulations. Furthermore, in Zhang et al. (2014a), the source term in the transport equation for ozone contains ozone self-decomposition and consumption by *NOM* and bromate. The latter consumption was represented by a second-order reaction. Discussion on how to model the turbulence-chemistry interaction associated with second-order reactions will be given in Section 4.5. Note that the first-order representations of source terms are empirical and not kinetics-based. The source term for the tracer is null.

A common practice in ozone disinfection modeling is to calculate the product of dissolved ozone concentration and contact time (CT) using Eqn. (6) with the source term set equal to ozone concentration. CT is commonly employed as the indicator of disinfection efficiency (USEPA, 2003; Zhang, 2006; Wols et al., 2010a,b,c; Zhang et al., 2014a).

In UV disinfection, the disinfectant is not a chemical but rather the energy of UV incident radiation. Eqn. (6) is also employed to calculate UV dose. In this case, the source term is equal to UV radiation (denoted as G in Table 1). The spatial distribution of UV radiation is independent from the flow but depends on location and light intensity of UV lambs. Thus it is not calculated by solving transport equations but by radiation models. More details about radiation models are described in Section 3.1.

2.4. Inactivation simulation

Additional reactions between microorganisms and disinfectant are included in the inactivation simulation stage. Wols et al. (2010a) has summarized and compared the existing approaches to estimate microorganisms survival ratio. An overview of inactivation or disinfection calculation methods is shown in Table 2. According to the study of Wols et al. (2010a), inactivation should be modeled via a particle tracking method or an Eulerian approach (that solves a scalar transport equation for the number of microorganisms directly) and either method should incorporate flow characteristics such as dead zones and short-circuiting, in order to predict disinfection more accurately. However, particle tracking methods are relative difficult to be implemented in traditional CFD codes because these are usually written in an Eulerian system. Thus, only Eulerian inactivation will be described in this review.

In Eulerian inactivation, a transport equation for the concentration of microorganisms is commonly considered to be the governing equation of the inactivation of microorganisms (Huang et al., 2004; Greene et al., 2006; Wols et al., 2010a):

$$\frac{\partial N_m}{\partial t} + u_j \frac{\partial N_m}{\partial x_j} - \frac{\partial}{\partial x_j}\left(D_i \frac{\partial N_m}{\partial x_j}\right) = S_{N_m} \tag{5}$$

where N_m is the concentration of microorganism m and S_{Nm} is the external volumetric source term for microorganism m. Various models have been developed for the source term of microorganisms. Details of these models are provided in Section 3.1.

Solution of the inactivation equation based on RANS is typically performed after the first three steps outlined earlier (flow solution, passive tracer solution and reaction process solution) have been successfully conducted. An overview of the four stages of disinfection process modeling by CFD is listed in Table 3. All components or stages of the outlined framework comprised remain under active research. Improvement of this framework and related technologies, such as computer power and solution algorithms should improve the applicability and reliability of disinfection process simulations.

3. State of current research in disinfection simulation using CFD

The primary interests of reported studies on modeling disinfection process can be categorized into the following three groups:

- Development of simulation method and framework for disinfection process
- Parameters (to be described below) studies of modeling disinfection process
- Optimization of contactor configuration

3.1. Development of simulation methods and frameworks for disinfection process

Framework and simulation methodology development have always been at the frontier of disinfection simulation research. Before CFD technology was applied to the area of disinfection process, early research developed several simplified models for the

Table 2
An overview of disinfection calculation methods (adapted from Wols et al. (2010a)).

Method	Required information
CT10-method	RTD (residence time distribution)
CSTR-method	Number of compartments
Segregated Flow Analysis	RTD
Micro-mixing analysis	RTD
Eulerian mean CT value	CFD (flow velocities, turbulent diffusivities, disinfectant concentrations, etc.)
Eulerian direct inactivation	CFD (flow velocities, turbulent diffusivities, disinfectant concentrations, etc.)
Particle tracking	Particle trajectory, CFD (disinfectant concentrations)

Table 3
An overview of the four stages of disinfection process modeling by CFD (adapted from Wols et al. (2010a)). Note that the flow simulation stage underlies the entire framework.

Stages	Methodologies and models	Physical quantities
Stage 1: Flow Simulation	RANS or LES based on Navier-Stokes Equations; Turbulence modeling for RANS or SGS modeling for LES.	Flow fields (e.g. velocity, pressure); Turbulent properties
Stage 2: Tracer Transport Simulation	Advection-diffusion equation for passive scalar	Tracer concentrations; Residence time distribution
Stage 3: Reaction Process Simulation	Species transport equations; Modeling for chemical source terms	Chemical concentrations (e.g. dissolved ozone); Incident radiation for UV disinfection; disinfection contact times
Stage 4: Inactivation Simulation	Species transport equations; Inactivation kinetic modeling	Concentrations of microorganisms; Microorganisms survival ratio

flow in disinfection contactors, such as the axis dispersion reactor (ADR) model (Chen, 1998; Kim et al., 2002, 2007) and the back flow cell model (BFCM) (Nguyen-Tien et al., 1985). However, these models cannot meet the demand of industry any longer due to limited applicability (usually the simplified models are only for contactors with simple geometries) and insufficient accuracy.

At the end of 1990s, researchers recognized the potential of CFD technology for improving disinfection modeling. Cockx et al. (1999) conducted simulations of the flow in two ozone disinfection towers using a two-phase flow CFD code. In their model (Cockx et al., 1999), a source term which represents mass transfer was introduced to achieve the dissolved gas concentration held in the reactor. Greene et al. (2002) developed a CFD-based framework to predict flow structure, mass transport and chlorine decay in a continuous flow pilot scale reactor. This framework was verified by a test-case comparison with physical experimental measurements. Greene et al. (2004) developed a CFD-based framework that incorporates experimentally derived terms for chlorine decomposition and microbial inactivation based on the work of Haas et al. (1995). The results from this model (Greene et al., 2004) showed good agreement with the physical experimental data set over a wide range of microbial inactivation rates.

