Computational Fluid Dynamics Based Models for Assessing UV Reactor Design and Installation

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Computational Fluid Dynamics Based Models for Assessing UV Reactor Design and Installation
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FOREWORD

The Water Research Foundation (Foundation) is a nonprofit corporation that is dedicated to the implementation of a research effort to help utilities respond to regulatory requirements and traditional high-priority concerns of the industry. The research agenda is developed through a process of consultation with subscribers and drinking water professionals. Under the umbrella of a Strategic Research Plan, the Research Advisory Council prioritizes the suggested projects based upon current and future needs, applicability, and past work; the recommendations are forwarded to the Board of Trustees for final selection. The Foundation also sponsors research projects through the unsolicited proposal process; the Collaborative Research, Research Applications, and Tailored Collaboration programs; and various joint research efforts with organizations such as the U.S. Environmental Protection Agency, the U.S. Bureau of Reclamation, and the Association of California Water Agencies.

This publication is a result of one of these sponsored studies, and it is hoped that its findings will be applied in communities throughout the world. The following report serves not only as a means of communicating the results of the water industry’s centralized research program but also as a tool to enlist the further support of the nonmember utilities and individuals.

Projects are managed closely from their inception to the final report by the Foundation’s staff and large cadre of volunteers who willingly contribute their time and expertise. The Foundation serves a planning and management function and awards contracts to other institutions such as water utilities, universities, and engineering firms. The funding for this research effort comes primarily from the Subscription Program, through which water utilities subscribe to the research program and make an annual payment proportionate to the volume of water they deliver and consultants and manufacturers subscribe based on their annual billings. The program offers a cost-effective and fair method for funding research in the public interest.

A broad spectrum of water supply issues is addressed by the Foundation’s research agenda: resources, treatment and operations, distribution and storage, water quality and analysis, toxicology, economics, and management. The ultimate purpose of the coordinated effort is to assist water suppliers to provide the highest possible quality of water economically and reliably. The true benefits are realized when the results are implemented at the utility level. The Foundation’s trustees are pleased to offer this publication as a contribution toward that end.

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Chair, Board of Trustees
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EXECUTIVE SUMMARY

The use of ultraviolet (UV) disinfection for drinking water treatment is expected to increase, and computational fluid dynamics (CFD) is expected to play an increasing role in the design, implementation, and validation of UV disinfection systems. A CFD model provides detailed simulations of flow fields and hydraulic behavior within the piping and reactor that may impact reactor performance. In addition, UV radiation and dose models can be readily incorporated into or combined with CFD-based hydraulic models for simulation of the reduction equivalent dose (RED). Thus, CFD-based models may provide an alternative for expensive biodosimetry validation methods and a potential substitute for revalidation. Although CFD has not yet been accepted as a stand-alone validation method, it may be used to build confidence in the validation process and address “what if” scenarios if different configurations are being evaluated.

RESEARCH OBJECTIVES

The goal of this work was to evaluate whether CFD-based models could be used to accurately model the hydraulics, UV intensity distribution, and RED in commercial UV reactors with different reactor and piping configurations. In particular, the primary objective was to demonstrate whether CFD-based models could be used to compare the performance of installed UV disinfection systems relative to validated systems with different piping configurations (potentially caused by retrofits or space limitations at the installed site). Based on input from the Project Advisory Committee (PAC), the prioritized tasks for this project were as follows:

1. Use CFD to evaluate the impact of changes in inlet and outlet piping on performance (see “Simulations of IDI Reactor” in Chapter 3 and Chapter 5).
2. Demonstrate how the relative performance of an installed UV system can be compared to a validated system (i.e., provide the methodology needed to demonstrate that the installed system is at least as good as the validated system) (see Chapter 5).

Additional activities that were also identified as important if time and funding permitted were as follows:

3. Demonstrate how CFD can be used to redefine the validated dose monitoring equation (RED) based on changes in the installed system (see “CFD-Based Dose Monitoring Equations” in Chapter 5)
4. Generate a CFD QA/QC checklist that regulators can use when evaluating CFD reports (see Chapter 6).
5. Conduct round-robin CFD benchmarking study (not performed; however, two codes were used to simulate the RED for two of the three different UV reactors simulated. See “Simulations of UV Intensity and RED for the IDI Reactors” and “Simulations of UV Intensity and RED for the Calgon Reactor” in Chapter 3).
Three different commercial reactors were simulated: (1) an IDI (Degremont Technologies) Ozonia Aquaray® H2O 20-inch reactor, (2) a Calgon Sentinel® 12-inch reactor, and (3) a Trojan Swift® 10L30 reactor. The IDI reactor was validated using three different piping and reactor configurations. Each IDI configuration was simulated to determine if the different approach hydraulics and subsequent dose distributions were adequately modeled relative to the trends in the data. The Calgon and Trojan reactors provided an opportunity to model other commercial reactors with different piping, lamp, and sensor configurations. Although these reactors were not validated under different piping configurations, the suite of different operational conditions (i.e., flow rate, UVT, different lamps on or off, lamp power) during the validation tests provided a good basis to assess and compare the capabilities of the CFD-based models.

The results of the modeling showed that CFD-based simulations were able to capture the salient trends in measured RED as a function of different flow rates, UV transmittances, and lamp power. In addition, the use of different pipe sizes and the comparison of runs with and without a baffle plate showed notable impacts on the measured RED in the IDI validation tests. The simulated performance of these different IDI configurations matched the observed trends. Simulations of the Calgon and Trojan reactors also resulted in good matches between simulated and measured data for a wide range of operating conditions. A summary of the primary objectives is provided below.

Use CFD to Evaluate the Impact of Changes in Inlet and Outlet Piping

Simulations of the IDI validation tests consisted of three different configurations that impacted the approach hydraulics into the reactor. The L-rig (without baffle plate) used inlet and outlet pipes that were larger than the diameter of the reactor, so the flow converged into the opening of the reactor. The M-rig used pipes that were smaller than the diameter of the reactor, so the flow expanded into the reactor. Tests were also performed on the M-rig with and without a baffle plate near the inlet of the reactor. The baffle plate was intended to “straighten” the flow before passing through the reactor.

Results of both the tests and simulations showed that the L-rig performed better than the M-rig (without baffle) for equivalent operating conditions (and for operating conditions when the L-rig would be expected to perform worse; e.g., when the flow rate was greater in the L-rig). The M-rig tests with the baffle plate performed better than tests without the baffle plate for similar operating conditions. These results indicate that CFD simulations can be used to assess the impact of different piping configurations on approach hydraulics and reduction equivalent dose.

Demonstrate Relative Performance of an Installed UV System Compared to a Validated System

A method was presented to compare the performance of an installed reactor configuration relative to a validated reactor configuration that may have a different piping configuration. A plot is generated of the simulated RED of the installed configurations as a function of the simulated...
RED for the validated configuration. The operational conditions are identical for the installed vs. validated runs. Points falling above the $y = x$ (see Figure 5.3) line indicate that the installed configuration performs better than the validated configuration, and vice versa. The proposed method is consistent with guidance in USEPA (2006, Appendix D.6). In addition, a revised dose monitoring equation can be generated based on the results of the simulations of the installed configuration.

Simulations of the different IDI configurations showed that this method is capable of demonstrating whether an installed configuration will perform at least as well as the validated configuration. The simulated results of the IDI configurations matched the observed trends in the measured RED among the L-rig, M-rig (with baffle), and M-rig (no baffle) configurations.

Generate a QA/QC Checklist that Regulators Can Use When Evaluating CFD Reports

A checklist has been created that distills the important features and processes for CFD-based modeling of UV disinfection systems. While this checklist is not exhaustive, it presents a number of key issues that should be considered by the modeler, manager, or regulator when CFD-based models are used to predict the performance of UV disinfection systems (see Chapter 6).

Additional details regarding the important findings and relevant issues associated with the CFD-based models developed in this report are provided below.

Hydraulic Modeling

- Based on previous studies investigating Reynolds-Averaged Navier-Stokes (RANS) based turbulence models that did not show significant differences, only one turbulence model (realizable k-$\varepsilon$) was used in this study. Other models that simulate turbulent fluctuations directly (e.g., large eddy simulation) should be studied in the future.
- Grid convergence studies and comparisons to head-loss data showed that the hydraulic models were in general agreement with the actual flow fields.
- Turbulence parameters (e.g., $k$ and $\varepsilon$) should be initialized using appropriate equations to ensure proper convergence of the flow field and turbulence parameters.
- The discrete random walk (DRW) particle tracking model (which includes perturbations to the particle movement based on turbulent fluctuating velocity components) can yield different results than the particle tracking model without DRW at lower flow rates ($Re \sim 100,000$). At lower flow rates, the turbulent kinetic energy (which is proportional to the turbulent fluctuating velocity components) are more predominant relative to the mean velocity magnitude. Therefore, the random motion is more pronounced in the particle paths. At higher flow rates ($Re \sim 1,000,000$), the mean velocity magnitude is predominant and the particle paths are smoother (they follow the mean velocity). Therefore, for turbulent conditions encountered in UV reactors, the DRW particle tracking model is recommended.
- Different piping configurations and the presence of a baffle plate had a notable impact on the approach hydraulics and measured RED in the IDI reactor validation tests. These impacts were successfully modeled.
UV Radiation Modeling

- Two different UV radiation models were used: UVXPT and the discrete ordinates radiation model in FLUENT.
  - UVXPT modeled the effects of absorption in the water, reflection/refraction at the quartz sleeve, spectral dependencies, lamp output distribution (spectral and directional), and UV sensor characteristics (spectral and directional).
  - The discrete ordinates model in this study assumed single-band gray radiation. Reflection and refraction at the quartz sleeve was neglected, and the lamp UV radiation was applied diffusely on the outside of the sleeve. Sensitivity studies showed that this approximation was valid. The effects of wall reflection were included, as well as shading from features within the reactor (e.g., UV sensors, lamps, wiper screw).

- The UV output of the lamps used in the models can be calibrated by comparing the measured and predicted UV sensor readings. However, if the UV intensity model does not rigorously capture the features of the UV sensor that affect the measured UV intensity (e.g., acceptance angle, reflection from the lens, spectral dependencies, etc.), the simulated lamp output power cannot solely be calibrated to the sensor readings. In these cases, an alternative approach is to calibrate the simulated lamp output power so that the simulated RED matches the measured RED (see Appendix C for more details). The calibration run that is chosen should match as closely as possible to the operating conditions that are simulated (number of lamps, flow rate, UVT, etc.).

- Wall reflection can significantly affect the UV intensity distribution within the reactor at high UVT (> 88%). Wall reflection depends on the finish of the reactor’s walls and can exceed 50 percent with electro-polished steel. Wall reflection is readily included in the Fluent DO radiation model, and wall reflection has been recently incorporated into UVXPT. We therefore recommend including wall reflections when the UVT is greater than ~88%. Processes such as fouling and aging of the wall surfaces will tend to reduce the wall reflectivity, but these processes were not investigated in this study.

Inactivation Kinetics

- The action spectra or wavelength response of the microbes is used in UVXPT to model germicidal dose delivery with UV systems using polychromatic medium pressure lamps. One important source of error with action spectra measurements that has been recently reported is the use of bandpass filters. Those filters typically have a full width at half maximum of 10 nm. This causes errors on the order of 25% because the dose-response observed with a given filter can be more affected by wavelengths above or below the nominal wavelength of the filter. One recommendation for future validation of MP UV systems is that the dose-response of the test microbe should be measured with both LP and MP collimated beams. Comparison of the LP and MP dose-response calculations will provide insight into the validity of the MP dose calculation and potentially define a correction factor that can be applied to the UV dose distribution predicted using CFD-based dose models.
Simulations of RED

- The average relative errors in predicted RED using the Fluent DO radiation model ranged from approximately \(~6–40\%\) for the IDI and Calgon reactors, depending on features used in the model (e.g., DRW vs. no-DRW, reflection vs. no reflection), lamp configuration, UVT, and choice of run for model calibration. The average relative errors using the UVXPT model ranged from approximately \(~10–30\%\) for the IDI, Calgon, and Trojan reactor simulations. Errors above 20\% in UVXPT were typically caused by simulations that neglected wall reflection with high UVT. Larger errors in Fluent were typically caused by the selection of calibration runs for the lamp output that were not consistent with the configuration of the current simulation and (in the Calgon simulations) when only one lamp was operational.

ADDITIONAL RESEARCH

Based on the results of this work, the following additional research is recommended:

- Additional work is needed to evaluate the directional profile of emission from UV lamps. The emission profile depends on the optical density of the arc at the relevant wavelength of emitted light (Phillips, 1983). A small element along the lamp acts more like a Lambertian emitter as the optical density of the arc increases. While the output from a linear fluorescent lamp behaves like an ideal Lambertian emitter, the output of mercury lamps without fluorescent coatings (e.g., the 265 nm line of a medium pressure UV lamp) is more complex, behaving between what would be expected with a Lambertian and point source emitter. If the behavior is not known, the angular dependence of the UV lamp’s output represents a potential source of modeling error.

- More work is needed measuring the reflection coefficient of reactor surfaces as a function of the wavelength of light, understanding the impact of the reactor surface finish on specular and diffuse reflection, and modeling the impact of specular and diffuse reflections on UV intensity fields and dose delivery. Experimental work is also needed to confirm the impacts of reflection on UV intensity, log inactivation and RED. Lastly, work is needed on understanding the regulatory impacts of reflection on UV dose monitoring at the water treatment plant application since reflection will be impacted by fouling and surface corrosion, yet UV sensors will not be monitoring the impact of these phenomena on UV dose delivery.

- If additional validation data become available that compare alternative piping and/or inlet/outlet configurations for UV reactors, the methods presented in this report should be applied to further assess CFD-based tools for predicting flow, UV intensity, and UV dose in those systems.
CHAPTER 1
INTRODUCTION

BACKGROUND

The use of ultraviolet (UV) disinfection for drinking water treatment is expected to increase as a result of the Long-Term 2 Enhanced Surface Water Treatment Rule (LT2ESWTR) (USEPA, 2006a) and Stage 2 Disinfection/Disinfection Byproducts Rule (USEPA, 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. Such validation uses costly biodosimetry methods and must be re-done if a utility desires to change their configuration or operation of the UV system.

A primary reason for the extensive UV system validation requirements is that a significant knowledge gap exists regarding hydraulic effects on UV disinfection performance. As a result of this gap, the USEPA’s UV Disinfection Guidance Manual (UVDGM) (USEPA, 2006c) has conservative recommendations for inlet/outlet hydraulic configurations and correction factors for the reduction equivalent dose (RED). In many cases, utilities will be retrofitting UV into existing treatment processes. Space may be limited, so the installed piping configuration may not be identical to the validated configuration, and the inlet/outlet piping configurations may not be able to meet recommendations provided by the UVDGM. Thus, utilities need a tool to assess hydraulic impacts on UV disinfection performance and to evaluate alternative configurations early in the design process. Moreover, a better understanding of the effects of inlet/outlet hydraulic configurations on UV disinfection performance will result in more pragmatic design recommendations, with the potential to significantly reduce capital costs in future UV installations.

Computational fluid dynamics (CFD) is a modeling tool that has been shown to successfully determine relative differences in UV reactor performance (AwwaRF, 2006). A CFD model provides detailed simulations of flow fields and hydraulic behavior within the piping and reactor that may impact reactor performance. In addition, UV radiation and dose models can be readily incorporated into or combined with CFD-based hydraulic models for simulation of the RED. Thus, CFD-based models may provide an alternative for expensive biodosimetry validation methods and a potential substitute for revalidation. Although CFD has not yet been accepted as a stand-alone validation method, it may be used to build confidence in the validation process.

LITERATURE REVIEW

A recent AwwaRF project #2682, Hydrodynamic Characterization of UV Reactors, (AwwaRF, 2006) evaluated prediction of UV system performance through experimental and numerical techniques that assessed UV intensity, hydraulics, UV dose distributions, and microbial inactivation levels. This project found CFD to be a useful tool for assessing UV reactor performance, but a general CFD protocol was not developed. AwwaRF Project #2768 (2007) provides a guide to implementing and modeling UV disinfection systems for water treatment plants. Specific recommendations for CFD modeling are provided along with operational and design guidance, but evaluations of commercial reactors were not performed. In addition, evaluation of the impact of
different piping configurations and their impact on approach hydraulics and simulated RED was not performed.

AwwaRF project #2682 (2006) provides a comprehensive review of the literature regarding testing and modeling of various components of UV disinfection systems, including low field characterization, turbulent modeling, UV intensity distributions, Langrangian vs. Eulerian dose modeling, microbial inactivation and transport, and UV disinfection design. The reader is referred to that report for a thorough review of the literature. Specific articles and reports are cited in this current report as individual topics and details are discussed.

SCOPE AND OBJECTIVES

The goal of this project is not to develop a universal CFD model that will be broadly applicable to UV disinfection systems. Rather, the objective of this project is to evaluate the effectiveness of CFD as a tool to assess the impact of design and operational changes on desired performance objectives such as UV dose distribution and the resulting reduction equivalent dose. These evaluations and applications will be demonstrated in the context of the protocol and guidance established in the UVDGM to facilitate potential regulatory acceptance of the use of CFD in demonstrating compliance of installed UV disinfection systems.

Based on input from the Project Advisory Committee (PAC), the prioritized tasks for this project were as follows:

1. Use CFD to evaluate the impact of changes in inlet and outlet piping on performance (see “Simulations of IDI Reactor” in Chapter 3 and Chapter 5).
2. Demonstrate how the relative performance of an installed UV system can be compared to a validated system (i.e., provide the methodology needed to demonstrate that the installed system is at least as good as the validated system) (see Chapter 5).

Additional activities that were also identified as important if time and funding permitted were as follows:

3. Demonstrate how CFD can be used to redefine the validated dose monitoring equation (RED) based on changes in the installed system (see “CFD-Based Dose Monitoring Equations” in Chapter 5)
4. Generate a CFD QA/QC checklist that regulators can use when evaluating CFD reports (see Chapter 6).
5. Conduct round-robin CFD benchmarking study (not performed; however, two codes were used to simulate the RED for two of the three different UV reactors simulated. See “Simulations of UV Intensity and RED for the IDI Reactors” and “Simulations of UV Intensity and RED for the Calgon Reactor” in Chapter 3).
CHAPTER 2
MODELING APPROACH

A brief review of the hydraulic, UV radiation, and dose models used in this study is provided in this section. Figure 2.1 summarizes the generic model components and their interaction. First, a geometric model of the UV reactor and piping is developed. The model is discretized (meshed), and CFD models are developed with appropriate boundary conditions to simulate the hydraulic behavior and flow fields. The geometry is also used in radiation models to simulate the UV radiation field within and near the UV reactor. Both the hydraulic results and the UV radiation fields are used to calculate the dose to particles moving through the system. The distribution of particle doses is then used to calculate an effective inactivation and reduction equivalent dose.

CFD HYDRAULIC MODEL

The CFD software FLUENT was used to simulate the hydraulic conditions within the UV disinfection systems. An inflow velocity was applied at the upstream end of the model using a uniform velocity distribution corresponding to the respective test conditions. The downstream boundary was an outflow boundary (assumes a zero normal gradient for all flow variables except pressure; appropriate when the exit flow is close to fully developed and when the details of the flow velocity and pressure are not known at the exit). All other surfaces were wall boundaries. AwwaRF (2006, project #2682) evaluated six different turbulence models (standard k-ε, k-ε, RNG, k-ω (88), k-ω (98), Reynolds Stress Transport Model, and the two-fluid model). Their results showed that although certain models were able to characterize the turbulence and flow in different locations, no single turbulence model significantly outperformed the others in general. In addition, Munoz et al. (2007) evaluated two turbulence models (k-ε and Reynolds stress model) and found that the same general flow pattern and velocity profiles were generated, with minor differences close to the reactor wall. In these cases, the standard turbulence model were sufficient. However, more detailed turbulence models such as Large Eddy Simulations may be necessary in specific cases and configurations where discrete models of eddy formation and transport impact the simulated RED. If significant discrepancies exist between the simulated and measured RED, then more detailed hydraulic processes turbulent models may be needed.

In this study, the k-ε realizable turbulence model was used in all cases with the standard wall function, which provides a commonly used approximation for the near-wall velocity for turbulent flows (Shih et al., 1995). The realizable k-ε model differs from the standard k-ε model in two ways: (1) the realizable k-ε model contains a new formulation for the turbulent viscosity and (2) a new transport equation for the dissipation rate, ε, derived from an exact equation for the transport of the mean-square vorticity fluctuation. The term “realizable” refers to the fact that the model satisfies mathematical constraints on the Reynolds stresses (must remain positive) by making a previously defined constant, C_μ, in the definition of the turbulent viscosity a function of the mean flow and turbulence quantities. Neither the standard k-ε model nor the RNG k-ε model is realizable and can violate the positivity of the Reynolds stress terms. The realizable k-ε model has been validated for a wide range of flows including jets, mixing layers, channel and boundary layer flows, and separated flows. The realizable k-ε model is likely to provide superior performance for flow involving rotation, boundary layers with strong adverse pressure gradients, separation, and
recirculation (Fluent, 2006). Additional details and governing equations of the realizable k-ε turbulence model are provided in Appendix A.

The models were all run to steady state in double precision. The solution was calculated with the SIMPLE algorithm utilizing a second order accurate discretization (per AIAA, 1998). The models were run to a converged solution, defined by an absolute residual of less than 0.001 for all solved variables. After the flow solution converged for each of the reactor models, particles were released at the inlet and tracked in time as they traveled through the system. Particle tracking was performed both with and without the discrete random walk model as part of the sensitivity analyses. The particle paths were used in conjunction with the UV radiation model described in the next section to determine a dose distribution.

**UV RADIATION MODELS**

A number of previous studies have developed and evaluated models to simulate the UV intensity (or fluence rate) distribution in UV reactors. Bolton (2000) and Liu et al. (2004) provide excellent reviews of these models.

UV intensity and RED analyses were performed in this study using UVXPT. The UVXPT software was developed by Carollo Engineers to model UV intensity fields, UV sensor readings, UV dose delivery, and microbial inactivation (Wright and Reddy, 2003). UVXPT uses Microsoft Excel as a user interface. The software is programmed in Visual Basic and is accessed using command buttons. Spectral and directional analyses of the UV intensity and sensor readings can be readily performed in UVXPT to account for dependencies on wavelength and refraction through
the air-quartz-water interfaces of the lamp sleeve. Wall reflection has been recently added to UVXPT, but shadowing from features within the reactor is neglected. See Appendix B for additional details of UVXPT.

Additional UV intensity and RED analyses were also performed using the discrete ordinates (DO) radiation model in FLUENT. The DO radiation model 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, reflection) can also be readily considered. In addition, a user-defined function (UDF) was implemented to calculate the cumulative dose of particles moving through the reactor. The cumulative dose (J/m²) was calculated as the product of the irradiation (W/m²) and the exposure time (s) at each step along the particle path. See Appendix A for more details on the DO formulations used in Fluent.

A previous study by Liu et al. (2004) concluded that the DO radiation model over predicted the intensity close to the lamps but under predicted the intensity far from the lamps because it did not include refraction. Refraction at interfaces can be included in the FLUENT discrete ordinates model, but the interfaces and geometries of different materials (e.g., lamp, air annulus, quartz sleeve) need to be discretely modeled. In the analyses using the Fluent DO radiation model, the radiation from the lamps was modeled as a diffuse source from the outer surface of the sleeves. Also, although up to ten wavelength bands can be modeled within the Fluent DO radiation model, the lamp radiation was modeled assuming a single germicidal wavelength (single band). Sensitivity analyses investigating the impact of reflection and refraction at the quartz sleeve is provided in “Sensitivity Studies of Reflection and Refraction” in Chapter 4.

