Evaluation of reflection and refraction in simulations of ultraviolet disinfection using the discrete ordinates radiation model

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ABSTRACT

Simulations of UV disinfection systems require accurate models of UV radiation within the reactor. Processes such as reflection and refraction at surfaces within the reactor can impact the intensity of the simulated radiation field, which in turn impacts the simulated dose and performance of the UV reactor. This paper describes a detailed discrete ordinates radiation model and comparisons to a test that recorded the UV radiation distribution around a low pressure UV lamp in a water-filled chamber with a UV transmittance of 88%. The effects of reflection and refraction at the quartz sleeve were investigated, along with the impact of wall reflection from the interior surfaces of the chamber. Results showed that the inclusion of wall reflection improved matches between predicted and measured values of incident radiation throughout the chamber. The difference between simulations with and without reflection ranged from several percent near the lamp to nearly 40% further away from the lamp. Neglecting reflection and refraction at the quartz sleeve increased the simulated radiation near the lamp and reduced the simulated radiation further away from the lamp. However, the distribution and trends in the simulated radiation field both with and without the effects of reflection and refraction at the quartz sleeve were consistent with the measured data distributions.

Key words | CFD, discrete ordinates, reflection, refraction, UV disinfection

INTRODUCTION

The use of ultraviolet (UV) disinfection for drinking water treatment is becoming more popular as a result of the Long-Term 2 Enhanced Surface Water Treatment Rule (LT2ESWTR) (US EPA 2006a) and Stage 2 Disinfection/Disinfection Byproducts Rule (US EPA 2006b). In order for utilities to receive inactivation credits for UV under the LT2ESWTR, systems must first be validated under the specific design configuration and operating conditions planned for full-scale treatment using costly biodosimetry methods. The US EPA’s UV Disinfection Guidance Manual (UVDGM) (US EPA 2006c) provides recommendations for modeling as a potential alternative and/or complement to these costly testing methods. However, standard protocols for modeling UV disinfection are still lacking, and features and processes that impact the accuracy of models and simulations are still being investigated. This paper focuses on processes involving reflection and refraction of UV radiation from walls and surfaces within the UV reactor that can impact the accuracy of UV radiation models and subsequent dose calculations.

Radiation emanating from a UV lamp through a quartz sleeve experiences both reflection and refraction at the air/quartz and quartz/water interfaces. Bolton (2000) found that neglecting reflection and refraction at these interfaces could yield errors up to 25% in fluence rate (irradiation or UV intensity) calculations. Liu et al. (2004) concluded that the discrete ordinates radiation model over predicted the intensity close to the lamps but under predicted the...
intensity far from the lamps because the discrete ordinates radiation model in Fluent (Fluent Inc. 2006) did not include refraction. Refraction at interfaces can be included in the Fluent discrete ordinates radiation model, but the interfaces and geometries of different materials (e.g., lamp, air annulus, quartz sleeve) need to be discretely modeled. Also, neither Bolton (2000) nor Liu et al. (2004) considered wall reflection (from the interior walls of the reactor chamber) in their models. Therefore, the objective of this study was to simulate the experiments of Liu et al. (2004) using a detailed discrete ordinates radiation model (including representation of the lamp, air annulus, and quartz sleeve) to determine the relative importance of reflection and refraction when all relevant processes are considered.

OVERVIEW OF EXPERIMENT

Figure 1 shows a sketch of the experiment conducted by Liu et al. (2004). A cylindrical nickel-plated stainless steel chamber was filled with water, and a low-pressure mercury UV lamp penetrated through the center of the chamber. Potassium iodide/iodate actinometers placed in spherical quartz vessels were suspended at 18 locations throughout the chamber to measure the spatial distribution of the UV radiation. An equation from Rahn et al. (2000) was used to relate measured quantities (e.g., temperature, change of absorption coefficient, volume of actinometer solution, cross-sectional area of the spherical vessels, exposure time), as well as reflection from the quartz vessel, to the incident radiation for each actinometer. Results were reported for a water UV transmittance of 88%. Figure 2 shows the location of the actinometer sensors in the UV reactor chamber.

