Computational modeling of ultraviolet disinfection
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ABSTRACT
The efficient design of ultraviolet light (UV) systems for water and wastewater treatment requires detailed knowledge of the patterns of fluid motion that occur in the disinfection channel. This knowledge is increasingly being obtained using Computational Fluid Dynamics (CFD) software packages that solve the equations governing turbulent fluid-flow motion. In this work, we present predictions of the patterns of flow and the extent of disinfection in a conventional reactor consisting of an open channel with an array of UV lamps placed with their axes perpendicular to the direction of flow. It is shown that the resulting flow is inherently unsteady due to the regular shedding of vortices from the submerged lamps. It is also shown that the accurate prediction of the hydraulic residence time and, consequently, the extent of disinfection is strongly dependent on the ability of the CFD method to capture the occurrence and strength of the vortex shedding, and its effects on the turbulent mixing processes.

Key words | computational fluid dynamics, turbulence, UV disinfection, vortex shedding

INTRODUCTION
The trend towards increased use of UV disinfection in preference to chlorination, which began in the mid 1980s when the US EPA identified UV disinfection as the “best available technology” for wastewater disinfection, has accelerated in recent years with the increase in public awareness of the drawbacks associated with chemical disinfection. By 2006, the number of wastewater treatment plants in the USA has grown to 900 (Leong et al. 2008). As energy costs continue to rise, there is a clear incentive in revisiting the hydraulic aspects of the design of UV systems with view to reducing the hydraulic losses associated with the flow of water around the submerged lamps. A reduction in the hydraulic losses leads directly to a reduction in the energy costs needed to pump the water through the channel whereas a good understanding of the details of the flow patterns can lead to more efficient designs utilizing fewer UV lamps operated at lower power input. Computational Fluid Dynamics (CFD) has now become the tool of choice in the study of fluid-flow problems and it is expected that this technique will eventually become the primary tool in the design of efficient UV disinfection systems as well (e.g. Lyn & Blatchley 2005; Liu et al. 2007; Pan & Orava 2007). In this paper, we focus on a particular aspect of the computations that does not appear to have hitherto received much attention, namely the accurate prediction of the periodic mean-flow unsteadiness that is observed to occur when the water flows around an array of UV lamps with axes vertical to the flow. This arrangement, which is shown in Figure 1(a), is often used in preference to horizontal lamps in systems designed to accommodate significant changes in the level of the water being treated. The observed flow unsteadiness is not due to fluctuations in the conditions that prevail at the channel inlet but, rather, to an intrinsic feature of the flows around vertical tubes at Reynolds numbers that exceed a critical value (e.g. Zdravkovich 1997). The consensus of experimental findings indicates that for a circular cylinder, this critical value is about 40 (based on cylinder diameter and bulk velocity). This value is easily exceeded in a conventional UV disinfection channel. Once this critical value is exceeded,
vortex shedding occurs and the flow around the cylinder separates alternately from either side forming vortices that are advected downstream by the mean flow where they interact with other lamps and with the vortices shed by them. The result is a fairly complex hydrodynamic flow pattern which is far removed from the conditions that prevail in a fully mixed, heterogeneous reactor. It is thus clear that the usefulness of CFD as a practical tool for the design of UV system depends critically on the ability of the computations to accurately predict the occurrence of vortex shedding, and its consequences on the efficiency of UV disinfection. This is demonstrated in this paper.