DOSE-RESPONSE MODELS

The dose associated with each particle path was converted to an equivalent inactivation and reduction equivalent dose (RED) using appropriate dose-response curves. For the IDI Ozonia Aquaray® H₂O bioassay validation tests, B. subtilis was used as the surrogate pathogen per the DVGW guidelines, and for the Calgon Sentinel® and Trojan UVSwift™ tests, MS2 Phage was used. Dose-response curves were modeled during validation testing using the following equations:

IDI Ozonia Aquaray® H₂O: \[ \log\left(\frac{N}{N_0}\right) = A - B \times (\text{Dose in J/m}^2) \]

Calgon Sentinel® and Trojan UVSwift™ 10L30: \[ \text{Dose (mJ/cm}^2) = A \times \log\left(\frac{N_0}{N}\right) + B \times \log\left(\frac{N_0}{N}\right)^2 \]

where \(A\) and \(B\) are fitting coefficients provided in the validation reports, \(N_0\) is the number of viable microbes introduced to the system, and \(N\) is the number of viable microbes remaining after exposure to the UV reactor. Thus, \(N/N_0\) is the survival ratio, and \(N_0/N\) is the inactivation ratio. Other dose-response curve fits were also considered as described in this report. The procedure for determining RED from a distribution of particle doses can be found in Munoz et al. (2007). In brief, the survival ratio is calculated for each particle \((N/N_0)\), using the appropriate dose-response curve, where \(i\) denotes each particle. The cumulative survival ratio is then calculated by summing the individual particle survival ratios and dividing by the total number of particles, \(n_0\) (assuming each particle has equal weighting or probability):
The RED is then calculated using the cumulative survival ratio in the appropriate dose response curve and solving for dose. So, for example, using the dose-response curve above for the IDI Ozonia Aquaray® H₂O validation tests, the RED is calculated as follows:

\[
\text{RED} = \text{Dose} = \frac{A - \log\left(\frac{1}{n_p} \sum_{i=1}^{n_p} \left(\frac{N}{N_0}\right)\right)}{B}
\]  

(2.2)

The non-linear nature of the dose-response curve yields an RED that is different than the average of the particle dose distribution. The Fluent DO radiation model used the dose-response models shown above that were provided in the validation reports for each of the reactors. This was appropriate because of the gray (single-wavelength) assumption used in the Fluent DO radiation model. Because UVXPT performs a polychromatic analysis, additional spectral considerations were evaluated as described in the next section.

**Action Spectra**

CFD-based dose modeling of UV reactors using MP lamps requires the action spectra of the microbe as an input to the model if polychromatic analyses are performed (i.e., in UVXPT). The action spectra is a plot of the UV sensitivity of the microbe as a function of wavelength. There have been a number of approaches used to define the action spectra of microbes. Many researchers have defined the action spectra as a plot of log inactivation as a function of wavelength obtained with a fixed UV dose. While this approach is valid if the dose-response at each wavelength follows first order kinetics, it causes errors if the dose-response at different wavelengths has shoulders and tailing and the kinetic constants that describe the shoulders, tailing, and exponential regions of the dose response have a different relative dependence of wavelength. Cabaj et al. (2001) reports modeling the dose-response of \(B. subtilis\) spores using:

\[
\frac{N}{N_0} = 1 - (1 - 10^{-k \times \text{Dose}})^B
\]

where \(k\) is a coefficient that describes the exponential region and \(B\) is a coefficient that describes the shoulder region. Cabaj et al. (2001) reports that the wavelength dependence of these coefficients is different and that these differences have an important impact on how UV dose is calculated using a MP collimated beam apparatus. Furthermore, Cabaj et al. (2001) state that germicidal UV dose defined as the integration of dose at each wavelength weighted by the action spectra is only an approximation if the microbe’s dose response has shoulders. In other words, the standard approach proposed to calculate a MP germicidal dose is valid with microbes with first order kinetics but can cause errors with microbes with shoulders, tailing, and exponential regions that have different functional dependencies on wavelength. Instead, the inactivation at each wavelength needs to be calculated using the inactivation kinetics at each wavelength and then integrated as a function of wavelength. The UVXPT algorithm currently calculates a germicidal UV dose using the action spectra of the microbe. For this study, the IDI system was modeled using the dose-response of \(B. subtilis\) but the action spectra of MS2 as defined by Rauth (1965) (see Figure 2.2).
The Calgon and Trojan systems were modeled in UVXPT using the dose response and action spectra of MS2 as reported by Rauth (1965).

VALIDATION METRICS

A number of methods exist to evaluate the accuracy and uncertainty of computational models relative to the behavior and performance of the physical systems being modeled. Figure 2.3 shows a flow chart of the general modeling and validation process. Conceptual models are generated to represent real-world systems, and computational models are generated from these conceptual models. Computational results are compared to data using appropriate validation metrics to assess the accuracy and suitability of the model.

In general, model validation must be flexible and allow varying levels of accuracy depending on the application being studied (AIAA, 1998). In particular, AIAA (1998) states that “as long as the trends predicted by the tools are consistent within the design envelope and an estimate of the error and uncertainty can be made, less-than-perfect accuracy of the simulation is commonly acceptable.” AIAA (1998) recommends that validation be performed using a building-block approach, where the system being modeled is broken down into smaller components for assessment and validation. In this study, comparisons are performed on several model components, including hydraulics (e.g., comparison of head loss), UV radiation (e.g., comparison of UV intensity at sensor locations), and dose (e.g., simulated vs. measured RED). Although not all model components are validated for each reactor configuration, the RED is used as a metric in all the analyses with at least one or more additional metrics to build confidence in the models.

Regression Plots

One method of validation is to plot the measured vs. predicted performance metrics (e.g., RED) and generate a linear regression in the form of \( y = mx \). The coefficient of determination (\( R^2 \)) can be used to determine the correlation and “goodness of fit” between the measured and predicted data, and the slope can be used to indicate whether the model is under predicting or over predicting the measured data for different scenarios. According to Devore (1982; p. 449), a reasonable rule of thumb is that the correlation is weak if \( 0 \leq |R| \leq 0.5 \), strong if \( 0.8 \leq |R| \leq 1.0 \), and moderate otherwise. Therefore, if \( R^2 > 0.64 \), a strong correlation between the measured and predicted RED exists.
Error Propagation and Uncertainty Analysis

Coleman and Stern (1997) suggest a validation metric that accounts for uncertainty in both the experimental data and simulated predictions. Standard uncertainty analysis and error propagation is used to determine the uncertainty in the measured data. Parametric, convergence, and order-of-accuracy studies are used to estimate the numerical uncertainties. The results yield error bars for both measured and predicted values, so for plots of measured vs. predicted RED, a “box” around each data point can be evaluated to determine if it encompasses the $y=x$ line. In this study, only measurement errors are considered. Uncertainty in measured RED and log inactivation reported by the manufacturers in the validation report are used to generate vertical error bars in selected plots of measured vs. predicted RED. If the vertical error bars cross the $y=x$ line, then the predicted results are assumed to match the measured data (see, for example, Figure 3.24 and Figure 3.44). The percentage of predicted values that match the experimental data can be compared to a
prescribed accuracy requirement (e.g., “90% of the predicted data should match the measured data plus or minus the measurement uncertainty”).

**Confidence Intervals**

Oberkampf and Barone (2006) suggest a validation metric that employs confidence intervals to account for uncertainty in the experimental data. In this application, the absolute relative difference between measured and predicted RED for each test (abs(measured RED – predicted RED)/measured RED) has been calculated. The mean, $E$, and standard deviation, $s$, for the sample of absolute relative differences between measured and predicted RED are also calculated. Then, a confidence interval (say, 90th percent confidence interval) about the mean of the absolute relative differences is calculated as follows:

$$
\left( E - t_{a/2,v} \frac{s}{\sqrt{n}}, E + t_{a/2,v} \frac{s}{\sqrt{n}} \right)
$$

where $t$ is the student-t distribution, $a$ is 0.05 for a 95th percent confidence interval, $n$ is the number of tests, and $v = n-1$ degrees of freedom. The confidence interval can then be compared to the percent error associated with the experimental measurements. If the 90th (or 95th, etc.) percent confidence interval is less than the relative measurement error, then the validation metric has been met.

**Chi-Squared Goodness of Fit Test**

Here we derive a chi-squared goodness-of-fit confidence metric that provides an indication of whether the discrepancies between simulated REDs and measured REDs are due solely to the uncertainty in each measured RED, or whether the discrepancies are due to CFD model limitations.

Suppose N distinct validation tests were conducted, yielding measured REDs $M_i \pm \sigma_i$, where $i = 1, 2, \ldots, N$ and $M_i$ is the mean of a number of repeated measurements with variance $\sigma_i^2$. Let $m_i$ be a random variable generated from a normal distribution of mean $M_i$ and variance $\sigma_i^2$. Then, the quantity $(m_i - M_i)/\sigma_i$ has mean 0 and variance 1.

When some random variables $Z_i$ have normal independent distributions with mean 0 and variance 1, then the sum $\chi^2$, defined by

$$
\chi^2 = \sum_{i=1}^{N} Z_i^2
$$

is distributed as a chi-squared distribution with N-1 degrees of freedom (Devore, 1982, p. 523).

Therefore, the sum

$$
\chi^2 = \sum_{i=1}^{N} \left( \frac{m_i - M_i}{\sigma_i} \right)^2
$$

is distributed as a chi-squared distribution with N-1 degrees of freedom.

Each of the tests were simulated using CFD, yielding simulated REDs $S_i$, where $i = 1, 2, \ldots, N$. We need to determine a confidence metric that provides an indication of whether the discrepancies between all $S_i$ and $M_i$ are due solely to the uncertainty in each measured RED, or whether the discrepancies are an indication of CFD model limitations.
For good CFD models, the sum
\[ \chi_S^2 = \sum_{i=1}^{N} \left( \frac{S_i - M_i}{\sigma_i} \right)^2 \]
should be nearly distributed as
\[ \chi^2 = \sum_{i=1}^{N} \left( \frac{m_i - M_i}{\sigma_i} \right)^2 \]
that is as a chi-squared distribution with N-1 degrees of freedom.

The simulated REDs yielded by a poor CFD model would have a large discrepancy from the measured REDs relative to the uncertainty in the measured REDs. Hence, the sum \( \chi_S^2 \) would be relatively large, and there would be a low probability that \( \chi^2 \) would yield a value at least as high as \( \chi_S^2 \).

In contrast, when \( \chi_S^2 \) is calculated by comparing measured REDs to simulated REDs from a good CFD model, there would be a high probability that \( \chi^2 \) would yield a value at least as high as \( \chi_S^2 \), which would be a relatively small number.

To quantify this, we define the P-value corresponding to some \( \chi^2 \) as the probability that \( \chi^2 \) would yield a value at least as high as \( \chi_S^2 \). That is, the P-value corresponding to \( \chi_S^2 \) calculated from N-1 degrees of freedom is:
\[ P_N(\chi_S^2) = 1 - \int_{0}^{\chi_S^2} f_N(x) \, dx \] (2.3)
where
\[ \chi_S^2 = \sum_{i=1}^{N} \left( \frac{S_i - M_i}{\sigma_i} \right)^2 \] (2.4)
and \( f_N \) is the probability density function of a chi-squared distribution with N-1 degrees of freedom.

A larger P-value (say, 0.9 or 90%) indicates a higher likelihood that the discrepancies between the simulated REDs and the measured REDs are due solely to the uncertainty in each measured RED. A smaller P-value indicates a higher likelihood that the discrepancies are due to CFD model limitations.

Although this approach merits discussion and presentation, its novelty precludes us from applying it to the tests and simulations in this study. In addition, this approach is likely to be very sensitive to outliers in the residuals between measured and simulated values, and its application will require an accurate assessment of the error (or standard deviation) of the measured values of each validated run.
CHAPTER 3
SIMULATION OF COMMERCIAL REACTORS

SIMULATIONS OF IDI REACTOR

IDI Reactor Configurations and Grid Development

The IDI (Degremont Technologies) Ozonia Aquaray® H2O reactor was modeled using two configurations, the M-rig, which utilized a single reactor installed in 12-inch piping, and the L-rig, which utilized two reactors in series installed in 24-inch piping.

The M-rig model, shown in Figure 3.1, started with a section of straight 12-inch diameter pipe 60-inches long (5 pipe diameters), leading to a 90-degree elbow. The piping then ran straight to a S-bend, which included two 90-degree elbows separated by a short spool section. The S-bend was followed by a concentric expansion, which connected to the reactor. The reactor included 6 lamp sleeves, the wiper power screw, the outside surfaces of the UV sensors, and baffles. A concentric reducer is located downstream from the reactor, followed by approximately 5 diameters of 12-inch diameter straight piping. For some test conditions a porous baffle plate was located within the piping between the concentric expansion and the reactor.

The L-rig model, shown in Figure 3.2, began with a section of straight 24-inch diameter pipe 120-inches (5 pipe diameters), leading to a S-bend, which included two 90-degree elbows, separated by a short spool section. The S-bend was followed by a concentric reducer, which was attached to the upstream reactor. A second reactor was attached to the downstream end of the first reactor and followed by a concentric expansion back to 24-inch diameter pipe, which ran straight for approximately 5 diameters to the model outlet.

For both the M-rig and L-rig model runs, a similar procedure was used to generate the model grids. The piping was meshed using GAMBIT primarily with hexahedral elements using a Cooper scheme, which includes boundary layer elements at the surface. The M-rig had 1,120 cells along the pipe cross-section, and the L-rig utilized 1,092 cells along the pipe cross-section. The pipe elements were held constant with a minimum cell dimension of 10 mm for the M-rig, and 20 mm for the L-rig for each case. Interface boundaries were used to transition the coarser piping grid to the finer reactor grid. The grid refinement runs were carried out for both the M-rig and L-rig configurations. The M-rig and L-rig utilized the same reactor grid, with the exception of the interface between the two reactors in the L-rig where the grid was slightly altered to match one-to-one. The reactor was meshed using a Cooper scheme through the center along the lamp axis, and a tetrahedral/hybrid mesh with a hexahedral core was used to transition to the outer walls. The minimum tetrahedral cell quality was 0.82, where a value of 0 indicates that all cell faces are equilateral in shape, and a value of 1 indicates a poorly shaped cell. Achieving higher quality cells is typically not practical when modeling intersecting curved surfaces. The overall number of skewed cells was further reduced using the polyhedral conversion tool within Fluent. The M-rig grids with and without the baffle were identical, except that the cells representing the solid baffle area were changed from solid to fluid when the baffle was not present. Figure 3.3 shows the model grid at a section through the piping, and along the surface of the reactor.

A grid sensitivity analysis was performed by progressively reducing the cell size within the reactor while holding the piping size constant (Wicklein et al., 2008). The M-rig was evaluated at
Figure 3.1 M-rig GAMBIT/FLUENT model of the Ozonia Aquaray® H₂O reactor and piping

Figure 3.2 L-rig GAMBIT/FLUENT model of the Ozonia Aquaray® H₂O reactor and piping
a flow rate of 4.44 mgd, and the L-rig was evaluated at a flow rate of 7.61 mgd for the grid sensitivity analysis. Over 100 points within the vicinity of the reactor were evaluated for the hydraulic grid sensitivity analyses. These points were prescribed at locations just upstream and downstream of the reactor on a uniform grid.

Table 3.1 summarizes the size of the model grids evaluated, the percent refinement, as well as the velocity magnitude correlation for the pairs of grid comparison (medium vs. initial, fine vs. medium). Figure 3.4 shows a plot of the comparison for the M-rig runs without the baffle. Figure 3.5 presents a plot of the data comparison for the M-rig with the baffle. Figure 3.6 presents the

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Grid</th>
<th>No. of cells in reactor</th>
<th>Percent increase in number of cells</th>
<th>No. of cells in piping</th>
<th>Total cells</th>
<th>Velocity magnitude correlation $R^2$</th>
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</thead>
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<tr>
<td>M-rig no baffle</td>
<td>Initial (G1)</td>
<td>494,989</td>
<td>—</td>
<td>669,706</td>
<td>1,164,695</td>
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<td>0.99</td>
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<tr>
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<td>Initial (G1)</td>
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<td>—</td>
<td>668,959</td>
<td>1,163,948</td>
<td>—</td>
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<td>Medium (G2)</td>
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<td>681,559</td>
<td>1,363,293</td>
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<td>671,959</td>
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<td>555,828</td>
<td>1,527,374</td>
<td>—</td>
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<td>32</td>
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</table>
Figure 3.4 Point data comparison between grids for M-rig runs without the baffle

Figure 3.5 Point data comparison between grids for M-rig runs with the baffle

Figure 3.6 Point data comparison between grids for the L-rig runs
comparison for the L-rig runs. For all runs the velocity comparison improved, or matched very closely, with each progressively refined grid.

Additional runs were made with the L-rig at a high flow condition of 19.97 mgd and at a low flow condition of 4.82 mgd to evaluate the reactor head loss. Figure 3.7 shows a comparison between the measured head loss and the calculated head loss. The CFD model calculates the head loss for low and mid flows very well, while there is a slight variation at the high flow case.

Hydraulic Simulations of IDI Reactors

Figure 3.8 and Figure 3.9 show a comparison of the velocity magnitude at the reactor centerline in plan and profile for the M-rig with and without baffle at 700 m$^3$/h (4.4 mgd). In section view, the velocity is higher at the bottom of the reactor and toward the right side looking downstream for the run without the baffle. With the baffle installed, the simulated velocity profile is altered downstream of the baffle, but non-uniformities still exist. Figure 3.10 show the velocity magnitude at the reactor centerlines in plan and profile in the L-rig configuration. The velocity is fairly uniform approaching the first reactor, and the velocity distribution is similar for both reactors.

Simulations of UV Intensity and RED for the IDI Reactors

UV Intensity Predictions of IDI Reactor Using UVXPT

The validation report for the IDI reactor provides UV sensor readings made by a DVGW reference sensor and the duty UV sensor used by the UV system. UV sensor readings were recorded as a function of water UVT and ballast power setting at water layer distance from the sensor port window to the lamp sleeve of 4.0, 7.5 and 11.0 cm.

Figure 3.11 shows the spectral and angular response of the DVGW sensor used in the model. The spectral and angular response was obtained by interpolating nominal response reported in DVGW standard. Because the angular response data in the DVGW standard was for an air-quartz-air interface, the data was adjusted for a water-quartz-air interface. The angular response
Figure 3.8 Velocity magnitude at reactor centerline sections in plan and profile for M-rig without baffle at 4.44 mgd

Figure 3.9 Velocity magnitude at reactor centerline sections in plan and profile for M-rig with baffle at 4.44 mgd
was transformed using Snell’s Law where the response at angle $\theta_a$ in air was assigned to angle $\theta_w$ in water using:

$$n_w \sin \theta_w = n_a \sin \theta_a$$

(3.1)

where $n_w$ and $n_a$ are the indices of refraction in air (1.0) and water (1.33). Figure 3.12 shows the UV output of the MP lamp obtained from measurements made by Degremont R&D. Figure 3.13 shows the index of refraction of water and quartz and the UV absorbance coefficient of quartz used.
by UVXPT. The data for quartz was obtained from GE for type 214 quartz at room temperature. Figure 3.14 shows the spectral UVA of the test waters obtained from the validation report.

Figure 3.15 shows the comparison of measured and predicted UV sensor readings. The measured UV sensor readings were obtained directly from the validation report. The predicted UV sensor readings were obtained by integrating the UV intensity at the UV sensor location accounting for the angular and spectral response of the UV sensors as follows:
where \( S \) is the predicted UV sensor reading, \( I(\theta, \lambda) \) is the UV intensity from the lamps incident on the UV sensor location \((x,y,z)\) predicted by UVXPT, \( \theta \) is the angle of the light incident on the UV sensor defined using the dot product of the vector defining the viewing direction of the UV sensor and the Poynting vector of the UV light, \( \lambda \) is the wavelength of light, \( R(\lambda) \) is the spectral response of the UV sensor defined as a function of \( \lambda \), and \( R(\theta_i) \) is the angular response of the UV sensor defined as a function of \( \theta_i \).

The data was fitted using the relation \( y=Ax \) with a slope of 1.046 and an R-squared of 0.9829. The quality of the fit suggests that the UV intensity and UV sensor algorithm used by UVXPT is providing reasonable predictions. The slope suggests a model error on the order of 5 percent which is comparable to the absolute error expected with DVGW reference sensors. For the 4 cm location, model predictions are lower at high UVT. This difference can be explained by the tolerance given in the validation report for the location of the sensor relative to the lamps.

The slope of the relation between measured and predicted UV sensor readings in Figure 3.15 was used to calibrate the output of the MP lamp. Essentially, the lamp output in W/cm/nm was increased by a factor of 1.0461. Figure 3.16 shows a comparison of measured and predicted UV sensor readings after calibration. As expected, the relation has an improved correlation with a slope of 1.0029.

**Inactivation Kinetics Used in UVXPT**

The IDI reactor was validated using *B. subtilis* spores. Figure 3.17 shows a plot of the dose-response data. The dose response shows distinct regions with shoulders at low UV doses and tailing with some curves at high doses. The data also shows significant variability in the dose-response from day-to-day testing. A key question for modeling the reactors is whether or not the variability represents measurement error, the true dose-response of the *B. subtilis* for that day of testing, or the true dose-response of *B. subtilis* for the sample evaluated. If the 1st or 3rd conjectures are valid,
then the average dose-response of the combined data set should be used to model the reactor. If the
second is true, then the dose-response for each day of testing should be used.

Curve fitting software was used to identify the best empirical fit to the data. While polynomial functions can provide the best fit, they do not provide reasonable extrapolation of the dose-response data at high doses. Extrapolation of dose-response data is needed because the dose distributions predicted using CFD-based models often include UV doses that extend beyond the measured range of the dose-response data from collimated beam tests. This can occur, for example, if particles are trapped in recirculation zones near the lamp. For the most part, very high doses have a minor impact on the log inactivation and RED predicted using CFD because the survival ratio (N/N_0) predicted using those high doses is close to zero. However, there are two cases where one needs to make a good extrapolation of the dose-response curve to ensure that the model predictions are reasonable. First, the function should fit the curvature of the dose-response and always provide increasing inactivation as UV dose increases. One should be careful of selecting a polynomial function that may provide a good fit with the measured dose-response but provide extrapolations at high doses that peak and then show decreasing log inactivation with increasing dose. This will be the case with the quadratic function that the UVDGM recommends for fitting microbial

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**Figure 3.16** Comparison of measured and predicted DVGW UV sensor readings with the IDI reactor after lamp output calibration

**Figure 3.17** UV dose-response data for *B. subtilis* spores used to validate the IDI reactor
dose-response. That function is selected to provide good interpolation but was never intended for extrapolation. The second case occurs when the predicted RED is near the upper limit of the measured UV dose-response curve. In that case, the log inactivation predicted using UV doses in the dose distribution that are immediately above the measured range of dose-response will have an impact on the predicted log inactivation and RED.

The analysis identified two functions that provided good fits as follows:

Logistic Function: \[ \log i = \frac{a}{1 + b \times \exp(-c \times Dose)} \]

MMF Function: \[ \log i = \frac{a \times b + c \times Dose^d}{b + Dose^d} \]

The terms \( a, b, c \) and \( d \) in these equations are coefficients determined by the fit.
Figure 3.18 and Figure 3.19 show the fits to the UV dose-response data using the logistic and MMF functions, respectively. Figure 3.20 shows the logistic and MMF fits to the combined dose-response data sets. Table 3.2 tabulates the coefficients for the curve-fits. Figure 3.20 highlights the main differences between the logistic and MMF fits. Both models account for the shoulders and tailing in the dose-response data. However, the Logistic Model predicts greater tailing at high doses, especially with extrapolation, than does the MMF model. In particular, the logistic model shows that the log inactivation asymptotically approaches a maximum value given by the coefficient “a” in the equation. In contrast, while the MMF model predicts diminishing returns in log inactivation at higher doses, log inactivation does not asymptotically approach a maximum value. Furthermore, the MMF model predicts a wide range in tailing with some dose-response curves showing minor tailing and others showing significant tailing.