In order to reduce the high computational cost of CFD, researchers have developed a compartmental hybrid model of the completely mixed flow reactor (CMFR) and the plug flow reactor (PFR) (Gresch et al., 2009; Mandel et al., 2012) models. Although this kind of model is computational-effective and easy to use, it has a relative low spatial resolution of the flow, which may cause serious accuracy problems. Additionally, the compartmental model is highly dependent on flow conditions. A minor change in reactor configuration or flow rate can dramatically impact the compartmental model's prediction. Thus, the compartmental model is helpful for rapid analysis but not practical for prediction.

Bolaños et al. (2008) discussed the applicability of CFD to simulate ozonation processes in ozone disinfection. This research proposed the set of Navier–Stokes equations with effective density and effective viscosity applied to two-phase flows if the dispersed phase elements are small. Results from the study of Bolaños et al. (2008) demonstrated that CFD is an efficient tool to study mixing flow characteristics and inactivation processes in existing water treatment plants and for predicting process performance of new designs.

Besides simulations of flow in lab-scale contactors, attempts at applying CFD to full-scale contactors in water treatment plants have been conducted (Do-Quang et al., 2001; Huang et al., 2004; Mizuno et al., 2005; Hofman et al., 2007a; Zhang et al., 2007, 2014a; Talvy et al., 2011; Launer et al., 2013). Hofman et al. (2007a) applied CFD to the Leiduin water treatment plant in Netherlands. The disinfection performance of the ozone treatment at the plant was predicted and compared with experimental data. Talvy et al. (2011) used CFD to assess the ozone disinfection in the Tailfer plant in Brussels, Belgium. Zhang et al. (2007) developed a multi-phase CFD framework to address all the major components of ozone disinfection processes at the Charles DesBaillets Water Treatment Plant in Montréal, Canada. Zhang et al. (2014a) have successfully applied a CFD model combined with a reaction kinetics model to simulate the flow in a full-scale ozone contactor operated by City of Tampa Water Department, FL, United States.

Wang et al. (2003) tested various combinations of turbulence stress models and numerical schemes of advection term in simulating flow and tracer transport in different contactor designs. The results show that the standard k-ε model can accurately predict flow pattern but cannot predict the residence time distribution well due to the underestimation of the average velocity toward the end of the tank simulated. Kim et al. (2009) was the first to apply LES for analysis of flow in reactors as prior studies had been based on RANS. Kim et al. (2010) concluded that the inability of RANS to capture turbulent flow structures in a baffled ozone contactor may lead to a poor prediction of tracer transport statistics such as t_{10} (i.e. the time it takes for 10 percent of the tracer injected at the inflow to reach the outflow). These statistics are often used for evaluating hydraulic efficiency. LES was proposed as a more accurate alternative to RANS due to its improved prediction of tracer transport statistics. Zhang et al. (2013a) revisited the numerical and experimental studies of Kim et al. (2010) and found that the poor performance of RANS compared to LES observed by Kim et al. (2009) may have been due to inappropriate use of the turbulence model. Zhang et al. (2013a) found that for the near-wall resolving grid used by Kim et al. (2009), RANS with a low-Reynolds number turbulence model such as the Lauder–Sharma k-ε model (Wilcox, 1994) leads to more accurate tracer transport statistics than RANS with the standard k-ε model (Wilcox, 1994), the latter having been used by Kim et al. (2009) for their simulations. Application of the standard k-ε turbulence model on coarser grids led to better results. The

reason for this is that the standard k-ε turbulence model is designed for coarse meshes that do not resolve viscous, near-wall dynamics.

Equations governing flow and tracer transport solutions (excluding the turbulence model) are general to disinfection simulation frameworks. Differences appear when modeling the reactions. For modeling chlorine disinfection, the commonly used reaction system consists of chlorine decay only (Greene, 2002; Greene et al., 2006). For modeling ozone disinfection, the most common considered reactions include ozone decomposition, reaction between ozone and instantaneous ozone demand (IOD) or natural organic matter (NOM) or total organic carbon (TOC), and bromate formation. A summary of the reaction systems used in CFD simulations of ozone disinfection is given in Table 4. For modeling of UV disinfection, the primary focus in this stage is the radiation modeling. A summary of the radiation models used in the modeling of UV disinfection process up to date is listed in Table 5.

Although various inactivation models have been developed for the source terms of advection-diffusion equations governing the concentration of microorganisms (Gyurek and Finch, 1998), only the Hom–Haas model and the Chick–Watson model have been put to practice in CFD codes. The Hom–Haas model can represent the inactivation kinetics more accurately than the Chick–Watson model (Haas and Karra, 1984a, b; Zhang, 2006). The source term expression given by the Hom–Haas model is

$$S_{N_m} = \frac{dN_m}{dt} = -xN_m\left(k_{\mu,m}C_l^y\right)^{1/x}\left[-\ln\left(\frac{N_m}{N_0}\right)\right]^{(1-1/x)} \quad (6)$$

where N_0 is the initial concentration of the microorganism m, $k_{\mu,m}$ is the inactivation rate constant for the microorganism m, C_l the disinfectant (i.e. ozone or chlorine) concentration, and x and y are constants. Table 6 lists literature-reported constants for various pathogens. Inactivation rate constants depend on the target species and temperature. For the case when $x = y = 1$ the Hom–Haas model reduces to the Chick–Watson model:

$$S_{N_m} = \frac{dN_m}{dt} = -k_{\mu,m}C_lN_m \quad (7)$$

Although the Chick–Watson model does not consider the effect of initial microorganism concentration and has a limited applicability, it has been more popular in practical modeling than the Hom–Haas model due to its simplicity (Huang et al., 2004; Bartrand, 2006; Bolaños et al., 2008; Wols et al., 2010a). Note that, the Chick–Watson model requires only one parameter (i.e. $k_{\mu,m}$) whereas the Hom–Haas model requires two more parameters (i.e. x and y).

The inactivation models used in UV disinfection are similar to those used in ozone and chlorine disinfections except that the disinfectant concentration in Equations (6) and (7) needs to be replaced with incident radiation, G. For example, in the Chick–Watson model, which has been widely used in modeling of UV disinfection (Chiu et al., 1999; Lyn et al., 1999; Ducoste et al., 2005), the source term can be written as

$$S_{N_m} = -k_{UV,m}GN_m \quad (8)$$

where $k_{UV,m}$ (unit: $m^2/(Ws)$) is the intrinsic rate constant of the microorganism m.