**METHOD**

The research presented here has been performed using a Computational Fluid Dynamics software package called COMET (Demirdzic et al. 1997). This is a finite-volume method which solves the time-dependent form of the equations that govern the conservation of mass and momentum in three dimensions. The solutions are obtained at a discrete number of nodes sub-dividing the flow domain. A typical distribution of nodes used in this study is shown in Figure 1(b). Since the Reynolds number of the flow in a typical UV disinfection channel is high (typically of the order of 6,000—based on UV lamp diameter and average flow velocity), turbulent flow conditions prevail and, following the usual practice, the governing equations are averaged over a suitable time interval to avoid the excessive computational resources required to solve for the instantaneous flow velocity (Pope 2000). The size of the time interval over which the averaging takes place is taken here to be the same as the computational time-step size (\(\Delta t\)). By averaging the momentum equations, unknown turbulent correlations (the Reynolds stresses) appear and these are determined using a turbulence model. The turbulence model used here is the $k−\varepsilon$ model. It is a two-equation eddy-viscosity model requiring the solution of an equation for the turbulence kinetic energy ($k$) and another for its dissipation rate ($\varepsilon$). These two parameters define the turbulent (or eddy) viscosity which, in turn, is used to calculate the Reynolds stresses. Details are found in Launder & Spalding (1972). The $k−\varepsilon$ model in its standard form is inadequate for the prediction of flows in which vortex shedding is present (e.g. Franke & Rodi 1993). The reasons for this have been discussed in Younis & Przulj (2006) who postulated that the discrete input of energy in the turbulence spectrum that occurs at the Strouhal frequency is not adequately represented by the model for the dissipation rate which is based on the assumption of spectral equilibrium. Younis & Zhou (2006), from analysis of energy transfer rates across a distorted energy spectrum, derived a modification to the dissipation-rate equation that accounts for the effects of vortex shedding on the energy spectral transfer process. The modification takes the form of an additional contribution to the rate of generation of $\varepsilon$ thus:

$$C_{\varepsilon1} = C_{\varepsilon1} + C_{\varepsilon2}\left(1 + C_\varepsilon \frac{k}{\varepsilon Q + k} \frac{\partial (Q + k)}{\partial t}\right)$$

(1)
where $Q = 1/2(U^2 + V^2)$ is the mean-flow kinetic energy and $C_i = 0.38$. This modification was shown to produce substantial improvement in the prediction of vortex shedding in a number of benchmark flows including the case of a circular cylinder with axis vertical to the flow (Younis et al. 2005).

Turning to the model for UV inactivation, the results reported in this paper were obtained with the Eulerian approach. In this approach, each control volume used to sub-divide the flow domain is assumed to be equivalent to a completely mixed reactor wherein the microbial concentration and the UV intensity field are uniformly distributed. The concentration ($C$) of the viable component of the target microorganism is then obtained from the solution of the equation:

$$\frac{\partial C}{\partial t} + u(x,y,t) \frac{\partial C}{\partial x} + v(x,y,t) \frac{\partial C}{\partial y} = \frac{\partial}{\partial x}(\nu_t \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(\nu_t \frac{\partial C}{\partial y}) - R(C,t)$$

(2)

where $\nu_t$ is kinematic eddy viscosity, $\sigma_c = 0.9$ is the turbulent Schmidt number and the velocity components $u(x,y,t)$ and $v(x,y,t)$ are the outcome of the fluid-flow simulations. The maximum value of $C$ occurs at entry to the UV channel and is thereafter reduced with exposure to UV radiation. The mechanism for this reduction (disinfection) is introduced via the term $R(C,t)$ which represents the response of the target microorganism to the delivered UV dose. Thus if $R(C,t)$ is not included, the value of $C$ throughout the channel will eventually equal that at inlet. In this work, $R(C,t)$ is modeled using the first-order Chick-Watson kinetics model:

$$R(C,t) = KC(x,y,t)I(x,y)$$

In this model, the UV intensity $I(x,y)$ due to a single UV lamp is obtained from:

$$I(x,y) = \frac{S}{L} \int_{-L/2}^{L/2} \frac{1}{4\pi r^2 + z^2} \exp\left\{ -[\alpha_w(1 - D/2r) + \alpha_q(t_q/r)(r^2 + z^2)^{1/2}] \right\}$$