The differences between the fits of the dose-response data represents an important source of error when dose distributions, be they measured or predicted, are used to predict log inactivation and REDs with UV reactors. Ideally, the dose-response curve during validation should be measured well beyond the range of REDs used to validate the reactor if the validation data is later used to validate CFD-based model predictions. Since tailing tends to occur beyond four log inactivation, a guideline would be to measure the dose-response up to six log inactivation.

Because CFD models will often predict UV doses that extend beyond the range of the measured dose response of the validation microbes, one should also evaluate the impact of alternate fits to the dose-response on the relation between measured and predicted RED. If the impact is minor (e.g., less than the error between the measured and predicted REDs), it should not be a concern and the dose-response that gives the best correlation should be used.

When applying the CFD-based model to predict reactor performance, the UV dose-response of the pathogen or indicator microbe of interest should be defined to high enough log inactivation or UV dose that the impact of the extrapolation is minor. An example of the challenge is predicting 4 log inactivation credit for Crypto, *Giardia*, or adenovirus because the LT2ESWTR only defines UV dose-requirements up to 4 log. In that case, one can evaluate the impact of alternate extrapolations of the UV dose-requirements.
RED Simulations of IDI Reactor Using UVXPT

Particle tracks for the Ozonia Aquaray® H₂O 20" reactors were developed from the CFD models for the three validation configurations. Particle tracks with the M-rig were predicted using a CFD flowrate of 4.44 mgd while particle tracks for the L-rig were predicted at a CFD flowrate of 7.61 mgd. With each reactor configuration, particle tracks were developed for three grid mesh densities, identified as initial (G0), medium (G1) and fine (G2).

Figure 3.21 compares the measured *B. subtilis* RED with the M-rig without baffle plate to the RED predicted using the G1 mesh. REDs were predicted using the UV dose response modeled using the MMF fit to all of the dose-response data, as shown in Figure 3.20. The data shows an excellent correlation between measured and predicted RED at low UVTs of 92%. At 98% UVT, the relation between measured and predicted RED was fitted using a linear relation with a notable intercept and with a much lower R-squared. Based on data observed with the Calgon reactor, wall reflections may have an impact on the measured RED; the predicted REDs reported here do not account for reflections. See “Sensitivity Studies of Wall Reflection” in Chapter 4 for additional analyses of wall reflection.

Figure 3.22 compares the measured *B. subtilis* RED with the M-rig with baffle plate to the predicted RED. The correlation between measured and predicted RED at lower UVTs is notably less. Furthermore, at low UVTs, the CFD model for the M-rig with the baffle is predicting about 10% higher than with the M-rig without the baffle.

Figure 3.23 compares the measured *B. subtilis* RED from the L-rig without baffle plate to the RED predicted using the G1 mesh. Results show that the predicted REDs are consistently lower than the measured REDs by approximately 30% on average. These discrepancies may be caused turbulent hydraulic features (e.g., large or detached eddies), radiative processes (e.g.,

### Table 3.2

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Figure 3.21 Measured vs. predicted B. subtilis RED for the IDI reactor M-rig without baffle plate

Figure 3.22 Measured vs. predicted B. subtilis RED for the IDI reactor M-rig with baffle plate

Figure 3.23 Measured vs. predicted B. subtilis RED for the IDI reactor L-rig (one or two reactors without baffle plate)
reflection), and other features not captured in the current models that would act to increase the simulated dose.

**RED Simulations of IDI Reactor Using Fluent DO Radiation Model**

In addition to the UVXPT calculations of RED, simulations of UV radiation and RED were performed using the Fluent DO radiation model, which is integrated with the Fluent hydraulic model. Several advantages and disadvantages exist to using a radiation and dose model that is integrated with the hydraulic model. A primary advantage is the convenience of simulating the hydraulic, radiation, and dose processes in a single package. In addition, features and geometry that is included in the hydraulic model (e.g., sensors, baffles, wiper screws, etc.) are inherently included in the radiation and dose models. Disadvantages include the increased computational requirements if polychromatic analyses are needed or if small features (e.g., quartz sleeve, air annulus, internal sensor features) are modeled.

A total of 32 different IDI test configurations were simulated using the Fluent DO radiation model. A single-wavelength-band radiation model was implemented to represent an effective germicidal wavelength. Simulations and sensitivity analyses presented in Chapter 4 (Ho et al., 2008, 2009) showed that several factors were potentially important to the simulated RED:

- Particle tracking parameters (number of particles injected, use of discrete random walk model, initialization values for turbulent kinetic energy and dissipation parameters).
- Wall reflection
- Calibration method

The 32 cases were run with auto-convergence disabled for 1000 flow iterations, which was found to be sufficient to achieve convergence. For these runs, we implemented 20% (diffuse) reflection, discrete random walk (3 tries), and ~15,000 particle injection points. The reflectivity of steel ranges between 20% and 40% in the UVC range (Luckiesh, 1929, Figure 5). Sensitivity studies reported in Ho et al. (2008) showed that a value of 20% yielded good matches to data. In addition, because fouling is likely to reduce the reflectivity, a value of 20% was chosen. The studies in Chapter 4 showed that the use of 15,000 particles using the discrete random walk model with 3 tries was sufficient to produce a converged dose and RED. In addition, the turbulent kinetic energy was re-initialized to 1e-4 m²/s², and the turbulent dissipation rate was initialized as 1e-4 m²/s³, which correspond to the recommended values for the flow rate and dimensions of the system (AwwaRF #2768, 2007). The default initialization values in Fluent are 1 m²/s² and 1 m²/s³, respectively. These lower initialization values were found to reduce the turbulent viscosity and require fewer iterations for convergence.

The use of a measured RED value to calibrate the simulated lamp output is necessary when the simulated UV sensors do not accurately capture the features of the actual sensor that influence the measured UV intensity (e.g., acceptance angle, spectral response, reflectance from the lens, etc.). Although these features are considered in UVXPT, they are not considered in the Fluent model. Therefore, direct calibration of the simulated lamp output to the measured sensor readings can yield erroneous results, and the simulated lamp output must be calibrated to the measured RED.
Ho et al. (2009) showed that the choice of the run for calibrating the lamp output was important. In that study, the use of two different calibration runs (AV vs. AH) was intended to investigate the impact of the choice of the calibration run on subsequent simulations. These two runs were chosen to represent two different configurations (L-rig and M-rig no baffle) with approximately “average” values for flow rate, UVT, and power. Results showed that the simulated RED for runs using these two different calibration runs were not identical. In particular, runs that used the calibration test from the same configuration as the run itself (e.g., L-rig vs. M-rig without baffle) yielded better matches to data. Therefore, in the current study, the calibration run for each IDI configuration (L-rig, M-rig without baffle, M-rig with baffle) was chosen from a test using the same configuration with “average” values for flow rate, UVT, and power. Another option is to choose multiple runs for calibrating the lamp output and then average the results. Appendix C provides additional detail regarding the calibration process.

The process of running the numerous Fluent DO radiation simulations was automated by using a batch file. Each hydraulic simulation took about an hour to converge, and each radiation simulation took about an hour to converge running on a single Xeon dual-core 3 GHz processor with a Linux operating system. The batch file contained instructions to change the necessary input parameters when a run was finished and process the desired output. Therefore, after the batch file was written, the runs were automatically processed in a sequential fashion. Some batches were split on multiple processors to expedite the simulations. Appendix D contains a sample batch file that was used to automatically run and process the simulations.

Figure 3.24 shows the measured vs. predicted RED for all three configurations. Error bars representing an average error of plus or minus 6% in the measured RED (adapted from personal communication, Bruno Ferran, 10/9/2008) is also shown. Results show that a majority of the vertical error bars fall on the $y = x$ line. This indicates that the CFD-based models are capturing the salient trends in the measured RED as a function of different operational parameters (flow rate,
UVT, lamp output). The average absolute relative error for all the data is 6.1% with a 90% confidence interval of plus or minus 1.4%.

Results also show that the model tends to over predict the measured RED at larger RED values and under predict the measured RED at lower values. One explanation may be that the tests that were used to calibrate the lamp output had UVT values of ~87% (Tests AV, AH, and AE). Previous studies have shown that at UVTs of 88% or less, the impact of reflection is small (Ho et al., 2008 and Chapter 4). Therefore, the calibration of the lamp output to these tests did not actually represent the effects of reflection, which would be more pronounced at higher UVTs, causing a higher predicted RED. This effect is considered in more detail in the “Simulations of UV Intensity and RED for the Calgon Reactor” section later in this chapter.

SIMULATIONS OF CALGON REACTOR

Calgon Reactor Configuration and Grid Development

The model domain of the validated Calgon Sentinel® reactor is shown in Figure 3.25. The model began with a 12-inch diameter straight pipe section approximately 10 pipe diameters long. The straight piping was followed by a single 90-degree elbow approximately 4 pipe diameters upstream from the reactor. The reactor included the outer surface of the lamp sleeves, the sensor bodies, and included both horizontal and vertical baffles to direct flow toward the lamps. A second 90-degree elbow was located approximately 1 diameter downstream from the reactor, followed by a concentric expansion to 18-in diameter pipe.

The pipes were meshed with hexahedral elements using a Cooper scheme and included boundary layer elements at the surface. A grid sensitivity analysis was performed on the reactor grid by reducing the reactor cell size, increasing the total cell count of the reactor for two iterations from the initial grid, while maintaining a constant piping cell size with a range of 0.25-inches to 2 inches. The reactor was meshed using a tetrahedral/hybrid mesh with a hexahedral core. Table 3.3 summarizes the model cell count and results of the velocity magnitude comparison for the three model grids evaluated, and Figure 3.26 graphically shows the comparison. In all
sensitivity cases the model was run at the high flow rate. The velocity comparison was made at points located at the exit of the reactor, and the correlation coefficient is presented for the pairs of grid comparisons (medium vs. initial, fine vs. medium).

Data comparisons showed that the initial and medium grid only had a correlation coefficient of 0.85, whereas the medium and fine grids had a correction of 0.98. Therefore, the medium or fine grid produces a grid independent solution. The core element size in the medium grid reactor was 0.23-inches, with surface elements as small as 0.12-inches. The reactor grid contained 610,716 elements for total model size of 860,216 elements. Figure 3.27 shows a section of the grid through the piping, as well as the fine grid on the outer surfaces of the reactor.

Hydraulic Simulations of Calgon Reactor

The simulated velocity profile in the Calgon Sentinel® reactor at the high flow rate is shown in Figure 3.28. The figure shows both a vertical and horizontal section through the reactor center-line. The velocity in the 12-inch diameter piping approaching the reactor is 2.7 m/s. The baffles at the entrance to the reactor constrict the flow area increasing the velocity and directing flow toward the lamps. Flow accelerates around the upstream lamps, reaching a velocity of 5.5 m/s above and below the upstream lamps. The velocity is very low in the wake region behind the baffles. The peak velocity around the downstream lamp is approximately 4.5 m/s. In plan view, the wake region behind the leading sensor appears to extend past the downstream lamp.
Simulations of UV Intensity and RED for the Calgon Reactor

*UV Intensity Predictions of Calgon Reactor Using UVXPT*

The validation report for the Calgon reactor provided UV sensor readings measured using a DVGW compliant duty sensor manufactured by IL Metronics. The scaling factors used by the PLC to convert the output duty sensors in mA to mW/cm² were calibrated by comparison to a DVGW compliant reference sensor manufactured by IL Metronics. Duty sensor readings were recorded as a function of water UVT and ballast power setting for a fixed water layer distance. Figure 3.29 shows the spectral and angular response of the duty sensor used in the model. NIST measured the spectral and angular response as part of the Water Research Foundation project Design and Performance Guidelines for UV Sensor Systems (Water Research Foundation #2977, 2009). Because the angular response data was measured with an air-quartz-air interface, the data was adjusted for a water-quartz-air interface using the approach described in “UV Intensity Predictions of IDI Reactor Using UVXPT” in Chapter 3. The validation report for the Calgon reactor gave the relative UV output of the MP lamp. The absolute output in W/cm/nm was estimated assuming a typical germicidal output of a MP of 12 W/cm calculated by integrating the output from 225 to 320 nm weighted by the action spectra of MS2 phage (Rauth, 1965). Figure 3.30 gives the absolute UV output of the lamp estimated using this method. Figure 3.13 shows the index of refraction of water and quartz and the UV absorbance coefficient of quartz used by UVXPT. The data for quartz was obtained from GE for type 214 quartz at room temperature. Figure 3.31 shows the spectral UVA of the test waters obtained from the validation report.
Figure 3.32 shows the comparison of measured and predicted UV sensor readings. The data was fitted using the relation $y=Ax$ with a slope of 1.2003 and an R-squared of 0.9994. The quality of the fit suggests that the UV intensity and UV sensor algorithm used by UVXPT accounts for the relative impact of UVT and ballast power setting with a high degree of accuracy. The slope of 1.2, which indicates that the measured sensor readings are consistently ~20% higher than the predicted values, is not unexpected because the absolute output of the MP lamp was an estimate.

The slope of the relation between measured and predicted UV sensor readings in Figure 3.32 was used to calibrate the output of the MP lamp in UVXPT. The lamp output in W/cm/nm was
increased by a factor of 1.200. Figure 3.33 shows a comparison of measured and predicted UV sensor readings after calibration. As expected, the relation between predicted and measured UV intensities improved with a slope of 1.0002.

The UV intensity model within UVXPT was modified during this study to include specular reflection. Details on the modification are provided in Appendix B. Figure 3.34 shows the reflection coefficient defined as a function of wavelength.
Figure 3.32 Comparison of measured and predicted DVGW UV sensor readings with the Calgon reactor

Figure 3.33 Comparison of measured and predicted DVGW UV sensor readings with the Calgon reactor after lamp output calibration

Figure 3.34 Reflection coefficient of stainless steel (adapted from Luckiesh, 1929)
The Calgon reactor was validated using MS2 phage. Figure 3.35 shows a plot of the dose-response data. The dose response has statistically significant curvature and slight day-to-day variability. The October 19th data was noisier with one data point that appears to be an outlier. Curve fitting software was used to identify the best empirical fit to the data. The analysis identified the following function as providing the best fit.

Exponential Association Function: \[ \log_i = a \times (1 - \exp(-b \times \text{Dose})) \]

Figure 3.35 shows the fits to the UV dose-response data using the exponential association function, and Table 3.4 shows the coefficients that were used.

The models show distinct tailing when extrapolated beyond the range of the measured UV dose-response curves. There is also a distinct difference between the dose response measured on October 19 and the data measured on the other days. That difference will cause an error in the RED
predicted by the CFD models. We suspect that removing the outlier in the measured October 19 dose response will eliminate much of this difference.

**RED Simulations of Calgon Reactor Using UVXPT**

The UVXPT model was applied using the initial mesh and particle tracks. The UV output of the MP lamp used in the UVXPT simulation was calibrated by comparing predicted UV sensor readings to UV sensor readings measured during UV validation testing. All of the particle tracks made their way through the reactor. For rapid analysis, UVXPT scaled the time steps of the particle tracks obtained with the high flow rate Fluent hydraulic simulation to simulate particle tracks expected at other flow rates. Figure 3.37 shows examples of the predicted dose distribution with the Calgon reactor. Test conditions for each image in Figure 3.37 are as follows:

<table>
<thead>
<tr>
<th>Date</th>
<th>a</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>10/5/05</td>
<td>10.9</td>
<td>0.00475</td>
</tr>
<tr>
<td>10/17/05</td>
<td>7.68</td>
<td>0.00745</td>
</tr>
<tr>
<td>10/18/05</td>
<td>7.29</td>
<td>0.00804</td>
</tr>
<tr>
<td>10/19/05</td>
<td>24.4</td>
<td>0.00207</td>
</tr>
</tbody>
</table>

Table 3.4 Coefficients used in exponential association function for the Calgon reactor

Figure 3.37 UV dose distributions for the Calgon Sentinel® reactor
• Top left: UVT = 69.8%, flow = low, lamp output = 55.55 %, and one lamp on.
• Top right: UVT = 98.3%, flow = high, lamp output = 84.44 %, and one lamp on.
• Bottom left: UVT = 69.9%, flow = extra low, lamp output ~ 26 %, and three lamps on.
• Bottom right: UVT = 98.6%, flow = medium, lamp output ~ 32 %, and three lamps on.

The Calgon reactor was validated at the Portland UV Validation test Facility using MS2 phage as a test microbe. Figure 3.38 shows a plot of measured RED versus the RED predicted using the equations developed during validation. The relation between measured and validated RED was fit using the relation $y=Ax$ with a slope of 1.0173 and an R-squared of 0.9718. The standard deviation of the residuals, defined as the difference between the measured and validated REDs, was 3.15 mJ/cm².

Figure 3.39 shows a plot of measured versus UVXPT-predicted MS2 RED. Figure 3.40 shows a plot of validated versus UVXPT-predicted MS2 RED. The UVXPT model did not include wall reflections. The following observations are made from the data:

• The plot of measured versus UVXPT-predicted RED was fitted with the relation $y=Ax$ with an R-squared of 0.9379 while the plot of validated versus UVXPT-predicted RED was fitted with an R-squared of 0.9711. The higher R-squared occurs with the plot of validated versus UVXPT-predicted RED because the validated RED values are less impacted by experimental noise during validation testing.
• For a given UVT, the relation between validated and UVXPT-predicted RED is fitted with the relation $y=Ax$ with an R-squared ranging from 0.9848 to 0.9938. The high R-squared shows that the model is accounting for the impacts of flowrate, lamp on/off status, and relative lamp output reasonably well.
• At low UVTs from 70 to 88 %, the slope of the relation between measured and predicted RED for a given UVT ranges from 0.9529 to 0.9586 and averages 0.9552. This observation suggests that the CFD-model is providing good predictions of dose delivery by the reactor at those UVTs. An important observation is that these results were obtained without any “CFD calibration factor.” If the model provides accurate
predictions without application of a CFD factor, then it is accounting for the hydraulics through the reactor caused by the upstream and downstream piping (which include a ninety degree bend upstream) and baffle plates and lamps within the reactor.

- At high UVTs above 88%, the slope of the relation between measured and predicted RED for a given UVT increases with UVT. The slope is 1.0038 at 94% UVT and 1.1529 at 98% UVT. The increased slope likely occurs because the UVXPT model is not incorporating wall reflections.
- The observation that the CFD model obtained for a high flowrate provides good predictions at all other flow rates implies that the scaling of the time step used by UVXPT

Figure 3.39 Measured vs. UVXPT predicted MS2 RED for the Calgon Sentinel® reactor. UVXPT model does not include reactor wall reflections.

Figure 3.40 Validated vs. UVXPT predicted MS2 RED for the Calgon Sentinel® reactor. UVXPT model does not include reactor wall reflections.
is a reasonable approach. This conclusion is specific to this reactor and its inlet and outlet piping. The validity of the approach should always be verified before using it with other UV reactors and piping configurations.

With 40 percent specular wall reflection included in the UVXPT model, Figure 3.41 and Figure 3.42 show, respectively, the relation between measured and UVXPT-predicted MS2 RED and the relation between validated and UVXPT predicted MS2 RED. The following observations are made from the data:

- The plot of measured versus UVXPT-predicted RED in Figure 3.41 was fitted with the relation $y = Ax$ with a slope of 0.9355 and an $R^2$-squared of 0.9626 while the plot of

![Figure 3.41 Measured vs. UVXPT predicted MS2 RED for the Calgon Sentinel® reactor. UVXPT model includes specular reflection from the reactor walls.](image1)

![Figure 3.42 Validated vs. UVXPT predicted MS2 RED for the Calgon Sentinel® reactor. UVXPT model includes specular reflection from the reactor walls.](image2)
validated versus UVXPT-predicted RED was fitted with the relation \( y = Ax \) with a slope of 0.9189 and an R-squared of 0.9851. Inclusion of reflection significantly improved the correlation between the measured and validated REDs and the UVXPT-predicted RED.

- The UVXPT model calibrated using the UV sensor readings predicts high by about 9 percent. The model error may reflect error in the calibration of the UV sensors. The duty UV sensors used in the validation were calibrated during validation by comparison to DVGW compliant reference sensors. The uncertainty of the duty UV sensor calibration is estimated as 7.9 percent and the uncertainty of the reference UV sensor calibration is estimated as 8.9 percent. The model error may also be due to the UVXPT model not including shadowing of UV light by lamps. Shadowing of UV light by lamps is a complex phenomena due to the refraction and reflection of UV light by the lamp sleeves and the absorption and re-emission of UV light by the lamp plasma (Phillips, 1983). The overall impact of shadowing will be to reduce the UV intensity within the reactor.

- The close agreement between the validated and UVXPT-predicted RED, the slope of the relation could be used to further calibrate the UVXPT model, resulting in a one-to-one relation. The calibrated UVXPT model would then predict the validated RED to within 4.49 mJ/cm² as a 95th percent prediction interval. This value is comparable if not better than the uncertainty of interpolation typically observed with UV validation, which ranges from 4 to 12 mJ/cm².

- The R-squared with the relation between validated and UVXPT-predicted MS2 REDs is higher than that with the relation between the measured and validated MS2 REDs. The observation suggests that the CFD-based model is accounting for change flow, UVT and lamp power setting and lamp on/off status with an accuracy comparable to the validation equation. The observation provides confidence that a calibrated CFD-based model can accurately predict UV reactor performance for conditions that have not been validated, such as flow above or below the validated range, various combination of on/off lamps, different hydraulic conditions through the reactor, and changes in reactor design.

Figure 3.43 shows the ratio of UVXPT predicted RED with and without wall reflections as a function of UVT. The ratio increases from 1.01 at 70 percent UVT up to 1.25 at 98 percent UVT. The ratio also varies at a given UVT with higher values associated with higher REDs. This relation with RED likely occurs because higher log inactivation and associated RED is more impacted by the lower end of the UV reactor’s dose distribution. The lower end of the dose distribution is impacted by particle trajectories through the UV reactor that pass through the lower UV intensity regions close to the UV reactor walls. Those lower UV intensity regions closer to the reactor walls are more impacted by reflection.

It should be noted that the work on the impact of reflections on dose delivery by UV reactors presented in this report is preliminary. While a 40 percent reflection coefficient provided good agreement between model predictions and validated RED with the UVXPT model, a 20 percent reflection coefficient provided good agreement between the discrete ordinates radiation model predictions and measured data (see the following section and the “FLUENT Simulations” section in Chapter 4). More work is needed measuring the reflection coefficient of reactor surfaces as a function of the wavelength of light, understanding the impact of the reactor surface finish on...
specular and diffuse reflection, and modeling the impact of specular and diffuse reflections on UV intensity fields and dose delivery. Experimental work is also needed to confirm the impacts of reflection on UV intensity, log inactivation and RED. Lastly, work is needed on understanding the regulatory impacts of reflection on UV dose monitoring at the water treatment plant application since reflection will be impacted by fouling and surface corrosion, yet UV sensors will not be monitoring the impact of these phenomena on UV dose delivery.

**RED Simulations of Calgon Reactor Using Fluent DO Radiation Model**

Nearly 100 validation tests were performed on the Calgon Sentinel® reactor under a wide range of operating conditions that varied the flow rate, UVT, number of lamps used, and lamp output power. A large sampling of these tests was chosen for the CFD simulations to span the range of operating parameters considered.