Most of the reported CFD studies on disinfection tanks have used commercial software due to its advantages of easy-to-learn, friendly interface, and stability. The most common used CFD commercial software are ANSYS Fluent, ANSYS CFX, and COMSOL. Free software, in-house codes, and open-source codes were also employed but only in a few studies (Bolaños et al., 2008; Wols et al., 2008a,b, 2010a; Kim et al., 2010, 2013a,b; Zhang et al., 2013a,b, 2014a,b). A summary of CFD codes used in reported studies on disinfection tanks is shown in Table 7.

3.2. Parameter studies of modeling disinfection process

Several parameters related to disinfection efficiency have been studied via CFD. These parameters can be divided into the following three categories:

- Operation parameters
- Configuration parameters
- Parameters in modeling

The operation parameters studied by CFD include: pH (Kim, 2005), temperature (Kim, 2005; Talvy et al., 2011), bubble size variation (Talvy et al., 2011), ozone-consuming substances (OCS) variation (Huang et al., 2004), and flow rate (Zhang et al., 2014a). The studied configuration parameters include: inlet configurations (Greene, 2002; Greene et al., 2002), the direction and magnitude of the inlet flow (Ta and Hague, 2004), the method of tracer injection (Zhang et al., 2008), sampling locations (Zhang et al., 2008), the ratio of length of flow to width of flow (Peplinski and Ducoste, 2001), dead zone volume percentage (Lee et al., 2011), and wall reflection of light (Chen et al., 2011). The parameters in modeling are those involved in development of the CFD model, such as the effect of turbulence model (Rauen et al., 2008), time step (Peplinski and Ducoste, 2002), turbulent intensity of inflow conditions (Huang et al., 2002), turbulent Schmidt number (Kim et al., 2013a) and so on. Rauen et al. (2012) have appraised the CFD models and modeling techniques commonly used in chlorine contactor tank studies. They suggested that further investigation should be conducted on the sensitivity of predictions to the variation of modeling components (e.g. discretization schemes, turbulence models, and boundary conditions), the dependence of the turbulent Schmidt number on the geometric and hydraulic characteristics of contactor, and computational performance improvement of the existing CFD codes. The impacts of studied parameters on disinfection efficiency or predicting disinfection efficiency are summarized in Table 8.

A better understanding of the relationships between disinfection efficiency and operation parameters is helpful for troubleshooting existing disinfection contactors in water treatment plants. For example, the CFD simulation (Talvy et al., 2011) of the flow in the Tailfer plant, in Belgium, helped to identify problematic issues caused by the low operating temperature. Another example is the study of Zhang et al. (2008) which found that sampling location has a significant influence on tracer RTD prediction, suggesting that multiple sampling points should be employed during physical measurements.

Table 4
A summary of the reaction systems used in CFD simulation of ozone disinfection.

Studies	Ozone decay	Reaction between ozone and IOD or NOM or TOC	Bromate formation
Cockx et al. (1999)	√	√	
Huang et al. (2004)	√	√	
Bartrand (2006)	√	√	√
Zhang et al. (2007)	√	√	√
Bolaños et al. (2008)	√		
Wols et al. (2010a)	√		
Talvy et al. (2011)	√		
Launer et al. (2013)	√	√	
Zhang et al. (2014a)	√	√	√

Table 5
A summary of the radiation models used in the modeling of UV disinfection process.

Radiation models	Expressions	Sources
Non-attenuate model	Algebraic equation for incident radiation G is $G = I = I_{max}\left(\frac{r_s}{r}\right)$ where r is the radial distance from the lamp, I_{max} and r_s are the light intensity and radius at lamp surface.	Wright and Hargreaves (2001)
Modified P-1 radiation model	Transport equation for the incident radiation G is $\nabla\cdot(\Gamma\nabla G) - aG = 0$ (1) $\Gamma = \frac{1}{3a}$ where a is the absorption coefficient $a = -100\ln(\mathrm{UVT})$ UVT is UV radiation transmission. Alternatively, (2) $\Gamma = \frac{1}{3(a+\sigma_s)-C_1\sigma_s}$ where a is the absorption coefficient, σ_s is the scattering coefficient, and C_1 is the linear-anisotropic phase function coefficient	(1) Yu et al. (2008), Chen et al. (2011) (2) Li et al. (2010)
Finite Line Source or Multiple Point Source Summation (MPSS) Model	Available in Liu et al. (2004)	Lyn et al. (1999), Bolton (2000), Liu et al. (2004), Sozzi and Taghipour (2006), Hofman et al. (2007b), Younis and Yang (2010)
Multiple segment source summation (MSSS)	Available in Liu et al. (2004)	Liu et al. (2004, 2007), Wols et al. (2010b, c, (2012)
Modified line source integration (LSI) model	Available in Liu et al. (2004)	Blatchley (1997), Liu et al. (2004), Zhao et al. (2009)
Infinite-line source model or radical model	$I(r) = \frac{I_0 T^{\alpha(r-R_i)}}{2\pi r}$ where r is the radial distance from the lamp, I_0 is the UV lamp output (energy rate per unit length), T is the UV transmittance of the fluid, R_i is the radius of the UV lamp sleeve, and α is the extinction coefficient multiplied by the concentration of the absorbing species. For this model, the radiation fluence rate and irradiance become identical.	Taghipour and Sozzi (2005), Sozzi and Taghipour (2006)
Presumed dose distribution or exponential probability density function (PDF)	$f(D) = \lambda\cdot\exp(-\lambda(D - D_{\min}))$ where D represents the UV dose, $D_{\min}$ is the shift in dose distribution and λ is a distribution factor.	Wols et al. (2011)
The Discrete Ordinates (DO) Radiation Model	Available in Fluent user's guide (2006).	Crapulli et al. (2010)

3.3. Optimization of contactor configuration

Contactor configuration optimization which aims to obtain the maximum disinfection efficiency is an important research direction in water and wastewater treatment industry. Note that here hydraulic efficiency is considered as an index of disinfection efficiency in accordance with the majority of the literature. Various residence time statistics have been used to quantify hydraulic characteristics of water disinfection systems, which should ideally approach those of a plug flow reactor. These statistics include θ_{10}, corresponding to the normalized time it takes 10% of the injected tracer mass to exit the monitoring section. Normalization of θ_{10} is made with the theoretical mean residence time (i.e. the volume of the system divided by the flow rate through the system). A second statistic is the dispersion index, σ^2, defined as the ratio between σ_t^2 and θ_g^2, where σ_t^2 is the variance of the residence time distribution (RTD) curve and θ_g is the normalized time to the center of mass of the RTD curve. Finally, the Morrill or simply the Mo index is defined as the ratio between θ_{10} and θ_{90}, where θ_{90} corresponds to the normalized time it takes 90% of the injected tracer mass to exit the monitoring section. Index θ_{10} has been traditionally used as an indicator for short-circuiting. A high value of θ_{10} corresponds to weak short-circuiting. Furthermore, σ^2 and the Mo index have been recommended as good indicators of mixing under high mixing and low mixing conditions, respectively (Teixeira and Siqueira, 2008). Low values of σ^2 or Mo correspond to relatively weak mixing.