(3)

where $S$ is the total power output of the single lamp, $L$ is the total length of a lamp placed at location $(x_i,y_i)$ in the channel, $r^2 = (x - x_i)^2 + (y - y_i)^2$, $z$ is the vertical coordinate, $\alpha_w$ and $\alpha_q$ are the absorption coefficients of radiation in water and in quartz tubing respectively, and $t_q$ = thickness of the quartz jacket. When a number ($N$) of lamps is present, the resulting UV intensity at a point $I(x_i,y_i)$ in the flow field is simply the sum of contributions from all the lamps. In the results that follow, the various parameters that appear in Equation (3) were assigned the same values as Chiu et al. (1999) namely: $S = 26.7$ W, $L = 147$ cm, $\alpha_w = 0.44$ cm$^{-1}$, $\alpha_q = 0.63$ cm$^{-1}$ and $t_q = 0.15$ cm.

In Equation (3), the vertical coordinate (i.e. the coordinate that is perpendicular to the $x$–$y$ plane–the plane of the simulations) is represented by the dimension $z$. Even though the present simulations were two dimensional, the UV intensity in the plane of simulations incorporated the contributions from the parts of the lamp that are located outside this plane. This was done by dividing the vertical length into equal segments on either side of the center plane (2,000 segments in total) and then by incorporating the intensity due to each segment into Equation (3). The resulting UV intensity field using 200 segments is shown in Figure 1(c). The maximum intensity level obtained in the immediate vicinity of each lamp was $I = 29$ mW/cm$^2$, which is identical to the value obtained by Chiu et al. (1999).

Evaluation of the disinfection efficiency was done by estimating the concentration of the target microorganism that remains viable at the channel outlet. This is done by evaluating the average concentration $C$ at the outlet plane:

$$c(t)_{\text{out}} = \frac{\int_{y=0}^{y=B} u(x = x_{\text{out}}, y, t)c(x = x_{\text{out}}, y, t)dy}{\int_{y=0}^{y=B} u(x = x_{\text{out}}, y, t)dy}$$

(4)
where $B$ is the channel width and then by calculating the average extent of disinfection $\mathcal{N}$ from:

$$
\mathcal{N} = \frac{c_{\text{out}}}{C_0}
$$

with $C_0$ being the concentration of the untreated target microorganism at entry into the channel.

## RESULTS AND DISCUSSION

The results reported here were obtained for the channel configuration shown in Figure 1(a). This configuration is the same as that studied computationally by Lyn & Blatchley (2005) and experimentally by Chiu et al. (1999).

The lamps have diameter $D = 0.025$ m. The average flow velocity at channel inlet was $U_0 = 0.24$ m/s which gives a Reynolds number of 6,000. The computational grid consisted of 44,400 nodes non-uniformly distributed with the largest concentration being in the vicinity of the UV lamps. The smallest nodes were thus in direct contact with the lamps with the ratio $n_c/D = 0.00244$ (where $n_c$ is the distance between the center of the node and the lamp wall).

The time-step size was set equal to 0.00036s. The computed results were checked and found to be independent of the grid and time-step size.

An overview of the patterns of disinfection can be seen in Figure 2. Plotted there are the predicted contours of $C$ at several instances in time. In these calculations, $C$ was assigned a constant value at inlet. Thus the time-dependent nature of the results is a direct outcome of the mean-flow unsteadiness due to vortex shedding. For clarity, the contours are color coded such that the color red represents viable, untreated, flow whereas blue represents flow that has received sufficient UV dose to achieve complete disinfection. Figure 2(a) shows the progress of a front of untreated water through the channel. The graduated change in color ahead of the front represents the rate of transport of $C$ but diffusion. Figure 2(b) shows the patterns of disinfection as predicted with the standard $k$–$\varepsilon$ model at time $t = 22.3$ s from the start of release. The model incorrectly predicts an essentially steady flow as evidenced by the regular interface dividing the treated from the untreated flows. An entirely different pattern of disinfection is obtained when the modified model is used. This can be seen in Figure 2(c) at $t = 22.3$ s, and in greater detail in Figure 3. The regular interface previously observed is now replaced by complex pattern of entrainment that bring untreated water closer to the lamps, and of associated eruptions occurring at regular intervals that transport treated water away from the lamps. The widths of the wakes at channel outlet provide an early, qualitative, indication of the beneficial effects of vortex shedding on disinfection.