Similar to the IDI simulations, a batch file was created to perform and process the simulations of the Calgon reactor automatically. Each hydraulic simulation took on the order of 1–2 hours to converge, and each radiation simulation took about an hour to converge running on a single Xeon dual-core 3 GHz processor with a Linux operating system. The parameter values that were changed in each simulation (water absorptivity (for UVT) and lamp output) were recorded and stored in the batch file (see Appendix D).

After the hydraulic simulation converged, nearly 15,000 particles were injected uniformly at the inlet using the DRW model with three tries (based on results from the IDI sensitivity analyses). All interior surfaces of the reactor were assumed to have 20% wall reflectivity. The DO radiation model was used to simulate a single-band UV intensity field. The simulated lamp output for two different runs (one with a high UVT of 98.5% (Test 45) and one with a low UVT of 76% (Test 64)) were calibrated to yield the same RED as the measured RED for those runs, which had “average” flow rates. Then, the lamp output for all other runs was scaled to these two calibrated runs (for two different sets of results) using the measured sensor readings (see Appendix C). The cumulative dose (J/m²) received was calculated for each particle traveling through the reactor, and

![Figure 3.43 Ratio of UVXPT-predicted RED for the Calgon Sentinel® reactor with and without 40 percent wall reflections](image-url)
the dose distribution was used together with the appropriate dose-response curve to yield the simulated RED for each simulation.

Two different runs were chosen for calibration because the IDI results indicated that the choice of calibration may be important to the simulated results. The objective of selecting a calibration run with a high UVT versus a low UVT was to confirm if wall reflection was important. At low UVT (<~88%), the impact of wall reflection is minimal because the radiation cannot penetrate significant distances through the water before being attenuated (Ho et al., 2008). Therefore, for runs calibrated to the low UVT test, the simulated results of high UVT tests should over predict the measured RED if UVT was important since wall reflection would be providing additional radiation within the reactor. Conversely, if wall reflection was not important, the simulations calibrated to the low UVT test should not show any bias for runs with high UVT. Also, if UVT was not important, runs calibrated to the high UVT case would under predict the measured RED of runs at low UVT since the wall reflection would have caused the calibrated lamp output to be too low.

Figure 3.44 and Figure 3.45 shows plots of the measured vs. predicted RED for the Calgon Sentinel® reactor using the DO radiation model. Figure 3.44 shows results where all the runs were calibrated to the high-UVT run, and Figure 3.45 shows results where all the runs were calibrated to the low-UVT run. As indicated by the red regression lines, the simulations calibrated to the high-UVT run show a better correlation to the measured data. Runs calibrated to the low-UVT test over predict the measured data by a greater amount as shown by the lower slope of the regression between the measured and simulated RED. As discussed above, this indicates that wall reflection is playing a significant role in the reactor performance for runs with high UVT (> 88%).

\[ y = 0.9535x \]
\[ R^2 = 0.9279 \]
figures also show error bars associated with the measured RED. These values were taken from the uncertainty in the log inactivation provided in the Calgon validation report. These uncertainty values (percentages) were propagated to the measured dose using the dose-response curves (quadratic equations) provided in the validation report. The vast majority of the simulated RED results fall within the error of the measured values (i.e., the error bars cross the y=x line). The average measurement error was 16%, and the average absolute relative error between measured and predicted RED was 17% with a 90% confidence interval of plus or minus 5.3% for the high UVT calibration and 22% with a 90% confidence interval of plus or minus 5.8% for the low UVT calibration.

Test results and predictions were also categorized by both lamp configuration (1, 2, or 3 lamps active) and UVT as shown in Figure 3.46 and Figure 3.47. Results show that the simulations of tests consisting of three lamps yielded the best linear regressions relative to the measured data (slope close to 1). The different UVT categorizations had less of an impact on the simulated RED.

For comparison, results from the UVXPT model are shown in Figure 3.48. The UVXPT model included wall reflections, and accounted for spectral and directional dependencies (e.g., refraction) in the UV intensity model. All 96 validation tests were simulated using UVXPT. To provide an equivalent comparison, the UVXPT model was also calibrated using the comparison of measured and predicted RED as given in Figure 3.41. Results show that UVXPT predictions correlate well with the measured data for all three ranges of UVT (slope close to one). However, the correlation depends on the number of lamps with a slope of 0.96 with 1 lamp operation, 1.03 with 2 lamp operation, and 0.99 with 3 lamp operation.
Table 3.5 summarizes the average absolute error in RED (absolute relative difference between measured and predicted RED) categorized by different lamp configurations and UVT for both the Fluent DO radiation model and the UVXPT model. The average absolute error in predicted RED is 17–22% for all the runs using the Fluent DO radiation model (with a 90% confidence interval of plus or minus ~5–6%) and 10% for all runs using the UVXPT model (with a 90% confidence interval of plus or minus 2.0%). The lower average absolute errors resulting from the Fluent DO radiation model are due to its more accurate representation of the UV spectrum and lamp performance.

Figure 3.46 Measured vs. predicted RED using the Fluent DO radiation model with 20% wall reflectivity, DRW (3 tries, ~15,000 particles), calibrated to high UVT. Left: Regressions categorized by lamp configuration. Right: Regressions categorized by UVT.

Figure 3.47 Measured vs. predicted RED using the Fluent DO radiation model with 20% wall reflectivity, DRW (3 tries, ~15,000 particles), calibrated to low UVT. Left: Regressions categorized by lamp configuration. Right: Regressions categorized by UVT.

The average absolute error in RED categorizes by different lamp configurations and UV is summarized in Table 3.5 for both the Fluent DO radiation model and the UVXPT model. The average absolute error in predicted RED is 17–22% for all the runs using the Fluent DO radiation model (with a 90% confidence interval of plus or minus ~5–6%) and 10% for all runs using the UVXPT model (with a 90% confidence interval of plus or minus 2.0%). The lower average absolute errors resulting from the
UVXPT is probably due to the more rigorous treatment of the spectral, directional and reflective dependencies in the UV intensity model. With both the Fluent DO radiation and UVXPT model, the errors are greater when fewer lamps are used. A possible explanation is that as the number of lamps is reduced, the simulated RED becomes more sensitive to the actual flow pattern around those active lamps. Therefore, any discrepancies between the simulated and actual flow patterns would be accentuated in the simulated RED when fewer lamps are operational.

SIMULATIONS OF THE TROJAN REACTOR

Trojan Reactor Configuration and Grid Development

The Trojan Swift® 10L30 reactor was validated in a piping configuration that contains two S-bends upstream from the reactor, as shown in Figure 3.49. The model began with several pipe
diameters of straight pipe, 24-inches in diameter. The pipe size was increased to 30-inches in diameter through a concentric expansion. Two elbows downstream from the expansion formed an S-bend. After a short section of straight pipe, a two more elbows formed a second S-bend. The reactor was located downstream from the second S-bend. The reactor contains 10 lamp sleeves, 6 sensor sleeves, and a wiper screw. Approximately 4 pipe diameters of straight piping follow the reactor, then a concentric contraction for 30-inch diameter pipe, back to 24-inch diameter pipe.

In all cases, an inflow velocity was applied at the upstream end of the model using a uniform velocity distribution corresponding to the respective test conditions flow rate. The downstream boundary was an outflow boundary. All other surfaces were wall boundaries. The $k$-$\varepsilon$ realizable turbulence model was used in all cases, with the standard wall function. The models were all run to steady state in double precision. The solution was calculated with the SIMPLE algorithm utilizing a second order accurate discretization. The models were run to a converged solution, defined by an absolute residual of less than 0.001 for all solved variables.

A grid sensitivity analysis was performed by progressively refining the reactor model grid for three iterations. The cell size of the piping was not changed for the sensitivity runs to maintain a manageable overall model size. The reactor grid transitioned to match one-to-one at the interface with the piping grid. The piping was meshed with a Cooper scheme and cell length ranging from 0.75 inch to 2 inch. The reactor was meshed using a Cooper scheme for the central area with the lamp sleeves and a tetrahedral/hybrid mesh with a hexahedral core to transition to the outer walls. Table 3.6 summarizes the size of the model grids evaluated. The Trojan reactor grid sensitivity was done at a flow rate of 27.3 mgd (42.2 cfs).
For each sensitivity run, the velocity magnitudes at 100 points distributed before and after the reactor were compared between different grids. The correlation coefficients are presented for the pairs of grid comparison (medium vs. initial, fine vs. medium) in Table 3.6. For correlation coefficients close to 1, the simulated velocities were similar between the two grids. Figure 3.50 shows a plot of the comparison for the grid sensitivity runs. There was not much variation in grid comparison between the runs, all matched relatively closely. The fine grid had a cell size ranging from 0.1 inch to 1 inch.

### Table 3.6

<table>
<thead>
<tr>
<th>Grid</th>
<th>No. of cells in reactor</th>
<th>Percent increase in number of cells</th>
<th>No. of cells in piping</th>
<th>Total cells</th>
<th>Velocity magnitude correlation R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial (g1)</td>
<td>529,470</td>
<td>—</td>
<td>408,012</td>
<td>937,590</td>
<td>—</td>
</tr>
<tr>
<td>Medium (g2)</td>
<td>725,517</td>
<td>37</td>
<td>408,012</td>
<td>1,133,637</td>
<td>0.98</td>
</tr>
<tr>
<td>Fine (g3)</td>
<td>848,307</td>
<td>17</td>
<td>408,012</td>
<td>1,256,427</td>
<td>0.96</td>
</tr>
</tbody>
</table>

**Figure 3.50**  Point data comparison between grids for the Trojan grid sensitivity runs

The simulated velocity profile within the Trojan reactor at 27.3 mgd is shown in Figure 3.51 on both a horizontal and vertical cutplane through the reactor centerline. In plan view, the flow separation at the elbow just upstream from the reactor causes a higher approach velocity at one side of the reactor. The velocity approaching the lamps ranges from approximately 2 m/s at the side toward the inside of the elbow to 3.25 m/s on the side toward the outside of the elbow. In the profile section, flow accelerates around the lamps and sensors, with velocity ranging between 1.5 m/s in the open areas, to 3.5 m/s above and below the sleeves where flow acceleration is highest.
Figure 3.51 Simulated velocity profiles along cutplanes through the center of the Trojan Swift reactor. Top: side view. Bottom: plan view.

Simulations of UV Intensity and RED for the Trojan Reactor

**UV Intensity Predictions of Trojan UVSwift™ 10L30 Reactor Using UVXPT**

As indicated in Figure 3.49, the Trojan Swift reactor uses six UV sensor assemblies. Each UV sensor assembly is mounted into a quartz sleeve that projects into the reactor parallel to the lamps. Each UV sensor assembly consists of a rod on which is mounted one or two photodiodes on the outer circumference of the rod. Four assemblies have two photodiodes and two assemblies have one photodiode for a total of ten photodiodes per reactor. Figure 3.52 shows a photograph of the UV sensor assembly (from Water Research Foundation #2977).
The validation report for the Swift reactor provides UV sensor readings made by the Trojan UV sensor. UV sensor readings were recorded as a function of water UVT and ballast power setting at a water layer distance from the sensor port window to the lamp sleeve of 7.87 cm.

UVXPT was used to model the UV intensity within the UV reactor and the UV sensor readings. Figure 3.53 shows the spectral and angular response of the UV sensor used in the model, and Figure 3.54 shows the lamp output used to model the Trojan reactor. The spectral and angular response was obtained from Water Research Foundation project 2977, Design and Performance Guidelines for UV Sensor Systems. Because the angular response data given in Water Research Foundation 2977 was for an air-quartz-air interface, the data was adjusted for a water-quartz-air interface using the approach described in “UV Intensity Predictions of IDI Reactor Using UVXPT” earlier in this chapter. Figure 3.53 shows the UV output of the MP lamp obtained from AwwaRF.
project 2983 *Optimization of UV Disinfection*. The output was scaled to give a one-to-one relation between measured and predicted UV sensor readings (see Figure 3.58). Figure 3.55 shows the index of refraction of water and quartz and the UV absorbance coefficient of quartz used by UVXPT. The data for quartz was obtained from GE for type 214 quartz at room temperature. Figure 3.56 shows the spectral UVA of the test waters obtained from the validation report.

Figure 3.57 shows the dependence of the UV sensor readings on the angular orientation of the UV sensor around the lamp. Like many MP UV systems, the data shows that the UV lamp output varies about the circumference of the lamp with greater output from the top of the lamp. To account for this affect, the relative output from each lamp used in the model was scaled to give a UV sensor reading that showed a similar dependence.

Figure 3.58 shows the comparison of measured and predicted UV sensor readings. The data was fitted using the relation \( y = Ax \) with a slope of 1.00 and an R-squared of 0.9851. The quality of the fit suggests that the UV intensity and UV sensor algorithm used by UVXPT is accounting well for the relative impacts of UVT and lamp power setting.
Inactivation Kinetics Used in UVXPT

The Trojan reactor was validated using MS2 phage. Figure 3.59 shows a plot of the dose-response data. The dose response had statistically significant curvature.

Curve fitting software was used to identify the best empirical fit to the data. The analysis identified the following function as providing the best fit:

Exponential Association Function: \( \log i = a \times (1 - \exp(-b \times \text{Dose})) \)

where \( a = 8.399 \) and \( b = 0.007129 \).
Figure 3.59 UV dose-response data for MS2 phage used to validate the Trojan reactor

Figure 3.60 Exponential association function fit to the MS2 UV dose-response used to validate the Trojan reactor

Figure 3.60 shows the fits to the UV dose-response data using the exponential association function. The models show distinct tailing when extrapolated beyond the range of the measured UV dose-response curves.

**Action Spectra**

The Trojan system was modeled in UVXPT using the action spectra of MS2 as reported by Rauth (1965) (Figure 3.61).

**RED Simulations of Trojan Reactor Using UVXPT**

FLUENT software was used to generate particle tracks for the Trojan reactor with and without the random walk for three mesh densities. The CFD was conducted for a flowrate of 27.27 mgd. UVXPT scales the time step of the particle tracks using the ratio of the CFD flowrate and the flowrate of the operating condition of interest.
The Trojan reactor was validated at the UV Validation and Research Center of New York, Johnstown, NY. The reactor was validated using MS2 phage as a test microbe at flows from 2.85 to 42.4 mgd and UVTs from 79 to 98 percent. The validation data was fitted using a multivariate regression to the equation:

\[
RED = 10^A \times UVA^B \times UVA^C \times \left( \frac{S/S_0}{Q} \right)^D \times UVA^E \times UVA^F \tag{3.3}
\]

where \(RED\) is the MS2 RED, \(UVA\) is the UV absorbance of the water, \(Q\) is the flowrate, and \(S/S_0\) is the relative lamp output determined from the UV sensor readings, \(S\) and the UV sensor readings predicted for a new lamp operating at the 100 percent power setting in new and clean quartz sleeves. Figure 3.62 compares the MS2 RED measured during validation to that predicted using this equation. As shown, the relation between measured and predicted RED was fitted with the relation \(y = Ax\) with a slope of 1.0033 and an R-squared of 0.9806.
The UVXPT model was applied using the fine mesh. Figure 3.63 shows a plot of measured versus UVXPT-predicted MS2 RED. The UVXPT model did not include wall reflections. The following observations are made:

1. For a given UVT, the relation between measured and UVXPT-predicted RED is fitted with the relation $y=Ax$ with an R-squared ranging from 0.9653 to 0.9878. The high R-squared shows that the model is accounting for the impacts of flow rate and relative lamp output reasonably well.

2. The predicted REDs are lower than the measured REDs. In part, this difference is likely related to the calibration of the lamp output using the UV sensor readings. The UV sensor model does not account for the refraction and transmittance of light through the quartz tube holding the UV sensor. Refraction of light through the curved surface of the quartz tube will cause light to diverge from the UV sensor. Hence, the UV sensor model is likely underestimating the UV sensor readings and the calibration is underestimating the lamp output.

3. Like the Calgon model predictions, the differences between the measured and predicted REDs are greater at higher UVT. This observation may be explained by the contribution of reactor wall reflections.

4. The observation that the CFD model obtained for one flow rate provides good predictions at other flow rates implies that the scaling of the time step used by UVXPT is a reasonable approach. This conclusion is specific to this reactor and its inlet and outlet piping. The validity of the approach should always be verified before using it with other UV reactors and piping configurations.

The simulations used to develop Figure 3.63 assumed a Lambertian lamp output where the output from the line source is proportional to the cosine of the emitting angle. Figure 3.64 presents the relation between measured and predicted RED assuming a point source lamp output (i.e., the lamp output from each point source defining the lamp was equally weighted regardless of
the emitting angle. The lamp output was re-calibrated by comparing measured and predicted UV sensor readings. Figure 3.64 shows better agreement between measured and predicted RED at low UVTs compared to Figure 3.63, suggesting that the point source assumption is more valid than the Lambertian source assumption for the Trojan lamps. The average absolute relative error between measured and predicted RED is ~29% (with a 90% confidence interval of plus or minus 2.3%) for the Lambertian source assumption and ~16% (with a 90% confidence interval of plus or minus 2.5%) for the point source assumption.

Whether a small element along the length of a lamp should be modeled as a Lambertian radiator or a point source depends on the optical density of the arc at the relevant wavelength of emitted light (Phillips, 1983). A small element along the lamp acts more like a Lambertian emitter as the optical density of the arc increases. While the output from a linear fluorescent lamp behaves like an ideal Lambertian emitter, the output of mercury lamps without fluorescent coatings (e.g., the 265 nm line of a medium pressure UV lamp) is more complex, behaving between what would be expected with a Lambertian and point source emitter. If the behavior is not known, the angular dependence of the UV lamp’s output represents a potential source of modeling error.

Figure 3.65 compares the measured and UVXPT-predicted REDs where the UVXPT model assumes a point source lamp output and does not include wall reflections. Figure 3.66 compares the validation fitted REDs to the UVXPT predicted REDs obtained using the same model. The following observations are made from the data:

- The plot of measured versus UVXPT-predicted RED in Figure 3.65 was fitted with the relation $y = Ax$ with a slope of 1.08 and an R-squared of 0.972 while the plot of validation fitted versus UVXPT-predicted RED was fitted with the relation $y = Ax$ with a slope of 1.08 and an R-squared of 0.9933. Inclusion of reflection significantly improved the correlation between the measured and validation fitted REDs and the UVXPT-predicted RED.
- Given the close agreement between the validation fitted and UVXPT-predicted RED, the slope of the relation could be used to further calibrate the UVXPT model, resulting
Computational Fluid Dynamics Based Models for Assessing UV Reactor Design and Installation

The calibrated UVXPT model would then predict the validated RED to within 4.63 mJ/cm² as a 95th percent prediction interval. This value is comparable if not better than the uncertainty of interpolation typically observed with UV validation, which ranges from 4 to 12 mJ/cm².

- The R-squared with the relation between validation fitted and UVXPT-predicted MS2 REDs given in Figure 3.66 is higher than that with the relation between the measured and validation fitted MS2 REDs given in Figure 3.62. The observation suggests that the CFD-based model is accounting for change flow, UVT and lamp power setting and lamp on/off status with an accuracy comparable to the validation equation. The observation provides confidence that a calibrated CFD-based model can accurately predict UV reactor performance for conditions that have not been validated, such as flow above or below the validated range, various combination of on/off lamps, different hydraulic conditions through the reactor, and changes in reactor design.

Figure 3.65 Measured vs. UVXPT-predicted MS2 RED for the Trojan reactor where UVXPT model assumes a point source lamp output and includes wall reflections

Figure 3.66 Validation fitted vs. UVXPT-predicted MS2 RED for the Trojan reactor where UVXPT model assumes a point source lamp output and includes wall reflections
SENSITIVITY ANALYSIS OF PARTICLE TRACKING PARAMETERS

Sensitivity studies were performed to investigate the impact of several particle tracking parameters that are available in the Fluent hydraulic model. The parameters that were investigated included the following:

- Number of particles/tries using discrete random walk (DRW)
- Number of particles using no-DRW
- Impact of random eddy-lifetime
- DRW vs. no DRW as a function of flow rate

In the following sensitivity analyses, the Fluent DO radiation model was used.

Particle Injection and DRW

A sensitivity analysis was performed to expand on the work performed by Munoz et al. (2007) to investigate the impacts of various particle tracking inputs on the simulated performance (RED) of commercial UV reactors. The number of injected particles required to ensure a sufficiently invariant simulated RED was investigated. Furthermore, when the Discrete Random Walk (DRW) model is enabled for the particle tracking calculations, a random fluctuating velocity component (caused by turbulence) is added to the mean velocity at each time step along the particle trajectory. Therefore, for different runs (tries), a particle will take different paths with DRW enabled. This study also seeks to determine the number of repeated runs (tries) required to obtain a sufficiently invariant mean simulated RED.

Two geometries were considered in this study using the Ozonia Aquaray® H₂O UV reactor: (1) L-rig without baffle, only reactor #1 turned on and (2) M-rig without baffle. Two test conditions with different flow rates were chosen for each geometry and simulated in FLUENT. The particle tracking model was run on each of the 4 configurations using 10 different injection files (ranging from ~200–50,000 injection points). For each configuration, each injection file was run once without DRW and 20 times with DRW enabled. For both geometries, a high flow rate and a low flow rate test were chosen.

The lamp irradiation boundary condition for each case was fixed at a value that would, with DRW enabled, yield a simulated RED close to the measured RED. No wall reflection was simulated. The Random Eddy Lifetime option of the DRW model was enabled in this study, which randomized the characteristic eddy lifetime. For one configuration, a comparison was made between the simulated REDs yielded from enabling and disabling Random Eddy Lifetime. Table 4.1 summarizes the test conditions chosen for this sensitivity analysis.

Figures 4.1 through 4.4 show the simulated RED for each of the four reactor configurations using different configurations of particle tracking inputs. The simulated mean RED is plotted against the number of particles that were injected and traveled through the system for each run. For
multiple runs (tries), the same number of particles was injected for each run (try). In each plot, simulations with and without DRW enabled are shown.

Results show that there is a notable difference between the simulated RED with and without DRW, and this difference appears to be more pronounced at lower flow rates. This difference will be further explored in the sensitivity analysis that follows. It should be repeated that the simulated lamp output was calibrated using the runs with DRW enabled, so it is expected that the simulated RED with DRW enabled will match the observed RED values listed in Table 4.1. The variability of the simulated RED also appears more dependent on the number of injected particles when the flow rate is low, where a greater number of particles yields lower variability in the simulated RED between tries. Also, with increased numbers of tries, the variability is reduced, even with fewer particles injected.

In all cases, the variability in the simulated RED drops to less than several percent if greater than 5,000–10,000 particles is used for any number of tries. Even in the case of the lowest flow

<table>
<thead>
<tr>
<th>Test ID</th>
<th>Geometry</th>
<th>Flow rate (m³/h)</th>
<th>Test UVT (%)</th>
<th>Measured RED (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM</td>
<td>L-rig, reactor #1</td>
<td>380</td>
<td>81.85%</td>
<td>511</td>
</tr>
<tr>
<td>BD</td>
<td>L-rig, reactor #1</td>
<td>2050</td>
<td>91.83%</td>
<td>304</td>
</tr>
<tr>
<td>AF</td>
<td>M-rig no baffle</td>
<td>420</td>
<td>81.85%</td>
<td>390</td>
</tr>
<tr>
<td>P</td>
<td>M-rig no baffle</td>
<td>1200</td>
<td>90.36%</td>
<td>325</td>
</tr>
</tbody>
</table>

Figure 4.1 Simulated mean RED for different particle injection configurations for the L-rig, Test AM, 380 m³/h, UV T = 81.85%
Figure 4.2 Simulated mean RED for different particle injection configurations for the L-rig, Test BD, 2,050 m³/h, UVT = 91.83%

Figure 4.3 Simulated mean RED for different particle injection configurations for the M-rig, Test AF, no baffle, 420 m³/h, UVT = 81.85%
Computational Fluid Dynamics Based Models for Assessing UV Reactor Design and Installation

Figure 4.4 Simulated mean RED for different particle injection configurations for the L-rig, Test P, no baffle, 1,200 m$^3$/h, UVT = 90.36%

rate, Test AM (flow rate 380 m$^3$/h), the % Error in Mean RED was within 1% for any number of
tries when near 14,000 particles were used.