It is well-known that reduction of dead zones and short-circuiting leads to improved disinfection efficiency (Wols et al., 2008a,b; Bolaños et al., 2008; Kim et al., 2010; Amini et al., 2011; Zhang et al., 2013b). Increasing the number of baffles is a commonly used approach to reduce dead zones and diminish short-circuiting. Several studies have concluded that an increase of the number of baffles usually leads the fluid flow to approach plug-flow conditions characteristic of a plug-flow reactor (Wols et al., 2008a,b; Kim et al., 2010; Amini et al., 2011). Essential for achieving plug-flow conditions is the use of spatial separation of the flow to limit diffusion between chambers. However, a minor side effect caused by the increment of baffles is that more energy needs to be spent for driving the flow through the contactor (Zhang et al., 2013b).

Instead of increasing the number of baffles, proper rearrangement of chambers may have the same effect of reducing dead zones and diminishing short-circuiting. In the study of Amini et al. (2011), it is shown that the hydraulic efficiency of a six-baffle wall contactor with a proper rearrangement can be higher than that of a contactor with nine baffle walls.

Proper adjustment of the locations of inlet, outlet and diffusers may also improve hydraulic conditions. The hydraulic efficiencies of nine configurations of a disinfection tank with different inlet and outlet locations were compared by Stamou (2008). The one with the best hydraulic efficiency was proposed for construction. Cockx et al. (1999) conducted two-phase flow simulations of an initial disinfection tank and a refurbished disinfection tank with an adjustment of the locations of ozone diffusers. Their numerical results found that the refurbished disinfection tank could achieve a higher inactivation level for *Cryptosporidium* at the same operation costs. Modifying the shape of the baffle (such as adding a turning vane at the baffle end) to make the flow turn smoothly, is another way to reduce dead zones (Wols et al., 2010a). Tafilaku et al. (2010) conducted a numerical study on three designs of a disinfection clearwell with concentric baffles, conventional serpentine baffles and modified serpentine baffles. The results show that the configuration with conventional serpentine baffles has the highest hydraulic efficiency among these three configurations.

Table 6
Reported constants in the Hom–Haas model for ozone inactivation (adapted from Zhang (2006)).

Microorganism	$k_{\mu,m}$	x	y	Source
Cryptosporidium parvum oocysts	$0.68 \times 1.08^{T-22}$	0.71	0.73	Gyurek (1999), Li and Gyurek (2001)
Giardia	$2.35 \times e^{0.0723 \times T}$	1	1	Carlson et al. (2001)
Viruses	$4.90 \times e^{0.07 \times T}$	1	1	Carlson et al. (2001)

Note that the T used in the expressions of calculating $k_{\mu,m}$ is water temperature (°C).

Minor modifications of existing contactors to improve disinfection efficiency have been made based on troubleshooting existing contactors via CFD. Such modifications include adding chamfers, increasing end gap and so on (Phares et al., 2009). Attempts at optimizing contactor configuration with the aid of CFD simulations are summarized in Table 9.

4. Challenges in disinfection process simulation

Up to date, most reported studies have focused on flow and tracer transport simulation, and few studies have involved the simulation of chemical reaction process as well (Cockx et al., 1999; Greene, 2002; Huang et al., 2004; Bartrand, 2006; Zhang, 2006; Zhang et al., 2007; Bolaños et al., 2008; Wols et al., 2010a; Talvy et al., 2011). Studies that have incorporated inactivation kinetics modeling into CFD are even fewer (Huang et al., 2004; Zhang, 2006; Zhang et al., 2007; Bolaños et al., 2008; Wols et al., 2010a; Talvy et al., 2011). The present review study found that the challenges existing in disinfection process simulation include: 1) unsteady flow structure effects, 2) multi-phase flow effect, 3) complexity of reaction system, 4) uncertainty of inactivation kinetics, and 5) closure problem for chemical source terms.

4.1. Unsteady flow structure effect

As mentioned earlier, the accuracy of flow simulation is critical to disinfection process modeling. The majority of studies have successfully employed RANS for flow and tracer transport simulation. The primary reason why RANS has been successful is because steady or quasi-steady short-circuiting exists in most contactors and the unsteady (intermittent) small-scale eddies inside dead zones have little impact on tracer transport (Zhang et al., 2013a). However, since RANS resolves the mean flow only, a significant error may appear once energetic unsteady flow structures develop in the flow. Recent reports have pointed out that under such conditions LES is a more suitable approach than RANS due to its capability of capturing unsteady flow features (Wols et al., 2010b; Kim et al., 2010; Zhang et al., 2014b).

In an UV disinfection application, Wols et al. (2010b) found that RANS wrongly predicts local flow features around a UV lamp. This phenomenon was mainly caused by Kármán Vortex Street which is a typical unsteady flow structure in a flow around a blunt body. LES was employed and matched the experimentally measured velocity profile better than RANS. Zhang et al. (2014b) investigated a baffled contactor and a column contactor which are typically used for ozone and chlorine disinfection. Results showed that LES is a more reliable strategy than RANS in simulating tracer transport in column contactors due to its ability to better predict the spatial transition to turbulence characterizing the flow. However, in baffled contactors where such transition does not occur and the flow is characterized by a quasi-steady short circuiting jet and dead zones, RANS performs as well as LES.

Besides the significant impact on tracer transport, unsteady flow structures are expected to have a considerable impact on reaction and inactivation processes. Further exploration of this issue using higher resolution approaches such as LES, detached LES (Spalart et al., 1997; Strelets, 2001) or even DNS should be explored in the future as computational power becomes more affordable.