Liu et al. (2004) acknowledged that reflection from the chamber walls could play an important role in the metallic reactor because the “interior wall surface was smooth with a high surface finish.” Radiation reflected from the walls would increase the measured radiation by the actinometers. Luckiesh (1929, Figure 5) reported that the reflectance of nickel and steel near the germicidal wavelength of 254 nm can be up to $\sim 40\%$. The impact of wall reflection is considered in the models discussed in the next section.

MODELING APPROACH

The discrete ordinates radiation model in Fluent, a commercial computational fluid dynamics software package, solves the radiative transfer equation over a domain of discrete solid angles. It calculates the radiation intensity as a result of absorption, scattering, and emission within the fluid, along with reflection and emission from surfaces.
within the fluid. Because it is implemented within the Fluent CFD code, the impacts of geometry within the reactor (e.g., shadowing and reflection from sensors, lamps, surfaces, etc.) can also be readily considered. This provides consistency with the hydraulic CFD simulations that typically include the effects of this geometry. In addition, a user-defined function (UDF) can be implemented to calculate the cumulative dose of particles moving through the reactor. The cumulative dose (J/m²) is calculated as the product of the irradiation (W/m²) and the exposure time (s) at each step along the particle path. In this study, only the discrete ordinates radiation model was used in Fluent to simulate the measured radiation distribution in the test performed by Liu et al. (2004, see Figure 1).

Figure 3 shows the mesh (employing half symmetry) that was used in the Fluent DO radiation model. The lamp was modeled as an external semitransparent wall with a radiative flux (W/m²) that corresponded to the lamp power and dimensions shown in Figure 1. For a 16 W lamp with a 41.38% UVC efficiency, the simulated radiative flux of the half-lamp was calculated to be 251 W/m². This boundary condition was applied as a diffuse irradiation source along the lamp surface at a single germicidal wavelength (single-band model).

The air annulus (1.1 cm thick) between the lamp and the quartz sleeve was discretized and assigned a refractive index of one. The quartz sleeve was treated as an internal semi-transparent wall and assigned a refractive index of 1.52 (Bolton 2000). The water (fluid) region was assigned a refractive index of 1.38 (Bolton 2000) and extended to the walls of the reactor chamber. A total of 28,080 cells were used in the model. Grid convergence studies performed with coarser meshes showed that the results did not change at this refinement level. An angular discretization ($\theta \times \phi$) of 5 x 5 for the solid angles was found to be sufficient to generate a smooth radiation profile around the lamp, and the pixilation was set to 3 x 3 (as recommended by the Fluent User’s Guide). Default values were used for the under-relaxation factor (1) and discretization solution control (first-order upwind). Runs took about a minute to converge using an Intel Xeon quad-core CPU running at 2.5 GHz.

The interior walls of the reactor chamber were specified as either a specular (mirror-like) or diffuse reflecting surface with a prescribed diffuse fraction and internal emissivity. The reflectivity and absorptivity for these opaque surfaces are calculated in Fluent as follows:

Diffuse reflectivity $= f_d(1 - e)$  
Specular reflectivity $= (1 - f_d)$  
Absorptivity $= f_d e$

where $f_d$ is the diffuse fraction and $e$ is the internal wall emissivity (note that the values in Equations (1)–(3) sum to one). For a purely diffuse surface reflectivity of 40% (Luckiesh 1929, Figure 5), the internal emissivity was set to 0.6 and the diffuse fraction was set to one. For a purely specular reflectivity of 40%, the diffuse fraction was set to 0.6 and the internal emissivity was set to one. For zero reflectivity, both the diffuse fraction and internal emissivity were set to one.
Reflection and refraction at the air/quartz and quartz/water interfaces along the internal and external surfaces of the sleeve were treated specularly in Fluent. The angle of refraction at each interface is calculated using Snell's law, and the amount of reflection at each interface is calculated using the Fresnel laws \cite{Bolton2000}. Therefore, bending and focusing of the emitted rays from the lamp are captured in the current model. To neglect reflection and refraction within the quartz sleeve, the refractive indices can all be set to one, or the sleeve and annulus can be removed entirely from the model (radiation boundary applied to external surface of sleeve). The latter approach was implemented in Ho et al. \cite{Ho2008}. If the radiation boundary is applied directly to the external surface of the sleeve, the equivalent radiation flux was calculated to be 102 W/m², which accounts for the increased surface area of the quartz sleeve relative to the lamp.