The test condition M-rig No Baffle Test AF (Flow Rate 420 m$^3$/h, UVT = 81.85%) was run
using nearly 14,000 particles, 20 tries with DRW, and with Random Eddy Lifetime, and 20 tries
with DRW but without Random Eddy Lifetime (hence with Constant Eddy Lifetime). Test AF had
a sufficiently low flow rate for the DRW model to have a notable impact on the simulated RED, yet
the difference between REDs for Random and Constant Eddy Lifetime was within 0.7% for any
number of tries. The choice of enabling vs. disabling Random Eddy Lifetime thus appears
inconsequential.

Figure 4.5 shows some images of simulated results from the Fluent DO radiation model of
the Calgon Sentinel reactor when one lamp (lamp 3) is on at a relatively low flow rate (Re ~100,000).
The particle paths with discrete random walk (DRW) at this flow rate are more random than the
particle paths without discrete random walk. Appendix E provides additional discussion regarding
the inputs to the DRW model (time scale constant and random eddy lifetime) and their dependency
on flow rate. It should be noted, however, that although these flow fields converged using the
default convergence criteria (0.001) for the continuity, velocity, turbulent kinetic energy, and tur-
bulent energy dissipation residuals, the simulated turbulent kinetic energy may have been too high.
At low flow rates, warnings were generated by the Fluent code that the simulated turbulent (eddy)
viscosity, which is proportional to the square of the turbulent kinetic energy, was limited to $1\times10^5$
times the prescribed water viscosity ($1\times10^{-3}$ N-s/m$^2$) in a number of cells, even after the hydraulic
solution converged (~150 iterations). As discussed in the next section, the DRW particle tracking
model incorporates the turbulent fluctuating velocity components in the particle motion at each
time step. These fluctuating velocity components are proportional to the simulated turbulent kinetic
Figure 4.5 Simulated incident radiation using the Fluent DO radiation model (top) with one lamp on. Particle traces colored by cumulative dose (J/m²) are shown without DRW (middle) and with DRW (bottom) implemented in the particle tracking model after auto-convergence at 151 iterations.
energy (and turbulence intensity), so larger values of the simulated turbulent kinetic energy will increase the randomness of the particle path. To investigate this, the convergence criteria were turned off, and this run was allowed to proceed for 1000 additional iterations; the turbulent viscosity ratio fell below $1 \times 10^5$ for all cells at about 300 iterations. Figure 4.6 shows the particle paths resulting from these additional iterations.

The mean RED with DRW (3 tries) after 1151 iterations was 30.53 mJ/cm$^2$ ($\sigma=0.0259$), and the simulated RED without DRW after 1151 iterations was 31.22 mJ/cm$^2$, a relative error of only 2%. In contrast, the mean RED with DRW (3 tries) after 151 iterations (converged) was 25.07 mJ/cm$^2$ ($\sigma=0.134$), and the simulated RED without DRW after 151 iterations was 20.61 mJ/cm$^2$, a relative error of ~20%. This indicates that additional iterations may be needed, even after the hydraulic solution has converged with default convergence criteria. In turbulence models (such as the realizable $k$-$\epsilon$ model used here), iterations should be continued until the turbulent viscosity ratio drops below $1 \times 10^5$ (at which point the warning goes away), and it would be prudent to run several hundred additional iterations after that. The runs presented in this report using the Fluent hydraulic and DO radiation models should be redone with additional iterations to ensure the turbulent parameters have truly converged. Properly initializing the turbulence parameters (e.g., turbulent kinetic energy and turbulent energy dissipation) may improve the convergence. The default values of one used in Fluent are about four orders of magnitude too high for the geometry and flow conditions evaluated in this study. The next section and Appendix E provide additional discussion regarding the inputs to the DRW model (time scale constant and random eddy lifetime) and their dependency on flow rate.

Impact of DRW vs. Flow Rate

The previous sensitivity study indicated that the difference between simulated RED values with and without DRW enabled was more pronounced at lower flow rates. Ho et al. (2008) showed that the reason for the discrepancy at lower flow rates could be caused by the increased random turbulent velocity fluctuations that are added to the mean velocity components in the DRW model. If the contribution from these fluctuating velocity components are more significant relative to the mean velocity components at lower flow rates, then the DRW model could result in more significant differences at lower flow rates. A quantity called the turbulence intensity is equal to the turbulent fluctuating velocity component ($u'$) divided by the average velocity ($u_{avg}$). This value decreases with increasing flow rate (Reynolds number) as shown in Figure 4.7. Thus, the principle of a decreasing turbulent kinetic energy and turbulent intensity with increasing flow rate is valid, and using the DRW particle tracking model may yield more notable differences at lower flow rates.

SENSITIVITY STUDIES OF WALL REFLECTION

FLUENT Simulations

Models of UV disinfection systems typically simulate the hydraulics and UV-intensity fields independently of one another. Often, the UV-intensity models do not include the effects of shadowing and wall reflections that can be induced by surfaces and geometric features within the UV reactor, even though these features are typically modeled in the hydraulic system using CFD. The use of integrated hydraulic and radiation models, which honors a consistent representation of the geometry and features within the UV reactor, is assessed in this section.
Figure 4.6 Particle traces colored by cumulative dose (J/m²) for Test 74 (low flow) without DRW (top) and with DRW (bottom) implemented in the particle tracking model after 1,151 iterations.
The CFD software, Fluent, is used in our current studies to simulate the hydraulics within the UV reactor and piping. Fluent, which is used widely throughout industry and academia, also contains several radiation models that can simulate UV irradiation within the reactor. For problems with participating media over a wide range of optical thicknesses (e.g., water UVT ranging from 70–100%), the discrete ordinates (DO) radiation model is the best option. The DO radiation model solves the radiative transfer equation for a finite number of solid angles, prescribed by the user. Details of the DO radiation model can be found in the Fluent User’s Guide. A step-by-step user’s guide (developed as part of this work) to implementing the DO radiation model for UV disinfection problems is provided in Appendix A. This guide, as well as pre-processors (to generate a uniform distribution of particle injections), post-processors (to calculate the RED from the particle dose distribution), and user-defined functions developed for Fluent, will be posted to our web site (www.sandia.gov/cfd-water) to assist modelers in using Fluent (and other CFD codes with integrated radiation models) to simulate UV disinfection systems.

Two configurations of the Calgon 12” Sentinel were evaluated to perform sensitivity analyses using the Fluent DO radiation model: (1) UVT = 88% (ID #57) and (2) UVT = 98.6% (ID #46). Sensitivity to the lamp power, number of particles injected, and wall reflection was investigated. Comparisons were also made between the UV intensity fields calculated by Fluent and UVXPT.

Comparisons between the simulated UV-intensity fields of UVXPT and Fluent (with wall reflection) are shown in Figures 4.8 through 4.11. Results are plotted along three vertical transects and one horizontal transect within the reactor. These plots also show the Fluent results as a function of different lamp outputs for the configuration with UVT = 88% (ID #57), which was used to calibrate the lamp power to the observed RED. A simulated lamp output of 2,700 W/m² applied to each sleeve was found to yield a good match with the observed RED for a UVT of 88%. This lamp output was then used for all subsequent runs and configurations.
Figure 4.8 Comparison between simulated UV intensities along a vertical transect (x=0.31 m) in the Calgon reactor using UVXPT and Fluent. Top: UVT = 88%, Bottom: UVT = 98.6%.
Figure 4.9 Comparison between simulated UV intensities along a vertical transect \((x=0.39\text{m})\) in the Calgon reactor using UVXPT and Fluent. Top: \(\text{UVT} = 88\%\), Bottom: \(\text{UVT} = 98.6\%\).
Figure 4.10 Comparison between simulated UV intensities along a vertical transect (x=0.47m) in the Calgon reactor using UVXPT and Fluent. Top: UVT = 88%, Bottom: UVT = 98.6%.
Figure 4.11 Comparison between simulated UV intensities along a horizontal transect (x=0.31, z=0 m) in the Calgon reactor using UVXPT and Fluent. Top: UVT = 88%, Bottom: UVT = 98.6%.
The plots shown in Figure 4.8 through Figure 4.11 reveal the following:

- A calibrated lamp out of 2700 W/m² yields UV intensities that match those of UVXPT fairly well along vertical transects aligned with the lamps (Figure 4.8 and Figure 4.10), especially at UVT = 88%.

- At UVT = 98.6%, the Fluent intensities are higher than those of UVXPT, especially near the walls. This discrepancy can be attributed to the inclusion of wall reflection in Fluent. This difference is even more pronounced along the vertical transect at x=0.39 m (Figure 4.9) and the horizontal transect (Figure 4.11).

- Figure 4.9 shows the impact of shadowing caused by the wiper screw in the center of the reactor. The Fluent simulation shows a slight lowering of the UV intensities in this location as a result of the shadowing.

- Figure 4.11 shows that along the length of the lamp, UVXPT predicts greater intensities near the middle and less near the ends relative to the results of Fluent. This can be attributed to the application of a diffuse irradiation boundary condition in Fluent. As discussed in Liu et al. (2004), the effects of refraction, which is included in the UVXPT model but not in the Fluent model, tends to bend and focus the rays perpendicular to the sleeve surface. 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.

Figures 4.12 through 4.15 shows plots of simulated radiation intensities using Fluent with and without wall reflection for UVT = 88% and UVT = 98.6%. For the simulation with wall reflection, the internal emissivity for the reactor walls was changed from 1 to 0.6, which yields a 40% reflectivity. A value of 40% was used based on the spectral reflectance at 254 nm reported in Luckiesh (1929) for polished steel. Reflection from the walls was assumed to be completely diffuse (diffuse fraction = 1) because they were bead blasted. The following observations of the plots in Figure 4.12 through Figure 4.15 are made:

- At UVT = 88%, the impact of wall reflections is small (but still noticeable) relative to the differences when UVT = 98.6%.

- At UVT = 98.6%, the simulation with wall reflection yields UV intensities that are up to 75% greater than the simulation without wall reflection at locations near the walls (Figure 4.12 and Figure 4.14) and near the center of the reactor between the lamps (Figure 4.13).

- Figure 4.15 shows that wall reflection also increases the simulated intensities along the horizontal transect between the vertically aligned lamps.

Figure 4.16 shows the simulated cumulative dose along particle paths with and without reflection for a UVT = 98.6%. The wall reflection increases the amount of irradiation received by the particles, so the simulated cumulative dose distribution is higher. Note that in these simulations, DRW was not enabled to ensure repeatability between runs with and without wall reflection. Particle paths with DRW would be more random and less uniform.
Figure 4.12 Comparison between simulated UV intensities along a vertical transect (x=0.31 m) in the Calgon reactor using Fluent with and without wall reflection. Top: UVT = 88%, Bottom: UVT = 98.6%.
Chapter 4: Sensitivity Studies

Figure 4.13 Comparison between simulated UV intensities along a vertical transect (x=0.39m) in the Calgon reactor using Fluent with and without wall reflection. Top: UVT = 88%, Bottom: UVT = 98.6%.
Figure 4.14 Comparison between simulated UV intensities along a vertical transect (x=0.47m) in the Calgon reactor using Fluent with and without wall reflection. Top: UVT = 88%, Bottom: UVT = 98.6%.
Figure 4.15 Comparison between simulated UV intensities along a horizontal transect (x=0.31, z=0 m) in the Calgon reactor using Fluent with and without wall reflection. Top: UVT = 88%, Bottom: UVT = 98.6%.
Figure 4.16 Simulated cumulative dose (red is high, blue is low) of individual particles released into the Calgon Sentinel reactor using the discrete ordinates radiation model with UVT = 98.6%. Top: 40% wall reflection. Bottom: no wall reflection.

Figure 4.17 shows the measured and simulated RED using Fluent with and without reflection for UVT = 88% and UVT = 98.6%. Because the lamp power (2,700 W/m²) was calibrated to the measured RED for the Fluent simulation with a wall reflectivity of 40% at UVT = 88%, the simulated RED matches the measured RED for that run. Without wall reflection, the simulated RED for UVT = 88% is about 6% less. At UVT = 98.6%, the difference between the simulated REDs with and without reflection is about 23% (with a wall reflectivity of 40%). Also, the Fluent results with a wall reflectivity of 40% over predict the measured RED by ~18%, and the Fluent results without reflection under predict the measured RED by ~10%. The use of a lower wall reflectivity of 20% (as suggested by Keith Bircher from Calgon) is also shown in Figure 4.17. The reduced wall reflectivity of 20% does not change the simulated RED significantly for a UVT = 88%. However, at UVT = 98.6%, the simulated RED is reduced by ~13% when the wall reflectivity is reduced from 40% to 20%, and the results match the data better (within 4%). These sensitivity studies indicate that wall reflection should be considered when the wall reflectivity is at least 20% and when the UVT is greater than ~88%.
This section focuses on processes involving reflection and refraction of UV radiation from walls and surfaces (in particular the interior and exterior walls of the quartz sleeve) 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 4.18 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. Results were reported for a water UV transmittance of 88%. Figure 4.19 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 ~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 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 4.18).
Figure 4.20 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 4.18. 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 × phi) of 5 × 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 × 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 or diffuse reflecting surface with a prescribed internal emissivity. The reflectance for these opaque surfaces is calculated as one minus the prescribed emissivity (emissivity equals absorptivity for gray surfaces). 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 (mirror-like)
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 (Bolton, 2000). 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. (2008). 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

**DO Radiation Model With Refraction**

Figure 4.21 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 4.22 shows a plot of the measured and simulated incident radiation (with and without reflection) at the 18 actinometer sensor locations in Liu et al. (2004). 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.
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 underpredict 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 4.18). 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 4.23 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 ($x \sim 3.98$, 7.28, and 10.7 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 4.18). 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.
Radiation Model Without Refraction

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 4.24 and Figure 4.25 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 4.24 shows results from simulations that include reflection (40%) from the interior walls of the chamber, and Figure 4.25 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 4.26 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 4.27 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).
Figure 4.26 Simulated irradiation field (W/m²) neglecting the effects of reflection and refraction at the quartz sleeve. An appropriate power flux is applied to the outer surface of the sleeve, which is modeled as a void in the domain.

Figure 4.27 Simulated incident radiation without reflection and refraction at the quartz sleeve. The solid line represents a simulation with no sleeve or lamp annulus, and the dashed line represents a simulation that included those features but with the indices of refraction set to one. Wall reflection is included. Data are shown as symbols with error bars representing plus/minus one standard deviation.
Summary of Reflection and Refraction Study

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.
CHAPTER 5
COMPARISON OF INSTALLED VS. VALIDATED SYSTEMS
USING CFD-BASED MODELS

The performance of UV disinfection systems can be impacted by a number of factors that affect the hydraulics and/or UV intensity fields in these systems. Some of these factors (e.g., flow rate, UV transmittance) are characterized during validation testing of the UV reactors. However, the impacts of these and other factors, such as variability in UV lamp configuration and changes to the inlet/outlet piping, can be difficult to characterize if the installed configuration is different than the validated configuration. In many cases, utilities will be retrofitting UV into existing treatment systems, so they may be limited in their ability to either match the validated configuration or fully characterize the installed configuration. Thus, utilities need a tool to assess the impact of factors that may affect the hydraulics or UV intensity fields in their systems. Moreover, a better understanding of the effects of inlet/outlet hydraulic configurations and lamp configurations on UV disinfection performance will result in more pragmatic design recommendations, with a potential to significantly reduce capital costs in future UV installations.

IMPACT OF APPROACH HYDRAULICS

The IDI validation tests consisted of three different configurations that impacted the approach hydraulics into the reactor. The L-rig (without baffle plate) used inlet and outlet pipes that were larger than the diameter of the reactor, so the flow converged into the opening of the reactor. The M-rig used pipes that were smaller than the diameter of the reactor, so the flow expanded into the reactor. Tests were also performed on the M-rig with and without a baffle plate near the inlet of the reactor. The baffle plate was intended to “straighten” the flow before passing through the reactor.

Results of the tests showed that the L-rig performed better than the M-rig (without baffle) for equivalent operating conditions (and for operating conditions when the L-rig would be expected to perform worse; e.g., when the flow rate was greater in the L-rig). The M-rig tests with the baffle plate performed better than tests without the baffle plate for similar operating conditions. Table 5.1 summarizes the results of the L-rig vs. M-rig (without baffle) tests, and Table 5.2 summarizes the results of the M-rig (with baffle) vs. M-rig (without baffle) tests that were used to compare the impact of approach hydraulics.

The tests shown in Table 5.1 and Table 5.2 were simulated as detailed in “Simulations of IDI Reactor” in Chapter 3. The simulations yielded trends in the predicted RED that matched the observed trends in all but one case (Test AF yielded a predicted RED that was greater than that of Test AX). Figure 5.1 illustrates the trends by plotting the simulated RED of both the L-rig and M-rig (with baffle) as a function of the simulated RED of the M-rig (without baffle). Again, the tests that were chosen showed that the L-rig performed better than the M-rig (without baffle), and the M-rig (with baffle) performed better than the M-rig without baffle. The data in the plot fall above the y=x line (except for one), indicating that the simulated performance of the L-rig and M-rig with baffle is generally better than (or at least as good as) the performance of the M-rig without baffle. This method of comparison is further detailed and used in the next section to evaluate the performance of installed reactors relative to validated reactors that have different piping configurations.
Table 5.1
Results of IDI simulations of L-rig without baffle vs. M-rig without baffle

<table>
<thead>
<tr>
<th>Test ID</th>
<th>Configuration</th>
<th>Flow rate (m³/h)</th>
<th>UVT</th>
<th>DVGW Sensor Reading</th>
<th>Measured RED (J/m²)</th>
<th>Predicted RED (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AP</td>
<td>L-rig</td>
<td>890</td>
<td>86.70%</td>
<td>63</td>
<td>380</td>
<td>363.2</td>
</tr>
<tr>
<td>AI</td>
<td>M-rig (no baffle)</td>
<td>890</td>
<td>86.70%</td>
<td>65.5</td>
<td>320</td>
<td>298.1</td>
</tr>
<tr>
<td>AU</td>
<td>L-rig</td>
<td>1000</td>
<td>86.70%</td>
<td>65</td>
<td>345</td>
<td>336.0</td>
</tr>
<tr>
<td>AI</td>
<td>M-rig (no baffle)</td>
<td>890</td>
<td>86.70%</td>
<td>65.5</td>
<td>320</td>
<td>298.1</td>
</tr>
<tr>
<td>AV</td>
<td>L-rig</td>
<td>800</td>
<td>86.70%</td>
<td>66</td>
<td>409</td>
<td>409.0</td>
</tr>
<tr>
<td>AH</td>
<td>M-rig (no baffle)</td>
<td>630</td>
<td>86.70%</td>
<td>66</td>
<td>403</td>
<td>403.3</td>
</tr>
<tr>
<td>AQ</td>
<td>L-rig</td>
<td>950</td>
<td>91.83%</td>
<td>119</td>
<td>519</td>
<td>538.9</td>
</tr>
<tr>
<td>AJ</td>
<td>M-rig (no baffle)</td>
<td>850</td>
<td>91.83%</td>
<td>122</td>
<td>464</td>
<td>472.0</td>
</tr>
<tr>
<td>AX</td>
<td>L-rig</td>
<td>500</td>
<td>81.85%</td>
<td>38</td>
<td>434</td>
<td>452.7</td>
</tr>
<tr>
<td>AF</td>
<td>M-rig (no baffle)</td>
<td>420</td>
<td>81.85%</td>
<td>37.3</td>
<td>390</td>
<td>464.3</td>
</tr>
<tr>
<td>AG</td>
<td>M-rig (no baffle)</td>
<td>480</td>
<td>81.85%</td>
<td>37.2</td>
<td>370</td>
<td>389.4</td>
</tr>
</tbody>
</table>

Table 5.2
Results of IDI simulations of M-rig with baffle vs. M-rig without baffle

<table>
<thead>
<tr>
<th>Test ID</th>
<th>Configuration</th>
<th>Flow rate (m³/h)</th>
<th>UVT</th>
<th>DVGW Sensor Reading</th>
<th>Measured RED (J/m²)</th>
<th>Predicted RED (J/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AK</td>
<td>M-rig (with baffle)</td>
<td>440</td>
<td>81.85%</td>
<td>37.3</td>
<td>456</td>
<td>484.1</td>
</tr>
<tr>
<td>AF</td>
<td>M-rig (no baffle)</td>
<td>420</td>
<td>81.85%</td>
<td>37.3</td>
<td>390</td>
<td>464.3</td>
</tr>
<tr>
<td>AE</td>
<td>M-rig (with baffle)</td>
<td>660</td>
<td>86.70%</td>
<td>63</td>
<td>432</td>
<td>431.6</td>
</tr>
<tr>
<td>AH</td>
<td>M-rig (no baffle)</td>
<td>630</td>
<td>86.70%</td>
<td>66</td>
<td>403</td>
<td>403.3</td>
</tr>
<tr>
<td>AL</td>
<td>M-rig (with baffle)</td>
<td>950</td>
<td>91.83%</td>
<td>124</td>
<td>511</td>
<td>535.6</td>
</tr>
<tr>
<td>AJ</td>
<td>M-rig (no baffle)</td>
<td>850</td>
<td>91.83%</td>
<td>122</td>
<td>464</td>
<td>472.0</td>
</tr>
</tbody>
</table>

COMPARISON BETWEEN SIMULATED RED FOR DIFFERENT PIPING AND REACTOR CONFIGURATIONS

One of the primary objectives of this work is to show how CFD modeling can be used to demonstrate whether an installed reactor system with a different piping configuration will yield performance that is at least as good as the validated system. In some instances, space limitations or retrofits will require that the inlet and/or outlet piping to the reactor be different than the piping configuration used in the validation test. Rather than redoing expensive biodosimetry tests on the installed configuration, the following computational approach is proposed to assess the performance of the installed system relative to the validated system:

1. Perform CFD simulations of the validated reactor system under different operating conditions (e.g., flow rate, UVT, lamp output). See, for example, sections “CFD Hydraulic Model” in Chapter 2, and “IDI Reactor Configurations and Grid

a. Ensure grid-independent solution by refining mesh until simulated metrics (e.g., RED, velocities) do not change.

b. Develop UV intensity models and calibrate lamp output according to measured sensor readings (and RED, if sensor model is not adequate; see the section “RED Simulations of Calgon Reactor Using Fluent DO Radiation Model” in Chapter 3).

2. Compare the simulated RED to measured RED for each operating condition and determine if a good linear regression exists (e.g., plot the measured RED as a function of the predicted RED, fit a linear regression to the data in the form of \( y = mx \), and determine if the slope and \( R^2 \) are close to one*).

a. If not, the models must be refined and improved (e.g., inclusion of reflection, appropriate number and location of particles injected, choice of UV intensity model, use of appropriate inactivation kinetics, etc.) until a good regression with the measured data exists as determined by an appropriate validation metric as discussed in “Validation Metrics” in Chapter 2. See Figure 5.2 for an example regression between measured and predicted RED (red symbols and red regression line).

b. If a good regression exists between the measured and predicted RED, proceed to the next step.