4.2. Multi-phase flow effect

For ozone disinfection process simulation, a multi-phase flow simulation should be more accurate than a single-phase flow simulation since it is closer to reality. However, the majority of previous studies tended to neglect the effect of gas phase in the disinfection process for two reasons: 1) unknown parameters, such as bubble size distribution, mass transfer coefficients, models for closure of the two-phases, etc.; 2) a single-phase flow simulation is algorithmically simpler and less computationally expensive. Only a small portion of studies have conducted multi-phase flow simulations (Cockx et al., 1999; Ta and Hague, 2004; Bolaños et al., 2008; Bartrand et al., 2009; Talvy et al., 2011).

Bartrand et al. (2009) found that for water flow down a vertical column contactor with a counter (upward) gas flow, an increment

Table 7
A summary of CFD codes used in reported studies on disinfection tanks.

Category	Code	Sources
Commercial software	ANSYS fluent (or fluent)	Huang et al. (2004), Taghipour and Sozzi (2005), Sozzi and Taghipour (2006), Elyasi and Taghipour (2006), Phares et al. (2009), Wilson and Venayagamoorthy (2010), Josset et al. (2010), Li et al. (2010), Chen et al. (2011), Talvy et al. (2011)
	ANSYS CFX (or CFX)	Wright and Hargreaves (2001), Stamou (2002, 2008), Greene et al. (2006), Bartrand (2006), Zhang et al. (2007), Gresch et al. (2009), Bartrand et al. (2009), Tafilaku (2010), Lee et al. (2011), Launer et al. (2013)
	COMSOL	Gualtieri (2006), Hofman et al. (2007a, b), Wols et al. (2010b, c), Wols et al. (2011), Wols et al. (2012)
	PHOENICS	Peplinski and Ducoste (2001), Zhao et al. (2009)
	STAR-CD	Khan et al. (2006)
	COMET (Demirdzic et al., 1997)	Younis and Yang (2010)
	ASTRID CFD code (developed by Electricite H de France, EDF).	Cockx et al. (1999)
Free software	FEMLAB (developed by Chalmers University of Technology)	Bolaños et al. (2008)
In-house code	Finlab (Labeur and Wells, 2007)	Wols et al. (2008a,b, 2010a)
	Hydro3D-GT (LES code)	Kim et al. (2010, 2013a, b)
	SSIIM (RANS code) (Olsen, 2005)	Kim et al. (2010, 2013a, b)
Open-source code	OpenFOAM	Zhang et al. (2013a, b, 2014a, b)

Table 8
The impacts of studied parameters on disinfection efficiency or predicting disinfection efficiency.

Category	Item	Relationship	Source
Operation parameters	pH	Low pH is favorable for achieving high inactivation efficiency.	Kim (2005)
	Temperature	As temperature decreases, predicted inactivation efficiency decreases.	Kim (2005), Talvy et al. (2011)
	Bubble size variation	Bubble size variation causes lower ozone gas–liquid transfer rate and consequently causes lower concentration of dissolved ozone and lower pathogen removal efficiency.	Talvy et al. (2011)
	Ozone-consuming substances (OCS) variation	The increase in OCS loading significantly increases *C. parvum* survival ratios.	Huang et al. (2004)
	Method of tracer injection	Method of tracer injection slightly affects tracer RTD results.	Zhang et al. (2008)
	Kinetics and mixing state	Disinfection efficiency is affected by both mixing and kinetics (and their interaction).	Greene (2002), Greene et al. (2006)
	Dead zone volume percentage	Higher dead zone volume percentage leads to lower disinfection efficiency.	Lee et al. (2011)
Configuration parameter	Inlet configuration	Inlet configurations, such as inlet baffle and inlet pipe, can significantly impact reactor hydrodynamics.	Greene (2002), Greene et al. (2002, 2006)
	The direction and magnitude of the inlet flow	For a single-column contactor with side entry, the flow pattern was found to be crucially dependent on both the direction and magnitude of the entry velocity from the inlet pipe.	Ta and Hague (2004)
	Sampling locations	Sampling location has a significant influence on tracer RTD prediction or measurement.	Zhang et al. (2008)
	Flow length to flow width ratio	High flow length-to-width ratio results in a high level of disinfection credit for a given concentration of disinfectant.	Peplinski and Ducoste (2001), Li et al. (2006)
	Baffle spacing or baffle numbers	A perfect baffle spacing exists to achieve the possible highest hydraulic efficiency.	Kim et al. (2013b)
	Wall reflection of light	At higher inactivation levels, the effect of wall reflection is more influential.	Chen et al. (2011)
Parameters in modeling	Time step interval	Larger time step serves to increase the amount of tracer dispersion.	Peplinski and Ducoste (2001)
	Turbulent intensity of inflow	Tracer RTD prediction can be strongly dependent on turbulent intensity of inflow boundary condition.	Huang et al. (2002)
	Turbulent Schmidt number	Turbulent Schmidt number requires calibration since it is found to depend on geometry of disinfection tank.	Kim et al. (2013a)

of gas flow rate would promote stronger short-circuiting in both physical experiments and numerical simulations. Based on the simulation results, the explanation for this was that the upward flow of liquid phase within the bubble plume and reduction of the effective column cross sectional area through which downward-flowing liquid passes result in stronger short-circuiting. However, for a baffled contactor, especially a full-scale baffled contactor, the impact of gas flow on water flow may be less significant due to a lower ratio of gas flow rate to liquid flow rate. For example, the ratio of gas flow rate to liquid flow rate for a typical full-scale baffled contactor in a water treatment plant is 1.6%–3.3% (Talvy et al., 2011) while that for a column contactor the ratio is 7.6%–45% (Bartrand et al., 2009; Bolaños et al., 2008). Furthermore, in a column contactor, the gas flows in opposite direction to the bulk water flow and thus can significantly affect the overall flow, whereas in a baffled contactor, the gas flow can potentially influence the water flow only in the chambers where the gas diffusers are located, thereby making the effect of the gas flow on the overall flow negligible. In order to better understand the role of gas flow in disinfection processes for both column and baffled contactors, further exploration via simulations and physical experiments is required.