**MODELING RESULTS**

**Inclusion of reflection and refraction at the quartz sleeve**

Figure 4 shows the simulated radiation field including the effects of reflection and refraction through the quartz sleeve. The reflectivity of the chamber walls was set to 40% (diffuse). Results for diffuse wall reflection were nearly identical to the results for specular wall reflection, so only the diffuse wall reflection results are shown.

The incident radiation decreases with increasing radial distance from the lamp as a result of absorption in the water (UVT = 88%) and the increasing circumferential area. Figure 5 shows a plot of the measured and simulated incident radiation (with and without reflection) at the 18 actinometer sensor locations in Liu et al. \cite{Liu2004}. The results show that the simulated results are generally consistent with the measured data. The average absolute relative error between the measured and simulated data is 19% for the simulations with wall reflection and 33% for the simulations without wall reflection. The relative difference between the simulations with and without reflection ranged from...
several percent near the lamp (sensors 13–18) to nearly 40% further away from the lamp (sensors 1–6). Sensors 1–6 were positioned near the interior walls of the chamber, so reflection of UV radiation from these walls had a more significant impact on these locations.

The simulated results from the discrete ordinates radiation model do not show a significant bias at locations near versus far from the lamp. In general, the simulated results tend to under predict the measured values at all locations, even close to the lamp. It should be noted that Liu et al. (2004) state that the actinometers close to the lamp (e.g., sensors 13–18) may become saturated and therefore underestimate the true incident radiation at some of those locations. A possible reason for the under prediction may be the exclusion of the length of lamp extending above and below the reactor chamber (see Figure 1). In the simulation, only the portion of the lamp within the boundaries of the reactor chamber were modeled. Additional UV radiation from the top and bottom portions of the lamp outside of the chamber may have contributed additional energy to the system.

Figure 6 shows the simulated incident radiation as a function of vertical position within the chamber. The data and simulated results are grouped according to radial distance \((x = 3.98, 7.28, \text{ and } 10.7 \text{ cm})\) from the lamp center. Although the locations of the sensors vary slightly from these radial positions, the sensors are clustered closely around these three radial positions (see Figure 1). The results show that the simulated irradiation is lower towards the top and bottom of the chamber, especially close to the lamp. The inclusion of wall reflection (40% reflectivity) increases the simulated radiation throughout the vertical transects, not just close to the side, top, and bottom walls. The relative impact of wall reflection is more pronounced at larger radial distances. In general, the predicted results are lower than the measured data at all locations, consistent with the previous observations.

These results show that the inclusion of reflection and refraction in the Fluent discrete ordinates radiation model can yield consistent trends with the measured data in Liu et al. (2004). The next section evaluates the results of the discrete ordinates radiation model when reflection and refraction at the quartz sleeve are neglected.