*According to Devore (1982; p. 449), a reasonable rule of thumb is that the correlation is weak if \( 0 \leq |R| \leq 0.5 \), strong if \( 0.8 \leq |R| \leq 1.0 \), and moderate otherwise. Therefore, if \( R^2 > 0.64 \), a strong correlation between the measured and predicted RED exists. The accuracy can be judged by the residuals of measured and predicted RED values.
3. Using the same modeling approach that yielded a good regression with the validated data, develop a model of the installed system configuration (with different inlet and/or outlet piping).

4. Simulate the same operating conditions that were simulated for the validated configuration.

5. Plot the predicted RED of the installed configuration as a function of the predicted RED of the validated configuration for each run.
   a. If the data points fall above the $y = x$ curve, then the performance of the new configuration is better than the performance of the validated configuration.
   b. If the data points fall below the $y = x$ curve, then the performance of the new configuration is worse than the performance of the validated configuration.

6. A linear regression in the form of $y = mx$ can also be applied to the data. The data may not produce a linear regression (e.g., the installed configuration may not consistently perform better than the validated configuration for all operating conditions), but if it does ($R^2$ close to one), then the slope of the regression gives a convenient measure of the performance of the installed system relative to the validated configuration over the entire range of operating conditions simulated. See Figure 5.2 for an example of the regression between the simulated RED of a hypothetical installed and validated system (blue symbols and blue regression line).
   a. If the slope of the regression is greater than one, then the overall performance of the installed configuration is better than the performance of the validated configuration over the range of operating conditions simulated.
b. If the slope of the regression is less than one, then the overall performance of the installed configuration is worse than the performance of the validated configuration over the range of operating conditions simulated.

The above approach is consistent with the recommendations of the UV Disinfection Guidance Manual (USEPA, 2006, Appendix D.6). Figure 5.2 shows an example of this process using just a few results from the L-rig and M-rig (without baffle) simulations assuming that the M-rig (without baffle) was the validated configuration and the L-rig was the installed configuration. All simulations assumed 20% reflection and no-DRW, and the calibrated run corresponded to the system configuration being simulated (i.e., the lamp output was calibrated to test AV for the L-rig simulations and to test AH for the M-rig without baffle simulations). Values used from these selected simulations for each configuration were taken from Table 5.1. This example shows that the “installed” configuration yields simulated REDs that are approximately 14% greater than the simulated REDs for the validated configuration over the range of operating conditions considered (the slope of the regression is 1.14).

A more thorough comparison of this methodology was conducted with 24 tests using the validated M-rig no-baffle configuration (see Table 5.3). For demonstration purposes, we assume that the M-rig no-baffle configuration was the validated configuration, and that two new systems are to be installed using the L-rig and M-rig (with baffle) designs. The same operating conditions (flow rate, UVT, lamp power) for the 24 M-rig (no baffle) tests were applied to simulations of the L-rig and M-rig (no baffle) configurations.

Figure 5.3 shows plots of the simulated RED for the “installed” configurations (L-rig and M-rig with baffle) as a function of the simulated RED for the “validated” configuration (M-rig no baffle). The results are consistent with the observed trends from the actual validation tests. The L-rig and M-rig (with baffle) configurations yield higher REDs relative to the M-rig (no baffle) configuration. The L-rig appears to perform the best, with an average simulated RED that is approximately 65% higher than the M-rig (no baffle) configuration over the entire range of operating conditions. The M-rig (with baffle) configuration yields simulated REDs that are approximately 20% greater than the M-rig (no baffle) configuration over the range of operating conditions.

These results demonstrate that CFD-based models coupled with the above methodology can yield quantitative and qualitative assessments of the performance of installed UV disinfection systems relative to validated systems with potentially different reactor and piping configurations.

**CFD-BASED DOSE MONITORING EQUATIONS**

A multivariate regression can be developed based on the above simulation results to generate a revised dose monitoring equation (e.g., RED as a function of flow rate, UVT, lamp power) for the new (installed) configuration. With this approach, the revised dose monitoring equation will be based on the same runs used in the validation tests. If the simulated REDs of the installed configuration are significantly different (e.g., higher) than the simulated RED for the validated configuration under the same operating conditions, over-dosing may occur using the original validated dose monitoring equation. In these cases, the revised dose monitoring equation may save the utility costs by reducing the lamp power required to achieve a particular dose. However, the use of the validated dose monitoring equation, if more conservative, may be considered more acceptable from a regulatory standpoint.
The use of a CFD-based dose-monitoring equation is mentioned as a possible alternative to an empirically based dose-monitoring equation in the UV Disinfection Guidance Manual (USEPA, 2006, p. 3–30), but the USEPA strongly recommends the use of an empirical dose-monitoring equation developed through validation testing. Also, RED credit can only be granted for the experimentally measured RED from the validation site (USEPA, 2006, p. D-27). For situations where a revised dose monitoring equation is warranted, the following provides instructions on deriving a revised dose monitoring equation from simulated results.

The dose-monitoring algorithm for the UV reactor is obtained by analyzing the relations between measured RED and flowrate, UVT and UV lamp output. The dose-monitoring algorithm of many commercial UV reactors is often an equation with the functional form:

\[
RED = 10^A \times UVA^B \times UVA^C \times \left( \frac{S}{S_0} \right)^{D \times UVA + E \times UVA^2} \times Banks^F \tag{5.1}
\]

Table 5.3
Summary of IDI test runs (M-rig no baffle) used to demonstrate performance comparisons between validated and installed configurations

<table>
<thead>
<tr>
<th>Test ID</th>
<th>Flow rate (m³/h)</th>
<th>Test UVT</th>
</tr>
</thead>
<tbody>
<tr>
<td>AF</td>
<td>420</td>
<td>81.85%</td>
</tr>
<tr>
<td>AG</td>
<td>480</td>
<td>81.85%</td>
</tr>
<tr>
<td>AH</td>
<td>630</td>
<td>86.70%</td>
</tr>
<tr>
<td>AI</td>
<td>890</td>
<td>86.70%</td>
</tr>
<tr>
<td>AJ</td>
<td>850</td>
<td>91.83%</td>
</tr>
<tr>
<td>A</td>
<td>760</td>
<td>87.90%</td>
</tr>
<tr>
<td>B</td>
<td>950</td>
<td>87.90%</td>
</tr>
<tr>
<td>C</td>
<td>1150</td>
<td>87.90%</td>
</tr>
<tr>
<td>D</td>
<td>850</td>
<td>81.66%</td>
</tr>
<tr>
<td>E</td>
<td>710</td>
<td>81.66%</td>
</tr>
<tr>
<td>F</td>
<td>570</td>
<td>81.66%</td>
</tr>
<tr>
<td>M</td>
<td>600</td>
<td>85.31%</td>
</tr>
<tr>
<td>N</td>
<td>790</td>
<td>85.31%</td>
</tr>
<tr>
<td>O</td>
<td>790</td>
<td>90.36%</td>
</tr>
<tr>
<td>P</td>
<td>1200</td>
<td>90.36%</td>
</tr>
<tr>
<td>G</td>
<td>570</td>
<td>97.95%</td>
</tr>
<tr>
<td>H</td>
<td>710</td>
<td>97.95%</td>
</tr>
<tr>
<td>I</td>
<td>850</td>
<td>97.95%</td>
</tr>
<tr>
<td>J</td>
<td>760</td>
<td>97.95%</td>
</tr>
<tr>
<td>K</td>
<td>950</td>
<td>97.95%</td>
</tr>
<tr>
<td>L</td>
<td>1150</td>
<td>97.95%</td>
</tr>
<tr>
<td>Q</td>
<td>1200</td>
<td>97.95%</td>
</tr>
<tr>
<td>R</td>
<td>790</td>
<td>97.95%</td>
</tr>
<tr>
<td>T</td>
<td>600</td>
<td>97.95%</td>
</tr>
</tbody>
</table>
where \( UVA \) = UV absorbance coefficient (cm\(^{-1}\)) of the water determined from the 1 cm UV transmittance \([UVA = -\log(UVT/100)]\) measured at 254 nm, 
\( \frac{S}{S_0} \) = Relative output from the lamps determined using the UV intensity, \( S \), measured by the UV sensor and the UV intensity, \( S_0 \), expected with a new lamp in a clean sleeve operating at a 100 percent lamp power setting, 
\( Q \) = Flowrate through the UV reactor, and 
\( \text{Banks} \) = Number of operating banks or rows of lamps (applicable if the reactor is configured with banks or rows of lamps).

The terms A through F are constants determined by fitting the equation to validation data using linear and/or non-linear regression. Linear regression can only be used if the dose-monitoring equation can be expressed as a linear equation. The linear form of the equation cited above is:

\[
\log(\text{RED}) = A + B \times UVA \times \log(UVA) + (C + D \times UVA + E \times UVA^2) \times \log\left(\frac{S}{S_0} \times \frac{Q}{Q}\right) + F \times \log(\text{Banks})
\]

The coefficients A through F can be determined by fitting \( \log(\text{RED}) \) as a function of the log transformed variables using the linear regression tool within Microsoft Excel (Tools > Data Analysis > Regression). The tool also provides p-statistics for each coefficient, which can be used to confirm that the coefficients are statistically significant (i.e., \( p<0.05 \)) and should be included within the dose-monitoring algorithm. Once statistically significant coefficients are identified, the Solver tool of Microsoft Excel (Tools > Solver) can be used to fine-tune the values of coefficients A through F.
to minimize the error defined as the sum of the squares of the differences between the measured and predicted REDs. The Solver tool can also be used to fit non-linear dose monitoring equations to validation data. Both the Data Analysis and Solver tools need to be added in Excel using Tools > Add-Ins.
CHAPTER 6
REVIEW AND CHECKLIST OF KEY FEATURES AND PROCESSES FOR CFD MODELING OF UV DISINFECTION SYSTEMS

The previous chapters have provided a detailed discussion of CFD modeling methods and simulations of UV disinfection systems. Approaches have been developed that have been shown to yield representative models of commercial UV reactor systems that can accurately predict trends in UV system performance based on changes in operating parameters (flow rate, UVT, lamp output) and piping configuration. Sensitivity analyses have also shown that certain model parameters (initialization of $k$ and $\varepsilon$) and processes (e.g., reflection) can be important under different operating conditions.

This chapter distills the important modeling features and processes into a checklist (Table 6.1) that can be used by regulators or managers to assess the quality of modeling conducted for UV disinfection systems. Hyperlinks are provided in the checklist to relevant sections in this report for additional details. This checklist will help to ensure that important processes, features, and parameters are appropriately considered and applied to build confidence in CFD-based models of UV disinfection systems.

<table>
<thead>
<tr>
<th>Item</th>
<th>Description</th>
<th>Yes</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Numerical model is based on drawings provided by the manufacturer or measurements of the actual system</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Key features of the reactor (e.g., lamps, sensors, baffles) and piping (e.g., elbows, bends) are represented (see Chapter 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Grid independence study performed and demonstrated (see Chapter 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Basis provided for choice of turbulence model, or alternative turbulence models evaluated, for the specific problem being analyzed (see Chapter 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Turbulence parameters initialized properly (see Chapter 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Hydraulic results have converged as evidenced by residuals and “sensible” flow/particle paths (see Chapters 3 and 4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Hydraulic results have been compared to test data over a range of flow rates (e.g., head loss) (see Chapter 3) and shown to be within acceptable limits (see Chapter 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Basis provided for particle tracking model inputs (e.g., number of particles injected, DRW vs. no-DRW). (see Chapter 4)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(continued)
<table>
<thead>
<tr>
<th>Item</th>
<th>Description</th>
<th>Yes</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>Basis provided for choice of UV radiation model (e.g., MPSS, MSSS, DO) (see</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chapter 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Basis provided for the simulated lamp output and spectral/directional</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>distribution (see Chapter 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Proper representation of reflection/refraction through the quartz sleeve, or</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>justification if not included (see Chapter 4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Inclusion of wall reflection at high UVT (&gt; 88%) or justification if not</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>included (see Chapter 4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>If discrete ordinates radiation model is being used, ensure solid-angle</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>discretization is sufficient to provide uniform radiation field around</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>lamps (see Chapters 3 and 4, Appendix A)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Simulated UV radiation field compared and/or calibrated to sensor readings,</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>RED, or another metric over a range of UVT and lamp power (see Chapter 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Dose Model</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Appropriate dose-response curves used in models to represent test microbe</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>(see Chapters 2 and 3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>Spectral dependence of dose response evaluated (See Chapter 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>If Lagrangian method is being used for dose model, particles were injected</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>sufficiently far upstream of any pipe bends that may influence flow</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>distribution</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>Sufficient particles injected to obtain converged dose distributions (see</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chapter 4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Simulation of RED</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>Method used to calculate RED from simulated dose distribution is consistent</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>with standard approach (see Chapter 2)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>Simulated values of RED compared to measured values of RED over a range of</td>
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<td>One or more validation metrics used to compare simulated RED with measured</td>
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<td>RED and determine overall accuracy of model (see Chapter 2)</td>
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<td>Simulated REDs for installed configuration plotted as a function of simulated</td>
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<td>Regression of plot in item 24 above falls above $y=x$ line, indicating that</td>
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<td>the installed reactor performance is generally better than (or at least as</td>
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<td>good as) the validated reactor performance (see Chapter 5)</td>
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CHAPTER 7
SUMMARY AND CONCLUSIONS

The goal of this work was to evaluate whether CFD-based models could be used to accurately model the hydraulics, UV intensity distribution, and reduction equivalent dose (RED) in commercial UV reactors with different reactor and piping configurations. In particular, the primary objective was to demonstrate whether CFD-based models could be used to compare the performance of installed UV disinfection systems relative to validated systems with different piping configurations (potentially caused by retrofits or space limitations at the installed site).

Three different commercial reactors were simulated: (1) IDI (Degremont Technologies) Ozonia Aquaray® H20 20-inch reactor, (2) Calgon Sentinel® 12-inch reactor, and (3) Trojan Swift® 10L30 reactor. The IDI reactor was validated using three different piping and reactor configurations. Each IDI configuration was simulated to determine if the different approach hydraulics and subsequent dose distributions were adequately modeled relative to the trends in the data. The Calgon and Trojan reactors provided an opportunity to model other commercial reactors with different piping, lamp, and sensor configurations. Although these reactors were not validated under different piping configurations, the suite of different operational conditions (i.e., flow rate, UVT, different lamps on or off, lamp power) during the validation tests provided a good basis to assess and compare the capabilities of the CFD-based models.

The results of the modeling showed that CFD-based simulations were able to capture the salient trends in measured RED as a function of different flow rates, UV transmittances, and lamp power. In addition, the use of different pipe sizes and the comparison of runs with and without a baffle plate showed notable impacts on the measured RED in the IDI validation tests. The simulated performance of these different IDI configurations matched the observed trends. Simulations of the Calgon and Trojan reactors also resulted in good matches between simulated and measured data for a wide range of operating conditions.

Additional details regarding the important findings and relevant issues are provided below.

HYDRAULIC MODELING

- Based on previous studies investigating RANS-based turbulence models that did not show significant differences, only one turbulence model (realizable k-ε) was used in this study. Other models that simulate turbulent fluctuations directly (e.g., large eddy simulation) should be studied in the future.
- Grid convergence studies and comparisons to head-loss data showed that the hydraulic models were in general agreement with the actual flow fields.
- Turbulence parameters (e.g., k and ε) should be initialized using appropriate equations to ensure proper convergence of the flow field and turbulence parameters.
- The discrete random walk (DRW) particle tracking model (which includes perturbations to the particle movement based on turbulent fluctuating velocity components) can yield different results than the particle tracking model without DRW at lower flow rates (Re ~ 100,000). At lower flow rates, the turbulent kinetic energy (which is proportional to the turbulent fluctuating velocity components) are more predominant relative to the mean velocity magnitude. Therefore, the random motion is more pronounced in the particle paths. At higher flow rates (Re ~ 1,000,000), the mean velocity
magnitude is predominant and the particle paths are smoother (they follow the mean velocity). Because of these potential differences, the DRW model should be used for turbulent flow conditions.

- Different piping configurations and the presence of a baffle plate had a notable impact on the approach hydraulics and measured RED in the IDI reactor validation tests. These impacts were successfully modeled.

**UV RADIATION MODELING**

- Two different UV radiation models were used: UVXPT and the discrete ordinates radiation model in FLUENT.
  - UVXPT modeled the effects of absorption in the water, reflection/refraction at the quartz sleeve, spectral dependencies, lamp output distribution (spectral and directional), and sensor characteristics (spectral and directional).
  - The discrete ordinates model in this study assumed single-band gray radiation. Reflection and refraction at the quartz sleeve was neglected, and the lamp UV radiation was applied diffusely on the outside of the sleeve. Sensitivity studies showed that this approximation was valid. The effects of wall reflection were included, as well as shading from features within the reactor (e.g., sensors, lamps, wiper screw).
- If the UV intensity model does not rigorously capture the features of the sensor that affect the measured UV intensity (e.g., acceptance angle, reflection from the lens, spectral dependencies, etc.), the simulated lamp output power cannot solely be calibrated to the sensor readings. In these cases, an alternative approach is to calibrate the simulated lamp output power so that the simulated RED matches the measured RED (see Appendix C for more details). The calibration run that is chosen should match as closely as possible to the operating conditions that are simulated (number of lamps, flow rate, UVT, etc.).
- Wall reflection can significantly affect the UV intensity distribution within the reactor at high UVT (> 88%) and a wall reflectivity of 20%. Wall reflection is readily included in the Fluent DO radiation model, and wall reflection has been recently incorporated into UVXPT. We therefore recommend including wall reflections when the UVT is greater than ~88%. Processes such as fouling and aging of the wall surfaces will tend to reduce the wall reflectivity, but these processes were not investigated in this study.

**INACTIVATION KINETICS**

- One important source of error with action spectra measurements that has been recently reported is the use or bandpass filters. Those filters typically have a full width at half maximum of 10 nm. This causes errors on the order of 25% because the dose-response observed with a given filter can be more affected by wavelengths above or below the nominal wavelength of the filter. One recommendation for future validation of MP UV systems is that the dose-response of the test microbe should be measured with
both LP and MP collimated beams. Comparison of the LP and MP dose-response calculations will provide insight into the validity of the MP dose calculation and potentially define a correction factor that can be applied to the UV dose distribution predicted using CFD-based dose models.

SIMULATIONS OF RED

- The average relative errors in predicted RED using the Fluent DO radiation model ranged from approximately ~6–40% for the IDI and Calgon reactors, depending on features used in the model (e.g., DRW vs. no-DRW, reflection vs. no reflection), lamp configuration, UVT, and choice of run for model calibration. The average relative errors using the UVXPT model ranged from approximately ~10–30% for the IDI, Calgon, and Trojan reactor simulations. Errors above 20% in UVXPT were typically caused by simulations that neglected wall reflection with high UVT. Larger errors in Fluent were typically caused by the selection of calibration runs for the lamp output that were not consistent with the configuration of the current simulation and (in the Calgon simulations) when only one lamp was operational.

EVALUATION OF INSTALLED VS. VALIDATED REACTOR CONFIGURATIONS

- A method was presented to compare the performance of an installed reactor configuration relative to a validated reactor configuration that may have a different piping configuration. A plot is generated of the simulated RED of the installed configurations as a function of the simulated RED for the validated configuration. The operational conditions are identical for the installed vs. validated runs. Points falling above the $y = x$ line indicate that the installed configuration performs better than the validated configuration, and vice versa. The proposed method is consistent with guidance in USEPA (2006, Appendix D.6). In addition, a revised dose monitoring equation can be generated based on the results of the simulations of the installed configuration.
- Simulations of the different IDI configurations showed that this method is capable of demonstrating whether an installed configuration will perform at least as well as the validated configuration. The simulated results of the IDI configurations matched the observed trends in the measured RED among the L-rig, M-rig (with baffle), and M-rig (no baffle) configurations.

CHECKLIST

- A checklist has been created that distills the important features and processes for CFD-based modeling of UV disinfection systems. While this checklist is not exhaustive, it presents a number of key issues that should be considered by the modeler, manager, or regulator when CFD-based models are used to predict the performance of UV disinfection systems.
ADDITIONAL RESEARCH

Based on the results of this work, the following additional research is recommended:

- Additional work is needed to evaluate the directional profile of emission from UV lamps. The emission profile depends on the optical density of the arc at the relevant wavelength of emitted light (Phillips, 1983). A small element along the lamp acts more like a Lambertian emitter as the optical density of the arc increases. While the output from a linear fluorescent lamp behaves like an ideal Lambertian emitter, the output of mercury lamps without fluorescent coatings (e.g., the 265 nm line of a medium pressure UV lamp) is more complex, behaving between what would be expected with a Lambertian and point source emitter. If the behavior is not known, the angular dependence of the UV lamp’s output represents a potential source of modeling error.

- More work is needed measuring the reflection coefficient of reactor surfaces as a function of the wavelength of light, understanding the impact of the reactor surface finish on specular and diffuse reflection, and modeling the impact of specular and diffuse reflections on UV intensity fields and dose delivery. Experimental work is also needed to confirm the impacts of reflection on UV intensity, log inactivation and RED. Lastly, work is needed on understanding the regulatory impacts of reflection on UV dose monitoring at the water treatment plant application since reflection will be impacted by fouling and surface corrosion, yet UV sensors will not be monitoring the impact of these phenomena on UV dose delivery.

- If additional validation data become available that compare alternative piping and/or inlet/outlet configurations for UV reactors, the methods presented in this report should be applied to further assess CFD-based tools for predicting flow, UV intensity, and UV dose in those systems.
APPENDIX A
MODELS AND GOVERNING EQUATIONS USED IN FLUENT

APPENDIX A.1: TURBULENT FLOW MODELING IN FLUENT

The hydraulics in UV disinfection systems is characterized by turbulent flows with fluctuating velocity fields. Quantities such as momentum, energy, and discrete-phase particles are transported and mixed in these fluctuating fields, and they fluctuate as well. The fluctuations can occur at small scales and high frequencies, so direct simulation of these fluctuating quantities can be computationally expensive. Methods that can simulate these fluctuating quantities such as large-eddy simulation are available and may be valuable to consider in future studies, but they were not considered in this study because of the large computational costs.

Instead, time-averaged governing equations (Reynolds-averaged Navier Stokes equations) were used to remove the small scales. Additional unknowns (k, ε) are introduced, and the modified Navier Stokes equations containing these variables are solved together with the turbulence models to determine these additional variables. As discussed in “CFD Hydraulic Model” in Chapter 2, the realizable k-ε turbulence model was chosen in this study because of its superior performance in handling flows with recirculation and separation. The governing equations for the realizable k-ε model are presented below (Fluent, 2006).