4.3. Complexity of reaction system

The overall complexity of the reaction system is represented via the source term in Equation (6) which is mainly caused by the variety of species presented in the system and the complexity of kinetics for each elementary reaction. Usually, the reaction system in a disinfection process consists of an excessively high number of elementary reactions to be covered by modeling. Thus, it is necessary to develop a truncated or reduced reaction mechanism. The reduced reaction mechanism should contain a minimum number of species while preserving the characteristics of the reaction system.

Table 9
The methods of optimizing contactor configuration.

Optimizing modifications	Objective	Examples
Increasing the number of baffles	Separate flow spatially to hinder diffusion in order to approach plug flow	Evans et al. (2003), Wols et al. (2008a,b), Kim et al. (2010), Amini et al. (2011), Zhang et al. (2013b)
Rearrangement of chambers	Change flow path to improve hydraulics	Hannoun et al. (1998, 2003), Tafilaku (2010), Amini et al. (2011)
Proper adjustment of the locations of inlet, outlet and diffusers	To diminish dead zone regions	Cockx et al. (1999), Wright and Hargreaves (2001), Stamou (2002, 2008), Angeloudis et al. (2014)
Modifying the shape of baffle	To diminish dead zone regions	Wols et al. (2010a)
Troubleshooting with minor modification such as adding chamfers and increase end gap	Weaken short-circuiting	Phares et al. (2009)

An approach to simplify a reaction system is based on time-scale analysis (Okino and Mavrovouniotis, 1999; Zhang et al., 2014a). The basic steps behind time-scale analysis are

- Identify regions exhibiting different time scale behavior;
- Identify species having fast reaction rate or fast time scale within each region and lump them into a smaller set of pseudo species;
- Simulate the dynamics of the reaction system by a smaller set of variables characteristic of each region.

Another approach is to consider only the global reaction of the species of interest. This is commonly used in chlorine and ozone disinfection process simulation.

Besides the number of reactions, the complexity of reaction kinetics serves to increase the difficulty of modeling as well. Typically, first-order reaction kinetics is sufficient to describe the reaction system. However, in reality, the reaction rate could be higher or lower than first order, or in other complicated forms. For example, the kinetics of ozone self-decomposition used in reported studies is of first-order reaction rate (Cockx et al., 1999; Huang et al., 2004; Bartrand, 2006; Zhang, 2006; Zhang et al., 2007; Bolaños et al., 2008; Wols et al., 2010a; Talvy et al., 2011); however, as reported by Gurol and Singer (1982), ozone decomposes by a second-order reaction. In practice, a first-order approach may lead to satisfactory results as long as the ozone consuming species do not reduce significantly. The uncertainty of the reaction rate constants also has a significant impact on the accuracy of predictions. Since reaction rate constants depend on environmental parameters, such as pH and temperature, it is critical to use appropriate reaction rate constants in modeling.

4.4. Uncertainty of inactivation kinetics

For chemical disinfection (e.g. ozone disinfection, chlorine disinfection), the specific mechanisms of microorganism inactivation are not well understood (Crittenden et al., 2005). Inactivation kinetics could be of either first-order reaction or second-order reaction or even higher-order reaction. And the inactivation rate depends on the properties of each microorganism, disinfectant, and environmental parameters, such as temperature and pH. Furthermore, the inactivation rate can vary by as much as six orders of magnitude from one microorganism to another, even for the same disinfectant (Crittenden et al., 2005). How to overcome the uncertainties in inactivation kinetics and rate constants remains a challenge in the modeling of disinfection process, especially with various microorganisms.

Several inactivation kinetic models have been developed. Gyurek and Finch (1998) have written a summary of inactivation kinetic models. In the experiments of ozone disinfection for HPC bacteria (Gyurek and Finch, 1998), the Incomplete gamma Hom (I.g.H.) model showed the best performance in describing the HPC bacteria survival curve. However, the most commonly employed inactivation kinetic model in CFD has been the Chick–Watson model which has the simplest formula, as described earlier.

Although inactivation kinetics models have been developed, there is still important information missing for conducting a CFD simulation involving inactivation. For instance, up to date, the appropriate amounts of ozone needed to inactivate *Cryptosporidium* oocysts in water at various temperatures and pHs have not been clearly defined (Juranek, 1995). As a result, previous disinfection modeling studies (Huang et al., 2004; Zhang, 2006; Zhang et al., 2007; Bolaños et al., 2008; Wols et al., 2010a; Talvy et al., 2011) have not considered the consumption of disinfectant by pathogens. Note that the existing inactivation models such as the Hom–Haas model and the Chick–Watson model are only for calculating the pathogen decay rate without considering the corresponding consumption of disinfectant. Fortunately, in practice the consumption by microorganisms is usually low. Thus it is acceptable to neglect the consumption by microorganisms in modeling.

4.5. Turbulence-chemistry interaction

In Table 1, the commonly used source terms for species transport equations were discussed. If the source term is represented by a second-order reaction, then information regarding turbulence-chemistry interaction in the form of a turbulence closure would be required. Closure for chemical source terms is important in the modeling of finite rate reactions. Usually the reactions in disinfection process can be categorized into finite-rate chemistry or slow chemistry. For slow chemistry, the turbulence-chemistry interaction is simple since mixing by turbulence is fast enough that the mixing is complete before the reaction occurs. A first-order moment closure method has been commonly used to treat the turbulence-chemistry interaction in slow chemistry. However, it is much more challenging to treat the turbulence-chemistry interaction in finite rate chemistry. Ranade (2002) and Fox (2003) have explained the closure problem encountered in the modeling of turbulent reactive flow with finite rate chemistry. In this section, a brief introduction of this closure problem and the potential solutions are reviewed.

4.5.1. Turbulence-chemistry interaction in disinfection process modeling

Closure of chemical source terms is required for RANS or LES, but not for DNS. In RANS, the governing equation of species transport phenomena, Eqn. (4), can be written in the following form:

$$\frac{\partial\langle C_i\rangle}{\partial t}+\langle u_j\rangle\frac{\partial\langle C_i\rangle}{\partial x_j}+\frac{\partial\left\langle C_i'u_j'\right\rangle}{\partial x_j}-\frac{\partial}{\partial x_j}\left(D_i\frac{\partial\langle C_i\rangle}{\partial x_j}\right)=\langle S_{C_i}\rangle \tag{9}$$

where $\langle\rangle$ denotes the Reynolds-averaging operation. The term $\partial\langle C_i'u_j'\rangle/\partial x_j$ is commonly modeled by the gradient-diffusion hypothesis (Pope, 2000) which has been mentioned in section 2.2.