### Neglecting reflection and refraction at the quartz sleeve

Reflection and refraction at the quartz sleeve can be omitted by setting the refractive indices of the quartz sleeve and the water to one. Figure 7 and Figure 8 show the simulated...
incident radiation distribution within the reactor chamber both with (solid lines) and without (dashed lines) reflection and refraction modeled at the quartz sleeve. Figure 7 shows results from simulations that include reflection (40%) from the interior walls of the chamber, and Figure 8 shows results from simulations that neglected wall reflection. The results show that the simulated incident radiation is increased everywhere when wall reflection is included, especially near the top and bottom walls in the vicinity of the lamp ($x = 3.98$ cm). The inclusion of wall reflection in the model tends to improve the match between predicted and measured data. The results also show that neglecting reflection and refraction at the quartz sleeve (dashed lines) increases the simulated radiation near the lamp ($x = 3.98$ cm) and reduces the simulated radiation further away from the lamp ($x = 10.7$ cm), consistent with the findings of Liu et al. (2004). However, the distribution and trends in the simulated radiation field both with and without the effects of reflection and refraction at the quartz sleeve are consistent with the measured data distributions. The conclusion by Liu et al. (2004) that neglecting reflection and refraction at the quartz sleeve causes significant over prediction of the incident radiation near the lamp and under prediction far from the lamp cannot be deduced from comparison with the data using the current models. The average absolute relative difference in simulated incident radiation between simulations with and without reflection and refraction at the quartz sleeve at radial distances of 3.98, 7.28, and 10.7 cm from the lamp center were approximately 6%, 4%, and 9%, respectively, for the simulations with wall reflection. When wall reflection was neglected in the models, the average differences were approximately 4%, 6%, and 11%, respectively.

Simulating and meshing the air annulus and quartz sleeve to capture the effects of reflection and refraction at the air/quartz and quartz/water interfaces may be computationally challenging using the discrete ordinates radiation model. Although the simulation of these features in this study was straightforward because of the small size of the
test, the inclusion of multiple lamps, sensors, large reactors, and long lengths of piping in the model may prohibit the simulation of the quartz sleeve and air annulus in an actual UV disinfection system. In Ho et al. (2008), commercial UV reactors were simulated, and the boundary condition for the lamp radiation was modeled as a diffuse source on the outer surface of the sleeve, which was calibrated to either sensor data or measured RED. The sleeve itself was an extruded cut (void) in the model domain. This greatly simplified the model and reduced the number of elements required in the discrete ordinates radiation model.

Figure 9 shows the simulated irradiation field when the radiation boundary condition was applied on the outer surface of the sleeve (reflection and refraction at the quartz sleeve were neglected). Figure 10 shows the distribution of simulated incident radiation using this method (solid lines). The results of the previous method where the air annulus and quartz sleeve were modeled but the indices of refraction were set to one are also shown (dashed lines). Results indicate that the two methods yield similar results. The average absolute difference between the two methods is only 2% along vertical transects at radial distances of \( x = 3.98 \) and 7.28 cm, and up to 5% further from the lamp (\( x = 10.7 \) cm).

**CONCLUSIONS**

A detailed discrete ordinates radiation model of the transmissivity test detailed in Liu et al. (2004) was developed in this study. The effects of reflection and refraction at the quartz sleeve were investigated, along with the impact of wall reflection from the interior surfaces of the chamber. Results showed that the inclusion of wall reflection improved matches between predicted and measured values of incident radiation throughout the chamber. The difference between simulations with and without reflection ranged from several percent near the lamp to nearly 40% further away from the lamp.

Comparisons between simulations with and without reflection and refraction at the interior and exterior surfaces of the quartz sleeve showed that neglecting reflection and refraction at the quartz sleeve increased the simulated radiation near the lamp and reduced the simulated radiation further away from the lamp, consistent with the findings of Liu et al. (2004). However, the distribution and trends in the simulated radiation field both with and without the effects of reflection and refraction at the quartz sleeve were consistent with the measured data distributions. The average absolute relative difference in simulated incident radiation between simulations with and without reflection and refraction at the quartz sleeve at radial distances of 3.98, 7.28, and 10.7 cm from the lamp center were approximately 6%, 4%, and 9%, respectively, for the simulations with wall reflection. When wall reflection was neglected in the models, the average differences were approximately 4%, 6%, and 11%, respectively.

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REFERENCES


Fluent, Inc. 2006 Fluent 6.3 User’s Guide. Fluent Inc., Lebanon, NH.