The continuity and Reynolds-averaged Navier Stokes equations can be written as follows for incompressible flows:

\[ \frac{\partial u_i}{\partial x_i} = 0 \] (A.1)

\[ \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \rho \frac{\partial}{\partial x_j} \left( u_i u_j \right) \] (A.2)

The Reynolds stresses, \( u_i u_j \), need to be modeled in order to solve Equations A.1 and A.2. The Reynolds stresses can be related to the mean velocity gradients:

\[ - \rho u_i u_j = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \rho k \] (A.3)

where the turbulent (eddy) viscosity, \( \mu_t \), is defined as follows:

\[ \mu_t = \rho C_t \frac{k^2}{\epsilon} \] (A.4)

The modeled transport equations for the turbulent kinetic energy, \( k \), and turbulent dissipation rate, \( \epsilon \), are as follows assuming incompressible flow, no buoyancy, and no source terms:

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) - \rho \mu_t \frac{\partial u_j}{\partial x_i} - \rho \epsilon \] (A.5)
\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho \varepsilon u_j) = \frac{\partial}{\partial x_j}\left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right) \frac{\partial \varepsilon}{\partial x_j}\right) + \rho C_1 \varepsilon S - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}}
\]

where

\[
C_i = \max\left\{0.43, \frac{\eta}{\eta + 5}\right\}, \quad \eta = \frac{k}{\varepsilon}, \quad S = \sqrt{2S_{ij}S_{ij}}
\]

and \(\sigma_k\) and \(\sigma_\varepsilon\) are the turbulent Prandtl numbers (1.0 and 1.2) for \(k\) and \(\varepsilon\), respectively, and \(C_2 = 1.9\). The difference between the realizable \(k-\varepsilon\) model and the standard and RNG \(k-\varepsilon\) models is that \(C_\mu\) is no longer constant:

\[
C_\mu = \frac{1}{4.04 + \sqrt{6 \cos \phi \frac{kU^*}{\varepsilon}}}
\]

where (for non-rotating reference frames):

\[
U^* = \sqrt{S_{ij}S_{ij}} \phi = \frac{1}{3} \cos^{-1}(\sqrt{6} W), \quad W = \frac{S_{ij}S_{jk}S_{ki}}{S^3}, \quad S = \sqrt{S_{ij}S_{ij}}, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)
\]

Standard wall functions are used to estimate the mean velocity near walls. The law-of-the-wall for the mean velocity is given as follows (Fluent, 2006):

\[
U^* = \frac{1}{\kappa} \ln(E y^*)
\]

where

\[
U^* = \frac{U_P C_\mu^{1/4} k_p^{1/2}}{\tau_w/\rho}
\]

\[
y^* = \frac{\rho C_\mu^{1/4} k_p^{1/2} y_P}{\mu}
\]

and

\(\kappa\) = von Karman constant (= 0.4187)
\(E\) = empirical constant (= 9.793)
\(U_P\) = mean velocity of the fluid at point \(P\)
\(k_p\) = turbulence kinetic energy at point \(P\)
\(y_P\) = distance from point \(P\) to the wall
\(\mu\) = dynamic viscosity of the fluid

The logarithmic law for the mean velocity is valid for \(30 < y^* < 300\). In Fluent, the log-law is employed when \(y^* > 11.225\). When the mesh is such that \(y^* < 11.225\), Fluent applies the laminar stress-strain relationship such that \(U^* = y^*\). It should be noted that \(y^*\) is approximately equal to \(y^+ (= \rho u_c y/\mu)\) in equilibrium turbulent boundary layers.
APPENDIX A.2: DISCRETE ORDINATES RADIATION MODELING IN FLUENT

The discrete ordinates (DO) radiation model solves the radiative transfer equation over a finite number of solid angles, each associated with a vector direction $\tilde{s}$ in the global Cartesian system ($x$, $y$, $z$). The DO radiation model does not perform ray tracing. Instead, the radiative transfer equation is transformed into as many transport equations as there are solid angles with direction $\tilde{s}$. The solution method is the same as that used for the momentum and energy equations. The radiative transfer equation in the direction $\tilde{s}$ can be written as follows:

$$\nabla \cdot (I(\tilde{r},\tilde{s}) \tilde{s}) + (a + \sigma_s) I(\tilde{r},\tilde{s}) = a n^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_{4\pi} I(\tilde{r},\tilde{s}') \Phi(\tilde{s} \cdot \tilde{s}') d\Omega' \quad (A.11)$$

where
- $\tilde{r}$ = position vector
- $\tilde{s}$ = direction vector
- $\tilde{s}'$ = scattering direction vector
- $s$ = path length
- $a$ = absorption coefficient
- $n$ = refractive index
- $\sigma_s$ = scattering coefficient
- $\sigma$ = Stefan-Boltzmann constant ($5.672 \times 10^{-8}$ W/m²K⁴)
- $I$ = radiation intensity, which depends on position ($\tilde{r}$) and direction ($\tilde{s}$)
- $T$ = local temperature
- $\Phi$ = phase function
- $\Omega'$ = solid angle

In this application, scattering is neglected, and the local temperature is set to one everywhere to omit the thermal emission term. Fluent can also allow modeling of non-gray radiation using up to 10 gray bands to account for spectral dependencies. However, in this study, only a single-band model was used to represent a germicidal wavelength.

The angular discretization for the solid angles is defined by the user. Figure A.1 shows the definition of the angles ($\theta$ and $\phi$) used to define the number of solid angles ($N_0$ and $N_\phi$) in the model. Each quadrant of the Cartesian coordinate system is discretized into $N_0 \times N_\phi$ solid angles, so in three dimensions, a total of $8 \times N_0 \times N_\phi$ solid angles is modeled. The default discretization in Fluent is $2 \times 2$, but we found that $5 \times 5$ solid angles in each quadrant (for a total of 320 solid angles) was necessary to produce a uniform radiation field around the lamps. In addition, the number of pixels ($N_{0p} \times N_{\phi p}$) was increased to $3 \times 3$ from the default value of $1 \times 1$ as recommended in the Fluent User’s Guide (Fluent, 2006). The pixelation discretizes the overhanging control angle of control volume faces that do not align with global angular discretization.
APPENDIX A.3: IMPLEMENTING THE DISCRETE ORDINATES (DO) RADIATION MODEL

The following is a step-by-step guide to implementing the DO radiation model in Fluent.

1. Read the case file (*.cas) and data (*.dat) files in FLUENT containing the desired model. The case file contains the mesh, boundary conditions, and other user settings. The data file contains the data results of previous simulations (e.g., flow simulation).
2. Run the DO radiation Model.
   a. Turn DO radiation model on (Define > Models > Radiation). Energy equation will automatically be turned on.
      i. The angular discretization controls the refinement of the DO model. The default for the theta and phi divisions is $2 \times 2$, which is coarse ($5 \times 5$ is better). Default for theta and phi pixels is $1 \times 1$ ($3 \times 3$ is recommended for specular or semi-transparent boundaries). Increasing the divisions will increase cost of computation. Increasing pixelation will also increase computation, but not as much (see Section 13.3.13 of the User’s Guide, Fluent, 2006).
      ii. The number of wavelength bands for a non-gray model can be specified as well (see Section 13.3.13 of the User’s Guide).
   b. Define appropriate materials for the model (Define > Materials)
      i. May have to change the fluid material type from air to water-liquid. Change solid materials if modeling quartz sleeve.
      ii. Change the absorption coefficient to reflect the UV transmittance (UVT) of the water, where:

        \[
        \text{UVT} = \frac{I}{I_0} = \exp(-ax), \text{ where } I/I_0 \text{ is the reduction in intensity over } x=1 \text{ cm} \\
        \text{ (Note that Fluent uses base e in this formula, not base 10)}
        \]

        Therefore, absorption coefficient, $a = -\ln(\text{UVT})*100$, where 100 is used to convert cm$^{-1}$ to m$^{-1}$

        Example: for a UVT of 0.9 (90%), the absorption coefficient is 10.5 m$^{-1}$
iii. Include refractive indices for semi-transparent boundaries, if desired.
c. Define radiation boundary conditions (Define > Boundary Conditions).
i. In our CFD models, different zones have been defined including the lamp sleeves, sensors, and the reactor body.

ii. For the sleeve, click Set:
   1. Under the Thermal tab, the refractive index can be set if radiation is being modeled through the sleeve (current models do not model the lamp and air annulus explicitly, only the sleeve).
      a. Emissivity can be set here, too. This plays a role in the diffusely reflected energy, $f_d(1-\varepsilon)q_{\text{in}}$, and the absorbed energy, $f_d\varepsilon q_{\text{in}}$. The specularly reflected energy is $(1-f_d)q_{\text{in}}$. “$f_d$” is the diffuse fraction, $\varepsilon$ is the emissivity, and $q_{\text{in}}$ is the radiative energy incident on the wall.
   2. Under the Radiation tab, set the BC Type to “semi-transparent.”
      a. Set the Diffuse Fraction to a value between 0 and 1. For a value of 1, all of the emitted radiation will be diffuse equal in all directions. For a value of zero, the emitted radiation will follow the beam direction (reflecting surfaces will be specular (i.e., a highly polished, mirror-like surface)). For circular lamps, the diffuse fraction must be set to 1 to apply the irradiation uniformly around the lamp (circumferentially).
      b. Set the Irradiation to be the intensity desired from each lamp sleeve. Calculate using lamp power (W) divided by the surface area of the sleeve. Correct for efficiencies or spectral distributions (if using non-gray radiation model).
      c. Uncheck the “Apply Irradiation Parallel to the Beam.” This will allow the specified irradiation to originate normal to the surface of the sleeve. Otherwise, the specified irradiation will originate in a direction parallel to the beam direction specified by the X, Y, and Z vector, and a component normal to each surface will be calculated.
d. The Beam Width (theta and phi) specifies the solid angle over which the irradiation is distribution (see Figure 13.3.13 in User’s Guide).

3. Alternatively, a thermal radiation boundary condition can be applied.
   a. Under the “Thermal” tab, click on “Radiation” for Thermal Conditions and set the External Radiation Temperature to a value that yields and equivalent lamp output power according to
   \[ q (W/m^2) = \varepsilon \sigma T^4 \]
   where \( \varepsilon \) is the external emissivity, \( \sigma \) is the Stefan-Boltzmann constant \( 5.67 \times 10^{-8} \text{ W/m}^2\text{-K}^4 \).
   b. Under the fluid zone (Define > Boundary Conditions > fluid > Set), click on Fixed Values and assign a constant value (say 1) to the fluid.
   c. Make sure that the Energy equations are activated in Solution Controls (Solve > Controls > Solution)

   iii. For the “reactor_body” and “sensor zones,” these boundary conditions can be treated as opaque walls with or without reflection.
      1. Under the Radiation tab, setting the diffuse fraction to 1 will allow diffuse reflection only if the internal emissivity is set to a value less than one in the “Thermal” tab.
      \[ \text{Diffusely reflected energy} = f_d (1-\varepsilon) q_{\text{in}} \]
      \[ \text{Absorbed energy} = f_d \varepsilon q_{\text{in}} \]
      2. Set the diffuse fraction to 0 to allow specular (mirror-like) reflection from these surfaces.

   d. To minimize the effect of thermal radiation from temperature differences between the fluid and the lamp sleeves, which have power being applied to them, reduce the temperature of the fluid to 1 K:
      i. If a previous data file with flow field results was read, use Solve > Initialize > Patch. Select Temperature as the Variable and “fluid” as the Zone to Patch. Change value to 1 K.
      ii. If a flow simulation has not been run yet, use Solve > Initialize > Initialize and scroll down to set the initial temperature to 1 K.

   e. Turn off flow models and only activate DO Model:
      i. Solve > Controls > Solution
         1. Activate only the Discrete Ordinates in Equations

   f. Run Model
      i. If a previous run has not been made, the model must be initialized first
         1. Solve > Initialize (specify initial parameters)
      ii. Solve > Iterate
         1. Choose number of iterations to be ~15–20 (shouldn’t take that many iterations to converge on the radiation solution; the default convergence criteria for the do-intensity values is a residual of 1e-6). Click Iterate.

   g. View Results
      i. Contours
         1. Display > Contours, choose Radiation… and Incident Radiation. You can view the incident radiation on the sleeve or other defined surfaces. This is the sum of all incident radiation on surfaces.
Appendix A: Models and Governing Equations Used in Fluent

a. To view the true irradiation boundary condition, use Wall Fluxes… and Beam Irradiation Flux.

b. To view the incident radiation directed toward a particular surface, choose Wall Fluxes... Surface Incident Radiation. This is useful for quantifying incident radiation entering the face of a sensor, for example.
   i. Alternatively, go to Report->Surface Integrals and select the surface you want to get a quantified report of the incident radiation entering the face of the sensor. The field variable should be Wall Fluxes... Surface Incident Radiation.
   ii. To view radiation from individual solid angles, use text command:

   Solve > “set expert” and make the following settings:
   • Use conservative form of energy equation? [yes]
   • Use alternate formulation for wall temperatures? [no]
   • Save cell residuals for post-processing? [no]
   • Keep temporary solver memory from being freed? [no] yes
   • Allow selection of all applicable discretization schemes? [no]

   Then, you can view the Radiation results for each individual solid angle (“Intensity Magnitude 0, 1, …”) in Display Contours. However, it is not clear how to associate the magnitudes with individual solid angles.

3. Run the particle tracking model.
   a. Copy or extract the “libudf” files and folders into the current working directory.
      There are separate “libudf” zip files for 3D and 3D DP. These are the user-defined function to calculate dose from the particles
      i. For Linux, the folder name in the working directory should be “libudf” and the required subfolder is “lnamd64,” which contains subfolders named by the version (e.g., “3d” or “3ddp”). Inside these subfolders are the required files.

b. Load the UDF into FLUENT
   i. Define > User-Defined > Functions > Compiled
      1. Click Load
   ii. Add dose scalar to discrete phase model
      1. Define > Models > Discrete Phase
         a. In the UDF tab, increase the number of scalars to 1
         b. In the Scalar Update field, change from “none” to “uv_dosage::libudf”
         c. In the Tracking tab, the max. number of steps can be increased to change the particle lengths.

c. Define Injections
   i. Define > Injections
      1. Click Create
         a. Under Injection Type, select either surface (to release particles from each element of the inlet, for example ) or file. If surface is selected, choose an appropriate surface (e.g., inlet). If file is selected, click on File... and select a file.
         b. In the Turbulent Dispersion tab, the Discrete Random Walk Model can be checked to randomly assign a random fluctuating velocity
component to the mean velocity. The number of tries indicates how many realizations will be simulated for the given set of injection points.

d. Compute dose to each particle
   i. Report > Discrete Phase > Sample
      1. Select the outlet for the Boundaries and the injection name for Release from Injections. Select as Output the “uv_output::libudf.” This will place an “output.dpm” in the same location where the injection file was read (if a file was used) or in the working directory. This file contains the cumulative dose distributions for each particle in [J/m²]. The dose is the cumulative product of the incident radiation [W/m²] and the time [s] along each step of the particle path.
         a. Be sure that the output.dpm file is not open or being read by Excel. If so, an error will result in Fluent.

e. Display histogram of dose
   i. Report > Discrete Phase > Histogram
      1. Click Read… and select the “output.dpm” file
         a. Make sure to read in the output.dpm file each time a new sample is created. Otherwise, it will plot the previously stored output.dpm file.
      2. Click on “UV-Dosage” in the Fields window (last parameter) and click Plot

f. Display particle tracks of dose
   i. Display > Particle Tracks
      1. Select Particle Variables… and “User Value 0” in the dropdown menu
      2. Select injection file
      3. Select Track Single Particle Stream or Skip factor (choosing all the particles is graphically intensive)

g. Display particle tracks of instantaneous irradiation
   i. Display > Particle Tracks
      1. Select Radiation… and “Incident Radiation” in the dropdown menu
      2. Select injection file

h. Write particle tracking data to files
   i. Solve > Particle history > Export Particle Data
      1. Choose Standard, which will create a *.fvp Fieldview file that contains x, y, z, and the selected scalar (e.g., time, incident radiation). Select a name for the file. Note that these files can be quite large if the number of steps for the particles is large.
         a. C:\Fluent.Inc\fluent6.3.26\help\html\ug\node1132.htm contains information on this format
i. Write particle path data to files
   i. Display > Pathlines
      1. Select desired scalar variable (e.g., incident radiation)
      2. Select surface to release paths
      3. Select a large step size if you just want points at the inlet and outlet of cells. If you want points in between, select a smaller step size (smaller than the cell size).
      4. Select the number of steps that each path will take.
      5. Select number of paths to skip.
      6. “Path coarsen” will remove points along a path (use 1)
      7. Click “Write to File” and choose “Standard” type
      8. Click “Write…”
      9. The resulting *.fvp file can be opened with a text editor or Excel. The output will contain x, y, z, scalar, and particle ID.
APPENDIX B
METHODS AND ALGORITHMS IN UVXPT

Because wall reflection may play an impact on the simulated dose distribution at high UVT, wall reflection was incorporated into the UVXPT model. Details of the associated algorithms and reflection models in UVXPT are provided below.

UVXPT ALGORITHMS

Point Calc

The subroutine PointCalc within UVXPT calculates the UV intensity field about a single point source as two arrays, Point1(r,z) and Point2(r,z), where r is the radial distance extending outwards from the point source and z is the axial distance along the length of the lamp from the point source. The array Point1(r,z) is dimensioned as a double precision array with 100 x 200 elements. The array Point2(r,z) is dimensioned as a double precision array with 100 x 100 elements.

The arrays Point1(r,z) and Point2(r,z) are used in the subroutine Lamp Calc to calculate the UV intensity field about half a lamp. The radial and axial spacing between array elements must ensure the array provides good resolution of the UV intensity field yet project sufficiently far in the radial and axial directions that important contributions of the UV intensity field to dose delivery are accounted for. Hence, radial distance, r, associated with the 100th element in the radial direction with both Point1(r,z) and Point2(r,z) is defined as:

\[
\frac{r_{OS} \times \exp^{-\alpha_w(254) \times (r-r_{OS})}}{r} \leq 0.001
\]

where \(\alpha\) is the UV absorbance coefficient of the water at 254 nm and \(r_{OS}\) is the outer radius of the quartz sleeve. With the array Point1(r,z), the axial distance, z, associated with the 200th element in the axial direction is defined as:

\[
z = \frac{L}{199}
\]

where \(L\) is the lamp’s arclength which is treated as 199 point sources. With the array Point2(r,z), the axial distance, z, associated with the 100th element in the axial direction is defined as:

\[
z = -\log(0.001)/\alpha_w(254)
\]

Using this approach, the both arrays extend further out in the radial direction and array Point2(r,z) extends further out in the z direction as the UV absorbance decreases.
The UV intensity field is calculated using the approach specified by Bolton (2000) with some important corrections. The germicidal UV intensity \( I(r,z) \) is calculated using:

\[
I(r,z) = \frac{\sum_{\lambda=200}^{300} G(\lambda)P(\lambda)}{4\pi\rho_A N_L} \times \frac{A_1}{A_2} \times \left(1 - R_{AQ}(\lambda)\right) \left(1 - R_{QW}(\lambda)\right) \times F \times e^{-\alpha_Q(\lambda)\rho_Q - \alpha_W(\lambda)\rho_W}
\]

where

- \( \lambda \) = wavelength of light in 1 nm steps
- \( G \) = action spectra of the microbe normalized at 254 nm
- \( P \) = UV output of the lamp in W per nm
- \( \rho_A \) = Distance light travels from the point to the inside radius of the sleeve
- \( \rho_Q \) = Distance light travels from the inside to the outside radius of the sleeve
- \( \rho_W \) = Distance light travels from the outside radius of the sleeve to the point of interest at \((r,z)\)
- \( N_L \) = Number of points defining a lamp, set to 199
- \( A_1/A_2 \) = Divergence of light as it travels from the inside radius of the sleeve to the point of interest at \((r,z)\)
- \( R_{AQ} \) = Reflectance at the air-quartz interface calculated using Fresnel’s Law
- \( R_{QW} \) = Reflectance at the quartz-water interface calculated using Fresnel’s Law
- \( F \) = Factor to define the lamp as a Lambertian source, \( F = 1.27324 \sin(\theta_1) \) (Sasges, 2008)
- \( \alpha_W \) = UV absorbance coefficient of water
- \( \alpha_Q \) = UV absorbance coefficient of quartz

The distance the UV light travels through air, quartz and water is defined using:

\[
\rho_A = \frac{r_{IS}}{\cos(\theta_1)}
\]

\[
\rho_Q = \frac{r_{OS} - r_{IS}}{\cos(\theta_2)}
\]

\[
\rho_W = \frac{r - r_{OS}}{\cos(\theta_3)}
\]

where

- \( \theta_1 \) = Incident angle of UV light on the air-quartz interface
- \( \theta_2 \) = Incident angle of UV light on the quartz-water interface
- \( \theta_3 \) = Refracted angle of UV light from the quartz-water interface

The incident and refracted angles are related using Snell’s Law as:

\[
SIN(\theta_1) = n_Q(\lambda) \sin(\theta_2) = n_W(\lambda) \sin(\theta_3)
\]

where

- \( n_Q \) = Index of refraction of quartz
- \( n_W \) = Index of refraction of water
The angle $\theta_1$ is iteratively solved using the relation:

$$z = r_{IS} \tan(\theta_1) + (r_{OS} - r_{IS}) \tan(\theta_2) + (r - r_{OS}) \tan(\theta_3)$$  \hspace{1cm} (B.9)

with convergence criteria of $|\theta_{1,k} - \theta_{1,k-1}| \leq 0.000 \ 000 \ 01$ radians where $k$ specifies the $k$th iteration.

The divergence of UV light, $A_1/A_2$, is calculated using:

$$A_1 = 2\pi r_{IS} \Delta z_1 \sin(\theta_1)$$  \hspace{1cm} (B.10)

and

$$A_3 = 2\pi r \Delta z_3 \sin(\theta_3)$$  \hspace{1cm} (B.11)

where $\Delta z_1 = \text{Difference in the axial distance travel from the point to the inside radius of the sleeve for light emitted and angles } \theta_1 \text{ and } \theta_1 + \text{d}\theta$.

$\Delta z_3 = \text{Difference in the axial distance travel from the point to the location (r,z) for light emitted and angles } \theta_1 \text{ and } \theta_1 + \text{d}\theta$.

The differential angle d$\theta$ is set to 0.0000001 radians. All calculated variables used to define $I(r,z)$ are dimensioned as double precision variables.

**Lamp Calc**

The subroutine Lamp Calc determines the UV intensity field about half of a lamp as an array $\text{Lamp}(r,z)$. The UV intensity field is determined using the Principal of Superposition of light from incoherent sources which states that:

$$I(r,z) = \sum_{n=1}^{199} I_n(r,z)$$  \hspace{1cm} (B.12)

where $I(r,z)$ is the UV intensity field about the half lamp at location $(r,z)$ and $I_n(r,z)$ is the UV intensity from the $n$th point along the length of that lamp. The array $\text{Lamp}(r,z)$ is dimensioned as a double precision array with 100 elements in the radial direction and 200 elements in the axial direction. The radial distance is the same as used with the array $\text{Point}(r,z)$. However, the axial distance is divided into two regions. The first region includes axial elements 1 to 100 and extends from the centre location of the lamp to a location $\Delta z/2$ from the lamp end where

$$\Delta z' = L/199$$  \hspace{1cm} (B.13)

The second region extends from axial elements 101 to 200 and extends from the end of the lamp to a distance beyond the lamp equal to the axial distance used to define the array $\text{Point2}(r,z)$. Using this approach to define the array $\text{Lamp}(r,z)$ provides good definition of the UV intensity field within and beyond the region of the lamp’s arc.

The contribution of the UV intensity field from each point along the length of the lamp to the location $\text{Lamp}(r,z)$ in the first region is determined by summing contributions from $\text{Point1}(r,z)$. The contribution in the second region is determined by exponential interpolation of the UV intensity field defined by $\text{Point2}(r,z)$.
CFD Dose Calc

The subroutine CFD Dose Calc integrates the particle track data generated by Fluent with the UV intensity field information in Lamp(r,z) to determine UV dose delivered to each virtual microbe. For each particle trajectory coordinate (x,y,z,t), the algorithm calculates the radial and axial distances from the centre of each lamp to a location (x,y,z) defined as the average of the mth and m+1 coordinate. The UV intensity at location (x,y,z) is determined using:

\[ I_m(x,y,z) = \sum_{i=1}^{L} I_i(r,z) \]  

where \( I_i(r,z) \) is the UV intensity at (x,y,z) due to the ith lamp. The values of \( I_i(r,z) \) are calculated using two dimensional exponential interpolation of the UV intensity data in the array Lamp(r,z).

The UV dose delivered to each particle is calculated using:

\[ D = \sum_{m=1}^{M} I_m(x,y,z) \times (t_{m+1} - t_m) \]  

where \( D \) is the UV dose and the particle trajectory is defined by \( M \) sets of (x,y,z,t) coordinates.