The most difficult term to close in Eqn. (9) is the Reynolds-averaged chemical source term $\langle S_{C_i}\rangle$. The nonlinearity of chemical source term increases the difficulty of modeling. Take natural organic matter (NOM) in ozone disinfection for example. Recall the source term for NOM in Table 1; thus, the Reynolds-averaged source term in the transport equation for concentration of NOM, would be

$$S_{[NOM]}=-k_{NOM}\left\{\langle[NOM]\rangle\langle C_l\rangle+\left\langle[NOM]'C_l'\right\rangle\right\} \tag{10}$$

where k_{NOM} is a second-order rate constant; $\langle C_l\rangle$ and C_l' are mean and fluctuation of the concentration of dissolved ozone respectively; $[NOM]$ and $[NOM]'$ are mean and fluctuation of the concentration of NOM, respectively.

The covariance term in Eqn. (10), i.e. $\langle[NOM]'C_l'\rangle$, must be closed or modeled since $[NOM]'$ and C_l' are fluctuations that are not accessible in RANS. This closure problem is similar to the Reynolds stress closure problem requiring the use of a model such as the k-ε turbulence model, discussed earlier. Note that LES is characterized by a similar closure problem for the reaction source term arising due to the spatial filtering of the equations (in similar fashion to the Reynolds-averaging operation in RANS).

Table 10
Summary of the closures for the chemical source term in disinfection process simulation.

Closure approach		Strengths	Limitations	Sources
Moment closures	First-order moment closures	Simple	Only suitable for slow chemistry	Fox (2003)
	Higher-order moment closures using the covariance of mixture fraction	Have the ability to model one-step chemistry	Poor prediction for multi-step chemistry	Fox (2003)
Lagrangian models	The IEM model	Simple and can be applied to check for sensitivity to micro-mixing effects	Does not consider flow effect	David and Villermaux (1975), Fox and Villermaux (1990), Fox (1991), Fox et al. (1994)
	Age-based model	Simple and can predict concentration at exit (outflow) of a reactor	Cannot be used to predict the concentration distribution inside a reactor	Fox (2003)
	Multi-environmental models	Have the ability to model slow, fast and finite-rate reaction	Empirical parameters existing in the model need to be fitted	Ritchie and Togby (1979), Mehta and Tarbell (1983), Ranade and Bourne (1991), Ranade (1993), Kolhapure and Fox (1999)
	Multi-environment presumed PDF models	Have the ability to model slow, fast and finite-rate reaction	The presumed PDF needs to be well selected for each situation	Fox (1998, 2003)
Linear eddy model		Have been applied to a wide variety of applications	Computationally-intensive	Kerstein (1988, 1990, 1992), Cremer and McMurtry (1998)

If the reaction rate is much slower or much faster than the turbulent mixing rate, the source term in (10) can be simplified by a first-order closure method (i.e. $\langle [NOM]' C_l' \rangle = 0$ in Eqn. (10) above) or set to zero, respectively (Fox, 2003). If the reaction rate is comparable to the mixing rate, the covariance term in (10) cannot be neglected. The covariance term could be a complicated function of the reaction rates and flow condition making it difficult to find a general method for obtaining a closure model over a wide range of chemical time scales.

4.5.2. Potential models for finite-rate turbulence-chemistry interaction in disinfection process

The physical significance of covariance terms is the interaction between reaction and turbulence mixing or turbulence-chemistry interaction. To model the turbulence-chemistry interaction could be even more challenging than to develop a pure turbulence model (i.e. a Reynolds stress model) due to the complexity of the interactions and the number of species in a reaction system (Georgiadis et al., 2009).

The existing models for finite-rate chemistry can be categorized into two groups: PDF (probability distribution function) models and non-PDF models.

The PDF models, especially the transport PDF models (Ranade, 2002), can provide a complete description of the reaction process. However, to solve the PDF model is a challenge for CFD codes which are based on Eulerian system. Usually, the PDF models are suitable for Lagrangian CFD approaches such as Monte-Carlo methods. These models are computationally intensive and difficult to implement in Eulerian CFD codes. A solution to this drawback is to use a presumed or pre-determined PDF model rather than solving for it. But, the presumed PDF model can be unreliable and inaccurate if the statistical data of the underlying physical experiment is not available as is the common situation. Thus currently, PDF models are usually not practical for modeling chemical disinfection processes.

Early attempts at using non-PDF models were simple, focusing on simulating the interaction of micro-mixing and chemical reactions. Examples include the engulfment model (Baldyga and Bourne, 1989) and the Interaction by Exchange with the Mean (IEM) model (David and Villermaux, 1975). However, the effects of large scale (or macro) flow structures, such as short-circuiting and dead zones occurring in disinfection contactors, were not considered in these models (Ranade, 2002). However, the simplicity of the IEM model makes it useful for verifying sensitivity to micro-mixing effects (Fox and Villermaux, 1990; Fox, 1991; Fox et al., 1994). The IEM model is a simple age-based model. The more complicated age-based models are based on residence time distribution (RTD) obtained from tracer tests. Since RTD is usually generated by the data measured at the exit of a reactor, the aged-based models cannot be used to predict the concentration distribution inside a reactor. Note that the age-based models are based on a Lagrangian system.

The linear eddy model (Kerstein, 1988, 1990, 1992) is another kind of model which aims to represent the turbulent mixing and reaction of a scalar quantity (e.g. a chemical species). The basic idea of the linear eddy model is to treat convection and diffusion separately as two different mechanisms acting on the evolution of chemical species. This provides a useful and insightful way to look into the turbulent mixing of the reacting species. Monte-Carlo simulation is required for the time evolution of chemical species thus making the linear eddy model generally inaccessible to the more popular Eulerian-based CFD codes.

Next the discussion turns focus on models which are more suitable to be implemented into Eulerian-based CFD codes. These models are moment closures, including both first-order and higher-order moment closures, and multi-environment models with and without a presumed PDF model.

