Environmental Modelling & Software 25 (2010) 573–582

Contents lists available at ScienceDirect

Environmental Modelling & Software

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

Evaluation of different disinfection calculation methods using CFD

B.A. Wols [a,b,*], J.A.M.H. Hofman [a,b,c], W.S.J. Uijttewaal [b], L.C. Rietveld [b], J.C. van Dijk [b]

[a] *KWR Watercycle Research Institute, 3430 BB Nieuwegein, The Netherlands*
[b] *Delft University of Technology, 2600 GA Delft, The Netherlands*
[c] *Waternet, 1108 AA Amsterdam, The Netherlands*

A R T I C L E I N F O

Article history:
Received 8 October 2008
Received in revised form
15 September 2009
Accepted 23 September 2009
Available online 7 November 2009

Keywords:
CFD
Particle tracking
Contact time
Disinfection
Disinfection calculation method
Ozone contactor

A B S T R A C T

Computational Fluid Dynamics combined with a particle tracking technique provides valuable information concerning residence times and contact times in chemical reactors. In drinking water treatment, for example an accurate estimation of the disinfection is important to predict the microbial safety. Ozone contactors are widely used for disinfection, but the complex geometry of the system causes suboptimal hydraulics and requires optimizations of the flow. This results in a lower ozone dosage, which may reduce the formation of unwanted disinfection-by-products and the consumption of energy. To that end disinfection needs to be calculated precisely, accounting for the complex hydraulics. Several calculation methods estimating the disinfection performance of ozone contactors were evaluated using Computational Fluid Dynamics. For an accurate disinfection prediction, the full distribution of ozone exposures (CT values) is needed, only a mean CT value or residence time distribution provides insufficient information for an accurate disinfection prediction. Adjustments to the geometry of the ozone contactor that reduce the short-circuit flows resulted in an increase in disinfection capacity, whereas the mean CT value remained the same. A sensitivity analysis with respect to the kinetics was conducted. The gain in disinfection capacity obtained by optimizing the hydraulics was significant for typical values used in practice.

1. Introduction

Because of recent developments in computer technology, Computational Fluid Dynamics (CFD) is increasingly applied to investigate and optimize hydraulic processes in a wide range of applications. For example, prediction of meteorological systems (Kovalets et al., 2008), wind flow and dispersion in urban environments (Solazzo et al., 2009), flooding by rivers (Elíasson et al., 2007) or predicting the efficacy of drinking water installations (Craig et al., 2002; Liu and Ducoste, 2006). It allows for detailed modelling of flow and (turbulent) mixing processes. Combined with Lagrangian (particle tracking) techniques valuable statistical information, such as residence time and contact time, is obtained. Residence time distributions are used to characterize the hydraulics and contact times define the conversion rate of chemical reactions. For disinfection processes in water treatment, the main goal is to guarantee sufficient microbial inactivation. Therefore, microorganisms need to be exposed to a sufficient high concentration of a chemical solution (oxidants such as ozone or chlorine) for a sufficient length of time. The contact time between a microorganism in the water and the chemical solution is mainly determined by the hydraulics. The distribution of contact times largely determines the efficiency of a treatment step. Especially for systems with large recirculation zones, differences in contact time can be large, so that hydraulic optimizations become necessary. A precise prediction of the disinfection, preferably at low computational costs, is then an important issue.

Worldwide, over 3000 ozone contactors exist that are used for disinfection purposes. The ozone contactor consists of a bubble column, where the ozone gas is injected and dissolved in the water, and a number of contact chambers to ensure enough reaction time of the dissolved ozone with the contaminants (Fig. 1). The geometry of the contactor results in a complex flow pattern that requires sophisticated modelling. Also, the production of disinfection-by-products, such as bromate, restricts the ozone dosage. An optimization of the ozone contactor is needed that reduces the production of bromate, whereas the microbial safety is ensured. Several authors used CFD as a tool to optimize ozone contactors (Cockx et al., 1999; Huang et al., 2004; Li et al., 2006; Zhang et al., 2007). They showed that improved hydraulics and/or microbial inactivation are obtained by changing the contactor geometry. However, the disinfection was calculated in different ways. Cockx et al. (1999) and Zhang et al. (2007) used the CT concept and calculated the CT value by solving the scalar transport equations (concerning advection, diffusion and a source term), from which they determined the inactivation out of

* Corresponding author. KWR Watercycle Research Institute, 3430 BB Nieuwegein, The Netherlands.
E-mail addresses: bas.wols@kwrwater.nl, b.a.wols@tudelft.nl (B.A. Wols).