Turning now to the details of the resulting flows, Figure 4 shows the predicted contours of the turbulent viscosity as obtained with the modified model. As expected, the flow around the UV lamps is quite complex and is characterized by strong interactions between the shed vortices with each other, and with downstream lamps.
The elevated levels of this parameter, which become more pronounced with downstream flow development, are indicative of the increased levels of turbulent kinetic energy that arise from the high shear rates in the separated wakes. This increase further confirms that the vortex shedding induced by the UV lamps plays an important role in increasing the turbulent mixing in the disinfection channel. Further evidence of this effect, and a demonstration of the need to employ a turbulence model that can adequately predict the occurrence and strength of vortex shedding, is presented in Figure 5. Plotted there are the pathlines of massless particles released at the channel inlet. Results obtained with both the standard and the modified forms of the $k-e$ model are presented. The most striking feature of the pathlines predicted by the standard model is their very small departures from the patterns that would be expected in steady-state flows. This is not surprising in view of this model’s known inability to capture vortex shedding of appropriate intensity. Thus, for example, there is no evidence of particles being entrained by the coherent structures, or of them being deflected by the strong shear that is set up in the cross-flow direction. This is in sharp contrast with the results obtained using the modified $k-e$ model which captures the significant deflection experienced.
by some particles e.g. one released from one side of the center plane which is then entrained by the wake of the leading lamp and subsequently deflected to the opposite side of the plane. The ‘capture’ of some particles in the reversed flow regions is also quite apparent as evidenced by their looped trajectories.

Comparisons of the residence time of the particles released at the channel inlet as predicted by the standard and the modified model are shown in Figure 6. In that figure, the particle release position, which is plotted on the horizontal axis, refers to the location of the particle release with respect to the centerline. Thus, for example, position 1 indicates a particle released at location $y/D = -3$, while position 13 refers to location $y/D = +3$ ($y$ is the distance measured from the centerline and $D$ is the lamp diameter). The effects of vortex shedding are seen to produce and overall increase the particles’ total residence time in the channel. This is consistent with the significantly more looped pathlines observed in Figure 5. This increase in residence time is expected to lead to increase in delivered dose and thus to improvement in disinfection efficiency. In terms of the extent of disinfection ($-\log_{10}(N)$), as evaluated from Equation (5), the simulations with the modified $k-\varepsilon$ model yield a value of 0.548 while the steady-state simulations yield the significantly lower value of 0.502. This result implies that there are distinct benefits to be gained by correctly estimating the strength of vortex shedding from the UV lamps.

CONCLUSIONS

Vortex shedding occurs from UV lamps having axes perpendicular to the flow and plays an important role in determining the efficiency of disinfection. The standard $k-\varepsilon$ model, which is arguably the most-widely used turbulence model in CFD for water-treatment applications, fails to capture the correct strength of the shedding process and, consequently, the extent to which this process modifies the flow and the total residence time. An extension to the standard $k-\varepsilon$ model which is derived from analysis of the distorted turbulence-energy spectrum in the presence of direct energy input at the Strouhal frequency is shown to capture the occurrence of the intense vortex shedding observed in experiments, and to correctly obtain the enhancement in turbulent mixing which arises from the interactions of the periodic separated vortices with adjacent lamps and with each other. The improvements in the extent of disinfection predicted with the modified model suggest that the design of UV disinfection channels can be made more efficient by the accurate prediction of the occurrence and strength of vortex-shedding from the UV lamps.

REFERENCES


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