4.5.2.1. First-order moment closures. In the situation that the chemical time scales are all large compared with the mixing time scale, i.e. the slow-chemistry limit, a simple first-order moment closure can be adequate. The 'default' closure in most commercial CFD codes is to assume that all scalar covariances are zero (Fox, 2003), which is the simplest first-order moment closure. However, if any chemical reaction is faster than the turbulent mixing, this approximation would result in a poor prediction. Thus, first-order moment closures should be used cautiously when applied to reactive flow with finite chemistry.

4.5.2.2. Higher-order moment closures. Several attempts have made at developing higher-order moment closures (Dutta and Tarbell, 1989; Heeb and Brodkey, 1990; Shenoy and Toor, 1990). The simplest closure approach is to relate the covariances of reactive scalars to the variance of mixture fraction which can be computed by solving inert-scalar-variance transport equations along with the transport equation for the mean mixture fraction (Fox, 2003). Although this approach has the ability to be applied to one-step chemistry, the extension of this approach to multi-step chemistry has been proven to be unreliable (Fox, 2003). A more general

higher-order moment closure strategy consists of solving the transport equations for the scalar covariances directly. However, as shown by Fox (2003), this strategy would generate difficult closure problems that need extra models which have not been developed yet.

4.5.2.3. Multi-environment models. Multi-environment models are another category of Lagrangian models. In these models, the well macro-mixed reactor is broken up into sub-grid-scale environments with uniform concentrations. For example, in a four-environment model (Villermaux and Falk, 1994), environment 1 contains fluid entering the system through the first feed stream; environments 2 and 3 contain partially mixed fluid; and environment 4 contains fluid entering the system through the second feed stream. Chemical reactions can only occur in environments 2 and 3. Such a model has been used to represent mixing in semi-batch reactors of different sizes studied by a novel parallel-competing test reaction and mixing of a stream of initiator in a recycle tubular reactor packed with static mixers for the polymerization of styrene (Villermaux and Falk, 1994). Multi-environment models have provided a flexible yet simple framework for modeling turbulent reactive flow. And it has been demonstrated that multi-environment models have the ability to simulate not only slow and fast reactions (Ranade and Bourne, 1991), but also finite-rate reactions (Ranade, 2002). However, since the relative volume of each environment and exchange rates between environments must be specified, it is a challenge to fit the parameters in the model when applied to general problems, especially problems with complex geometries.

4.5.2.4. Multi-environment presumed PDF models. As demonstrated by Fox (1998, 2003), it is possible to reformulate multi-environment models in terms of a multi-peak presumed joint PDF leading to a closed form of the chemical source term. Fox (1998) successfully applied a four-environment presumed PDF model to fully-developed turbulent flow with a two-step reaction in a one-dimensional tubular reactor. Comparing to a full PDF model, the principle advantage of multi-environment presumed PDF models is the fact that it is not necessary to integrate with respect to the joint composition PDF in order to evaluate the chemical source term since the latter has been closed. However, it requires particular attention to the definition of the micro-mixing terms when the model is extended to inhomogeneous flow (Fox, 1998), or to homogeneous flows with uniform mean scalar gradients (Fox, 2003).

There are a few other non-PDF models for simulation of reactive flow, for example, laminar diffusion flamelets (Peters, 1984, 2000) and the conditional-moment closures (Tsai and Fox, 1995). These models are not discussed here as they have been primarily designed for combustion. The potential closures for the chemical source term in disinfection process simulation are summarized in Table 10.

The above models have been mainly developed for RANS simulation. In LES, a similar closure problem exists for modeling the covariance of spatially filtered chemical source terms, which are to take into account the sub-grid turbulence-chemistry interaction. Closures based on LES have been developed for combustion (Fureby, 2008; Pitsch et al., 2008). However, to the authors' knowledge, no LES-based closure has been developed for water flows with finite-rate chemistry commonly seen in water and wastewater treatment plants. Nevertheless, semi-empirical methods, such as the Partially Stirred Reactor (Correa, 1993), the Eddy Dissipation Concept (EDC) (Berglund et al., 2008; Fureby, 2008) and Thickened Flame Model (TFM) (Colin et al., 2000) developed for LES simulation of combustion are valuable references for developing a closure method suitable for disinfection process simulation. Furthermore, Fox (2003) describes how the multi-environment presumed PDF models initially developed for RANS could be potentially extended to LES. And all the procedures in the RANS-based multi-environment presumed PDF models can be re-used in developing an LES-based multi-environment presumed PDF model with a few minor modifications.

5. Summary and prospectus

CFD applied to disinfection studies has become more prominent due to advancement of computing power and numerical methods. Studies reviewed here concentrated on the development of a simulation method or framework for disinfection process, the impacts of parameters on modeling disinfection, and optimization of the configuration of disinfection contactors. Relationships between parameters, such as operation parameters (e.g. pH and temperature), configuration parameters (e.g. flow length to width ratios), modeling parameters, and disinfection efficiency were summarized. Ways that can increase disinfection efficiency by optimizing contactor configuration were summarized as well. Challenges in simulation of disinfection process were identified and discussed. For example, challenges in resolving unsteady flow features may be overcome by advanced turbulence resolving approaches such as LES. Turbulence-chemistry interaction is the most challenging issue. Although several closures were discussed for turbulence-chemistry interaction in this review, it is not possible to validate the applicability of such closure models for turbulence-chemistry interaction unless the errors caused by unsteady flow features, multi-phase flow, and uncertainty of reaction system have been sufficiently reduced.

As CFD continues to become more accessible, new applications should be explored such as

- Studies of the impact of changes in reactor configuration (including the arrangement of diffusers) on disinfectant utilization efficiency. CFD could potentially be used to estimate the operational cost for different scenarios in order to find the minimum cost.
- Studies on the energy costs/savings incurred by disinfection approaches. Disinfection is an energy-consuming technology. For example, ultraviolet (UV) disinfection has a high consumption of electricity for UV lighting; ozone disinfection has a high level of electricity use for ozone generation.
- Applications to emerging disinfection technologies: disinfection by pulsed arc electrohydraulic discharge (Ching et al., 2001), ultrasound disinfection (Hoyer, 2002) and combined oxidants disinfection, such as UV and chlorine (Lotierzo et al., 2003) and ultrasound and chlorine (Plummer et al., 2002).

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