1364-8152/$ – see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.envsoft.2009.09.007

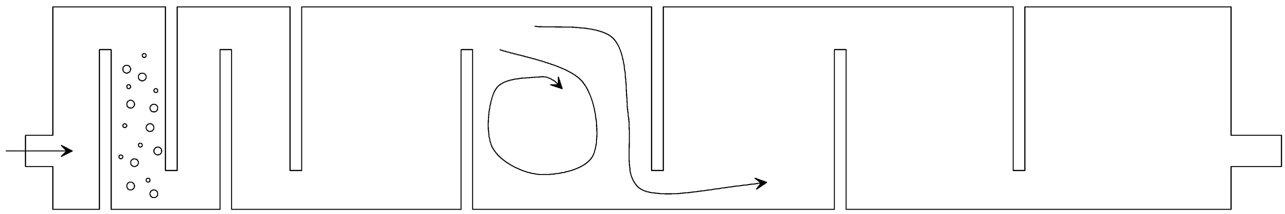

Fig. 1. Geometry of an ozone contactor, baffles cause complex hydraulics.

CT tables (USEPA, 1991; USEPA, 2006). Huang et al. (2004) calculated the microbial inactivation directly by solving the scalar transport equations for a concentration of microorganisms. Li et al. (2006) used a particle tracking technique to determine the residence time distribution, but no disinfection calculation was made here.

The objective of the research was to assess different calculation methods that predict the disinfection in ozone systems. An accurate prediction of the disinfection is beneficial, because it may restrict the ozone dosage, which reduces the formation of disinfection-by-products and reduces the energy consumption. Computational Fluid Dynamics was used as a tool to assess the disinfection calculation methods, because it can determine all the necessary quantities (residence time distributions, ozone concentrations, particle trajectories, CT values) needed for the disinfection calculation, so that a reliable comparison could be made. Moreover, these quantities are much easier obtained by CFD than by measurements. The complexity of a disinfection calculation method increases with increasing number of quantities taken from the CFD model, resulting in a more precise prediction of disinfection at a cost of higher computational time. The most complex disinfection method, the particle tracking method, tracks the paths of individual microorganisms to obtain a distribution of ozone exposures. The residence time distributions obtained from the particle sets were in correspondence with Eulerian calculations (Wols et al., 2008b), indicating that the particle tracks were representative for the fluid flow. The ozone exposure calculated for each particle provides additional information of the hydraulics of the system (particle paths, distribution of CT values), which are not provided by the other calculation methods. The particle tracking simulation comes closest to the actual movement of individual microorganisms in reality, which is expected to result in a very accurate disinfection prediction. For UV systems, Lagrangian methods also predict the microbial inactivation accurately (Ducoste et al., 2005; Sozzi and Taghipour, 2006). The other calculation methods using various assumptions to reduce computing time were assessed with respect to this particle tracking method.

Additionally, the effect of changing the flow by adjusting the contactor geometry was investigated. Next to the effect of hydraulic changes on the disinfection performance, a sensitivity analysis with respect to the kinetic constants (slow ozone decay and inactivation rate constant) was conducted.

