Environmental Modelling & Software 58 (2014) 71–85

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

Review

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

Jie Zhang*, Andrés E. Tejada-Martínez, Qiong Zhang

Department of Civil and Environmental Engineering, University of South Florida, Tampa, 4202 E. Fowler Ave., ENB 118, FL 33620, USA

ARTICLE INFO

Article history:
Received 19 September 2013
Received in revised form
27 March 2014
Accepted 3 April 2014
Available online 8 May 2014

Keywords:
Modeling
Computational fluid dynamics
Reactive flow
Water treatment
Disinfection

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.

* Corresponding author.
E-mail address: jiez@mail.usf.edu (J. Zhang).

http://dx.doi.org/10.1016/j.envsoft.2014.04.003
1364-8152/

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

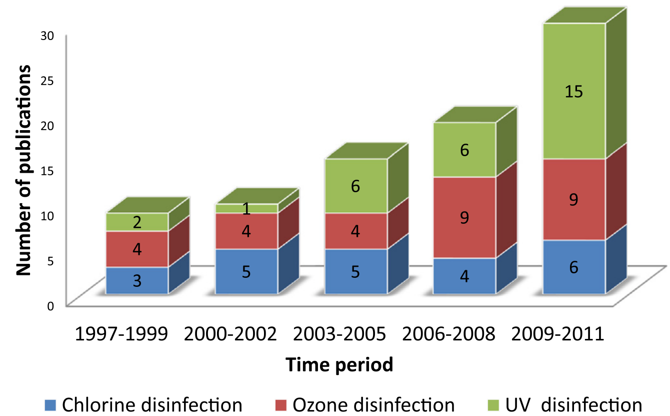

Fig. 1. Statistics of publications on CFD applied to disinfection (searched with Engineering Village and Web of Knowledge).

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

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