2. Methods

2.1. Comparing various approaches to estimate disinfection

The alternative disinfection calculation methods are based upon similar assumptions. First of all, the CFD model calculates the flow fields, turbulent kinetic energies and residence time distributions. These quantities form the starting point of most disinfection methods. The ozone decay process is assumed to be first order. Ozone decay coefficients ranging from 0.001 s^{-1} to 0.01 s^{-1} were used (van der Helm et al., 2007). The disinfection kinetics is represented by a classical Chick–Watson model, which defines the inactivation of microorganisms in the following manner:

$$\frac{dN}{dt} = -k_{\mu}CN, \tag{1}$$

where N is the concentration of microorganisms (n/L), k_{μ} is the inactivation rate constant (L/(mg min)) and C the dissolved ozone concentration (mg/L). Inactivation rate constants depend on the target species and temperature, for *Cryptosporidium parvum* oocysts values range from 0.1 L/(mg min) to 1.0 L/(mg min), see Rennecker et al. (1999) or Long Term 2 Surface Water Treatment Rule (USEPA, 2006). After integration, Eq. (1) is written as:

$$\ln\left(\frac{N}{N_0}\right) = -k_{\mu}\int Cdt, \tag{2}$$

where N_0 is the initial number of microorganisms (n/L). The time integration over the ozone concentration is the motivation for the CT value concept. The disinfection capacity is usually presented by the decimal elimination (*DE*) or log inactivation, which is equal to:

$$DE = -\log\left(\frac{N}{N_0}\right), \tag{3}$$

Given the kinetic constants (inactivation rate constant and ozone decay coefficient) and mean residence time, a maximal removal in case of perfect hydraulics can be formulated. This is represented by a perfect plug flow system, where every fluid element receives an equal ozone dose. When the finite time of the system, presented by the residence time, is taken into account (in case not all the ozone is consumed inside the system), the maximal log removal can be determined. For a first order ozone decay, the ozone concentration as a function of time $C(t) = C_0\exp(-k_s t)$ is substituted into Eq. (2). After integration from 0 to the mean residence time T_h and substituting the result into Eq. (3), the maximal log removal becomes:

$$DE_{\max} = \log(e)\frac{k_{\mu}C_0}{k_s}(1-\exp(-k_s T_h)), \tag{4}$$

where T_h is the hydraulic residence time (s) and k_s is the (slow) decay coefficient of ozone (1/s).

2.1.1. CFD Lagrangian (particle tracking) method

This method comes closest the actual movement of microorganisms, which are also discrete particles. Ducoste et al. (2005) and Sozzi and Taghipour (2006) use a similar approach to estimate the disinfection performance in UV reactors. Using a Lagrangian method the trajectories of individual particles are calculated. Fluctuations of the particles induced by the turbulent motions model the mixing processes precisely (Wols et al., 2008a). These particles are assumed to represent microorganisms that are small enough to move entirely with the fluid (particles without mass, no drag or lift forces are considered). The particles are uniformly injected at the inflow cross-section, where the velocity is also uniformly distributed over the cross-section, so that the particle sets are representative for the fluid volume. From the calculated flow field, a stationary ozone field (C) can be determined by solving an advection–diffusion–decay model, given by:

$$\frac{\partial C}{\partial t} + U_i\frac{\partial C}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) + k_s C = 0, \tag{5}$$

where U_i is the mean velocity (m/s) in x_i (x, y or z-direction) and D_{ij} the diffusion coefficient (m^2/s). Because the concentration of microorganisms is very small, it is assumed that the ozone consumption induced by microorganisms is negligibly small and the ozone is mainly consumed by organic matter. Thus, the particles have no effect on the ozone concentrations. The ozone concentrations are integrated over the particle path, which leads to the CT value of a particle. Every particle receives a certain CT value that corresponds to an inactivation level. Summation over all the particles gives the total inactivation, shown as the total amount N of surviving microorganisms:

$$\frac{N}{N_0} = \frac{1}{N_0}\sum_{i=1}^{N}\exp(-k_{\mu}\varphi_i), \tag{6}$$

where φ_i represents the CT value of particle i. Moreover, from the particle tracking important statistics (such as the distribution of CT values) are obtained that give valuable information about the performance of ozone systems.

2.1.2. CT_{10}-method

In the Surface Water Treatment Rule (SWTR) Guidance Manual (USEPA, 1991), the CT concept is applied, where the microbial inactivation is calculated from the product