QA/QC

As a QA/QC step, the Point Calc and Lamp Calc algorithms were set up within an Excel spreadsheet. The spreadsheet calculates the UV intensity at location (Sx,Sy,Sz) (cells F6:F8) caused by a lamp with lamp ends (Lx1, Ly1, Lz1) and (Lx2, Ly2, Lz2) (cells C3:C8). Other inputs to the algorithm are the lamp power (C2), the number of point sources used to model the lamp (C9), the inside and outside radii of the sleeve (cells C10:C11), the quartz UV A and index of refraction (cells C12:C13), and water UV A and index of refraction (cells C14:C15). The cells F2 to F5 are used to define (Sx,Sy,Sz) using the same coordinate system as used with the arrays Point1(r,z), Point2(r,z), or Lamp(r,z). Hence, the algorithm can be used as a QA/QC for the values calculated in these arrays. The cells C17:C19 are values calculated from the inputs and used by the spreadsheet. The cells A23:AE222 give the calculations of UV intensity from each point source defining the lamp. The cell F18 provides the UV intensity at location (Sx,Sy,Sz) determined using those calculations. The control button labeled “Run Macro” iteratively determines the propagation angles of light as it travels from the lamp through the sleeve to the point of interest. This button must be used to calculate the UV intensity at location (Sx,Sy,Sz) after an input has been changed.

The spreadsheet Point Calc calculations agreed with the Visual Basic code to within 6 significant figures. Future QA/QC will include calculation of the UV dose delivered to a particle track.

UVXPT REFLECTION ALGORITHM

UVXPT initially used in this project did not include subroutines for reflection and shadowing. Based on the findings of this work, UVXPT was modified to include spectral reflection. Reflection of light from surfaces can be categorized as specular or diffuse reflection (Figure B.1). Specular reflection occurs with smooth mirror-like surfaces and follows the Law of Reflection, which states the angle of reflection equals the angle of incidence. In vector form, the Law of Reflection can be expressed as:
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Figure B.1 Reflection models includes diffuse and specular reflection

\[ \tilde{n}_2 = \tilde{n}_1 - 2(\tilde{n}_1 \cdot \tilde{s})\tilde{s} \]  \hspace{1cm} (B.16)

where \( \tilde{n}_1 \) is a unit vector in the direction of the incident light, \( \tilde{n}_2 \) is a unit vector is the direction of the reflected light, and \( \tilde{s} \) is a unit vector defining the normal vector to the surface.

Diffuse reflection occurs with uneven or rough surfaces that cause the light to reflect in different directions. Diffuse reflection can be modeled by treating the reflected point as a point source emitter emitting evenly in all direction or as a Lambertian emitter where the intensity of the reflected light is proportional to the cosine of the reflected angle.

The internal wetted surfaces of UV reactors are typically either stainless steel or quartz. Metal surfaces tend to have high reflectivity (Phillips, 1983). Light is absorbed by free electrons and emitted as reflected light at the same wavelength. The physics of reflection is described by Maxwell’s equations and can be defined as a function of the refractive index, \( n \), and the absorption coefficient, \( k \) of the metal. These optical constants both vary as a function of wavelength. For wavelengths from 400 to 800 nm, the optical constants for 304 steel can be estimated using (Castelli et al., 2006):

\[ n = 0.0028\lambda + 0.100 \]
\[ k = 0.0033\lambda + 0.14088 \]  \hspace{1cm} (B.17)

Figure B.2 shows the optical constants of 304 steel predicted as a function of wavelength, including an extrapolation to 220 nm. The reflection coefficient of the light also depends on the angle of incidence. If the incident light is polarized such that the electric vector is perpendicular to the plane of incidence, the reflection coefficient is defined using:

\[ R_s = \frac{n^2 + k^2 - 2n \cos \theta + \cos^2 \theta}{n^2 + k^2 + 2n \cos \theta + \cos^2 \theta} \]  \hspace{1cm} (B.18)

where \( \theta \) is the angle of incidence of the light on the surface. If the light is polarized such that the electric vector is parallel to the plane of incidence, the reflection coefficient is defined using:

\[ R_p = \frac{(n^2 + k^2)\cos^2 \theta - 2n \cos \theta + 1}{(n^2 + k^2)\cos^2 \theta + 2n \cos \theta + 1} \]  \hspace{1cm} (B.19)

With unpolarized light expected from UV lamps, the reflection coefficient is the average of \( R_s \) and \( R_p \).
Using the optical constants for 304 stainless steel, the reflection coefficient at 400 nm for unpolarized light is estimated as 61 percent for a zero degree incident angle. Taylor (1934) reported that the reflection coefficient of stainless steel to be 30 percent at 296.7 nm. Luckeish (1929) reports reflection coefficients of steel from two sources (Figure B.3). One source states reflection coefficients of 33.3 percent at 253.7 nm, 35.3 percent at 274 nm, 43.0 percent at 309 nm, and 52 percent at 410 nm. A second source states coefficients of 34.8 percent at 226.5 nm, 35.7 percent at 231.3 nm, 39.6 percent at 257.3 nm, and 42.6 percent at 298.1 nm. Namba (1982) reported that the specular reflectance coefficient of AISI304 stainless steel at near normal incidence angles depended on the surface roughness and varied from 6 to 40 percent at 300 nm for surface roughness values ranging from 1.6 microns to 0.002 microns. The percentage of diffuse reflection is expected to increase with increased surface roughness.

The impact of specular reflection on the UV intensity field within the UV reactor will depend on the geometry of the internal surfaces. As shown in Figure B.4, the intensity of specular reflected light at a point within the reactor may be due to reflection from more than one location. With diffuse reflection, all surface locations within the line of sight of the point of interest will contribute to the UV intensity at that point of interest.
The intensity of the reflected light will also depend on the divergence or convergence of the reflected light. As shown in Figure B.5, the UV intensity of specular reflected light will decrease if the curvature promotes divergence but increase if the curvature of the surface promotes convergence.

Figure B.6 shows the ratio of the UV intensity with and without reflection caused by a point source within a cylinder with a reflection coefficient of 0.2. The water UVT was 98 percent. While the reflection coefficient is 0.2, the figure shows regions within the cylinder where the reflection ratio is as great as 2.9. The high reflection ratios occur because of the convergence of reflected light. With cylindrical mirrors, light from a point source will converge to form a line image (DeWeerd and Hill, 2005). With a point source within a cylinder, the light can converge to form multiple light images, as indicated in Figure B.6.

Figure B.7 shows a schematic of a UV reactor consisting of two intersecting cylinders where one cylinder houses three UV lamps within quartz sleeves (similar to the Calgon reactor modeled in this work). Figure B.8 shows the ratio of the UV intensity with and without reflection predicted within the reactor along the xz plane at y=0. The reflection coefficient of the reactor walls was 0.2. The predictions are made with one, two and three lamps on (Figures B.8, B.9, and B.10). The figures show complex reflection patterns that occur due to (1) reflection from multiple
Specular Reflection Algorithm

The UVXPT algorithm for specular reflection defines the internal surfaces of the reactor using equations for cylinders and planes in three dimensions. A cylinder is defined using its radius and two \((x,y,z)\) coordinates representing the beginning and end of the cylinder along the cylinder’s main axis. In this work, equations for cylinders were used to define the internal wetted surfaces of the two intersecting cylinders representing the Calgon, Trojan and IDI reactors. The UV sensor ports projecting into the reactor and the baffle plates were not modeled.

The algorithm treats each lamp as a line source consisting of fifty point source emitters. The algorithm also defines a 3 dimensional array to represent the internal space within the reactor. The spacing between grid points in the \(x\), \(y\) or \(z\) direction is selected to range from 0.5 to 2 cm.
The algorithm calculates the UV intensity at each grid point with and without the contribution of reflection. The UV intensity without the contribution of reflection is calculated using a polychromatic Point Source Summation (PSS) algorithm (Jacob and Dranoff, 1970):

\[
I(x,y,z) = \sum_{i=1}^{L} \sum_{n=1}^{N} \sum_{\lambda=200}^{320} I_{i,n,\lambda}
\]

(B.20)

where L is the number of lamps, N is the number of points defining each lamp, and:


Figure B.10 Ratio of UV intensity field with and without reflection with lamps 1, 2 and 3 on, 98 percent UVT, and a reflection coefficient of 0.2

\[
I_{i,n}(\lambda) = \frac{P(\lambda)G(\lambda)/N}{4\pi\rho^2} \times \exp\left(- (\alpha_q(\lambda)\rho_q + \alpha_w(\lambda)\rho_w)\right) \tag{B.21}
\]

where \( P(\lambda) \) is the UV output from the lamp per nm, \( G(\lambda) \) is the action spectrum wavelength response of the microbes, \( \rho \) is the direct (without reflection) distance from the point source on the lamp to the location \((x,y,z)\) within the reactor, \( \rho_q \) and \( \rho_w \) are the distances through the quartz sleeve and water, respectively, and \( \alpha_q(\lambda) \) and \( \alpha_w(\lambda) \) is the UV absorbance of the quartz sleeve and water, respectively. Note that \( \rho = \rho_q + \rho_w \).

To define specular reflection from each point source on the lamp to each grid point \((x,y,z)\), the algorithm identifies wetted surface points within the reactor that meet the relation:

\[
\hat{n}_2 = \hat{n}_1 - 2(\hat{n}_1 \cdot \hat{s})\hat{s} \tag{B.22}
\]

The UV intensity incident on the reactor surface is calculated using the PSS algorithm. The reflected intensity at each grid point \((x,y,z)\) is calculated using:

\[
I_{r,i,n}(\lambda) = I_w(\lambda) \times R(\lambda) \times \exp(-\alpha(\lambda)\rho_R)A_P/A_R \tag{B.23}
\]

where \( I_w(\lambda) \) is the UV intensity at the reflecting location on the reactor wall calculated using equation , \( R(\lambda) \) is the reflection coefficient, \( \rho_R \) is the distance through the water from the reflecting location to the grid point \((x,y,z)\), and \( A_P/A_R \) is the convergence/divergence factor for the reflected light. The convergence/divergence factor is calculated as the ratio of a differential area defined at the reflecting location, \( A_R \), to the projected area at the grid point, \( A_p \). The differential area is defined as a square element with one side oriented in the axial direction of the cylinder and the other perpendicular to that direction. The change in the area of that element as light is reflected is determined using ray tracing.
The UV intensity with reflection at each point on the grid is calculated using:

\[
I_R(x,y,z) = I(x,y,z) + \sum_{i=1}^{L} \sum_{n=1}^{N} \sum_{r=1}^{R} \sum_{\lambda=200}^{320} I_{r,i,n} (\lambda)
\] (B.24)

where \( R \) is the total number of reflecting locations that result in specular reflection from the point source on the lamp to the grid point \((x,y,z)\).

The ratio of UV intensity with and without reflection is calculated as:

\[
Ratio = \frac{I_R(x,y,z)}{I(x,y,z)}
\] (B.25)

The ratio is interpolated to estimate the ratio at each \((x,y,z,t)\) step of the Lagrangian particle tracks generated by Fluent. The UV dose delivered to each particle is determined using:

\[
D = \sum_{m=1}^{M-1} I_m(x,y,z) \times Ratio(x,y,z) \times (t_{m+1} - t_m)
\] (B.26)

Issues with this algorithm are as follows:

- The PSS algorithm used to calculate the UV intensity with and without reflection does not include the impacts of refraction through the sleeve. However, the ratio should provide a good first approximation of reflection on the UV intensity field within the reactor. While refraction can be included in the algorithm, it is expected to significantly increase processing time.

- The algorithm as written did not include the dependence of the reflection coefficient on the angle of incidence as defined by Equations A.10 and A.11. However, the impact is only significant at large angles that approach 90 degrees.

**Diffuse Reflection Algorithm**

The UVXPT algorithm for diffuse reflection calculates diffuse reflection from all surfaces within the reactor using a text file that defines the wetted surfaces within the reactor as triangular elements with a center point \((x,y,z)\) and area \(A\). The text file also defines a vector \((x_n,y_n,z_n)\) that is normal to the triangular element and points into the liquid.

The algorithm calculates the germicidal UV intensity incident on each wetted surface element using:

\[
I_w(x,y,z) = \sum_{i=1}^{L} I_i(r,z)
\] (B.27)

where \(I_w(r,z)\) is the UV intensity at \((x,y,z)\) due to the \(i\)th lamp. The values of \(I_i(r,z)\) are calculated using two dimensional exponential interpolation of the UV intensity data in the array \(Lamp\(r,z\).

The contribution of the \(i\)th lamp is included in the calculation if the dot product of the normal vector and the vector from the wall location \((x,y,z)\) to the centre of the lamp is positive. If the dot product is negative or zero, the algorithm assumes that the wall location is not in the lamp’s line of site.

The algorithm then treats each surface point as a Lambertian emitter with a germicidal power output of:

\[
P_w = R_w \times A_w \times I_w(x,y,z)
\] (B.28)
where $R_w$ is the reflectance coefficient of the surface element at 254 nm. The algorithm then calculates the UV intensity due to the wall sources over a three dimensional array defining the reactor space using:

$$I_R(x,y,z) = \sum_{s=1}^{S} \frac{1.27324 \times \cos(\beta) P_w e^{-\alpha_w(254) \times \rho}}{4\pi \rho^2} \quad (B.29)$$

where

- $\beta =$ Angle UV light is emitted from wall element
- $\rho =$ Distance from the wall element to the point $(x,y,z)$

This calculation is valid if the location in three-dimensional space is relatively far from the wall element but not valid as $\rho \rightarrow 0$. Hence, if the calculated contribution from a given wall element is greater than $R_w \times I_w$, the contribution is set to $R_w \times I_w$. The algorithm generates an output file containing the ratio of the UV intensity due to the wall elements to the UV intensity directly due to the lamps. The ratios are used to scale the UV intensity used to determine UV dose with the Lagrangian particles tracks.

Issues with this algorithm are as follows:

- The algorithm does not account for polychromatic reflections. With a MP UV lamp, one would expect more reflection of higher wavelength germicidal light and less reflection of lower wavelength light.
- The triangular elements defining the wall surfaces have areas ranging from $3.9 \times 10^{-6}$ to $4.5 \times 10^{-5}$ m². The equivalent radius is 0.2 to 0.7 cm. Because the elements have a discrete size, the algorithm does not do a good job of estimating the intensities close to the wall. This could be resolved by using smaller elements. However, the number of elements using this size is greater than 10,000 resulting in a high processing time.
APPENDIX C
CALIBRATION AND SCALING OF THE LAMP OUTPUT FOR THE FLUENT DO RADIATION SIMULATIONS

IDI RUNS

For each validation test, one DVGW sensor and one SDW1 sensor were used to measure radiation intensity. The distance between a sensor and the opposite sleeve varied among sets of tests. All tests with the same sensor distance were chosen for a multivariate regression to determine the sensor intensity as a function of UVT at 254 nm and lamp power reading. This function was determined to be:

$$S_0 = 10^x e^{y \cdot UVT} P^z$$

where $x$, $y$, $z$ are constants for a given sensor distance and sensor type, and $P$ is the power reading for the test. The power output was assumed to be equal for all six lamps.

1. **Calibration:**

   Choose a test to calibrate. Set the irradiation boundary condition for each of the six lamps to the same starting guess value, and adjust this value until the simulated RED equals the measured RED. Let the final irradiation boundary condition, which is equal for all six lamps, be $I_C$ [W/m²].

2. **Scaling:**

   Let $S_C$, $UVT_C$, and $P_C$ be the sensor reading, Test UVT, and power reading, respectively, of the calibrated run. Let $S_{0c}$ be the predicted sensor reading of the calibrated run, calculated using the regression equation.

   Let $S$ and $UVT$ be the sensor reading and Test UVT, respectively, of a run whose irradiation boundary condition we wish to scale. Let $S_0$ be the predicted sensor reading using the UVT of this run, but using the power reading of the calibrated run, $P_C$, in the regression equation.

   Then the scaled irradiation BC for the new run, $I$, which is equal for all six lamps, is given by:

   $$I = I_C \frac{S/S_0}{S_C/S_{0c}} = I_C \frac{S}{S_C} \frac{10^y e^{y \cdot UVT_C} P_C^z}{10^y e^{y \cdot UVT} P^z} = I_C \frac{S}{S_C} e^{y(UVT_C-UVT)}$$

The resulting expression scales the calibrated lamp irradiation value by the difference in lamp output power between the new and calibrated runs as measured by $(S / S_0)$ with a correction term $(e^{y(UVT_C-UVT)})$ for the potentially different UVTs used in the calibrated and new runs. If the UVTs are the same, the scaled lamp irradiation boundary is just equal to the calibrated lamp irradiation multiplied by the ratio of the sensor readings.
The new run is simulated using the same simulation settings as the calibrated run, with the exceptions of UVT, inlet velocity and irradiation boundary conditions. For instance, if 20% reflection on all surfaces is simulated for the calibrated run, then 20% reflection on all surfaces must be simulated for the new scaled run.

Note: for our calibration and scaling, the DVGW sensor readings at a distance of 110 ± 2 mm were used.

CALGON RUNS

The Calgon 12-in Sentinel Reactor consists of three lamps and three sensors. Each sensor faces one of the lamps. Hence, we refer to the sensor facing Lamp 1 as Sensor 1, the sensor facing Lamp 2 as Sensor 2, and the sensor facing Lamp 3 as Sensor 3. For any sensor, a general equation describing the UV sensor reading as a function of corresponding lamp ballast power and UVT at 254 nm, was determined by multivariate regression:

$$S_0 = 10^{A'}e^{B'UVT}P^{C'+D'UVT+E'UVT^2}$$

where $A'$, $B'$, $C'$, $D'$ and $E'$ are constants, and $P$ is the ballast power reading of the corresponding lamp.

1. **Calibration:**
   Choose a 3-lamp test to calibrate. Let the readings of UV Sensors 1, 2 and 3 be $S_1$, $S_2$, and $S_3$ respectively. Let the irradiation boundary conditions for Lamps 1, 2 and 3 be $I_1$, $I_2$, and $I_3$ [W/m²], respectively.

   Choose a starting guess value for $I_1$, then set $I_2 = (S_2/S_1)I_1$ and $I_3 = (S_3/S_1)I_1$. Then adjust $I_1$ (while adjusting $I_2$ and $I_3$) until the simulated RED equals the measured RED.

2. **Scaling:**
   Scaling is done on a per-lamp basis. Following are instructions for determining the irradiation boundary condition of Lamp $l$ for a run, where $l = 1, 2, 3$.

   Let $S_C$, $UVT_C$, and $P_C$ be the sensor reading, Test UVT, and ballast power reading of Lamp $l$ respectively for the calibrated run. Let $S_{0c}$ be the predicted sensor reading at the measured UVT and power reading of Lamp $l$ for the calibrated run, calculated using the regression equation.

   Let $S$ and $UVT$ be the sensor reading and Test UVT respectively for the run whose irradiation BC we wish to scale. Let $S_{0c}$ be the predicted sensor reading calculated using the UVT for this run, but with the power reading of Lamp $l$ for the calibrated run, $P_C$. 
Let $I_C$ be the irradiation BC of Lamp $l$ for the calibrated run. Then the scaled irradiation BC for Lamp $l$ of the new run, $I$, is given by:

$$I = I_C \cdot \frac{S/S_0}{S_C/S_0C} = I_C \cdot \frac{S}{S_C} \cdot \frac{10^A \cdot e^B \cdot UVT_c \cdot P_C^{C+D' \cdot UVT_C+E \cdot UVT^2_c}}{10^A \cdot e^B \cdot UVT \cdot P_C^{C+D' \cdot UVT+E \cdot UVT^2}}$$

$$\Rightarrow I = I_C \cdot \frac{S}{S_C} \cdot e^B (UVT_c-UVT) \cdot P_C^{D' (UVT_c-UVT)+E \cdot (UVT^2_c-UVT^2)}$$

The resulting expression scales the calibrated lamp irradiation value by the difference in lamp output power between the new and calibrated runs as measured by $(S/S_c)$ with a correction term, $e^B (UVT_c-UVT) \cdot P_C^{D' (UVT_c-UVT)+E \cdot (UVT^2_c-UVT^2)}$, for the potentially different UVTs used in the calibrated and new runs.

The new run is then simulated using the same simulation settings as the calibrated run, with the exceptions of UVT, inlet velocity and irradiation boundary conditions. For instance, if 20% reflection on all surfaces is simulated for the calibrated run, then 20% reflection on all surfaces must be simulated for the new scaled run.
APPENDIX D
SAMPLE BATCH FILES FOR AUTOMATED FLUENT RUNS

IDI RUNS
/file/read-case-data ozonia_M_rig_int_w_baff_g1_Y.cas
/define/models/radiation/discrete-ordinates yes 5 5 3 3
/define/materials/change-create water-liquid , no no no no yes constant 8.52
no no no no no
/define/boundary-conditions/wall sleeve_1,,,,,,,,,, 0.8,,,,,,,,,,,,, yes
semi-transparent,,,,,,,,, 3515.7 1 no ,,,
/define/boundary-conditions/copy-bc sleeve_1 sleeve_2 sleeve_3 sleeve_4 sleeve_5
sleeve_6 ,
/define/boundary-conditions/wall reactor_body,,,,,,,,,, 0.8,,,,,,,,,,,,, no 1 ,
/define/boundary-conditions/copy-bc reactor_body sensor_1 sensor_1_face sensor_2
sensor_2_face sensor_3 sensor_3_face ,
/define/boundary-conditions/copy-bc reactor_body sensor_4 sensor_4_face sensor_5
sensor_5_face sensor_6 sensor_6_face ,
/solve/patch fluid, temperature 1
/solve/set/equations
disco yes
temperature no
flow no
ke no
q q q
/solve/iterate 20
/file/write-case-data ,yes
;
/define/user-defined/compiled-functions load “libudf”
/define/models/dpm/user-defined “none” “none” “uv_output::libudf” “uv_dosage::libudf”
“none” 1
/define/models/dpm/numerics/tracking-parameters 100000 ,,
/define/injections/set-injection-properties no_rwm ,,,,,, “M_rig_15000.inj” ,,,
/define/injections/set-injection-properties rwm ,,,,,, “M_rig_15000.inj” yes yes 1 ,
/report/dpm-sample “rwm” () “outlet” () () no
!mv outlet.dpm outlet_Mwbaff-rig_Y_rwm_ie0.8_3515.7W_1.dpm
/report/dpm-sample “rwm” () “outlet” () () no
!mv outlet.dpm outlet_Mwbaff-rig_Y_rwm_ie0.8_3515.7W_2.dpm
/report/dpm-sample “rwm” () “outlet” () () no
!mv outlet.dpm outlet_Mwbaff-rig_Y_rwm_ie0.8_3515.7W_3.dpm
/file/write-case-data ,yes
;
CALGON RUNS
/file/read-case-data Calgon_0.3mgd.cas
/define/models/radiation/discrete-ordinates yes 5 5 3 3
/define/materials/change-create water-liquid , no no no no yes constant 35.81
no no no no no
/define/boundary-conditions/wall sleeve_1,,,,,,,,,, 0.8,,,,,,,,,,,,, yes
semi-transparent,,,,,,,,, 0.0 1 no ,,,
/define/boundary-conditions/wall sleeve_2,,,,,,,,,, 0.8,,,,,,,,,,,,, yes semi-
transparent,,,,,,,,, 0.0 1 no ,,,
/define/boundary-conditions/wall sleeve_3,,,,,,,,,, 0.8,,,,,,,,,,,,, yes semi-
transparent,,,,,,,,, 5230.9 1 no ,,,
/define/boundary-conditions/wall reactor_body,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
/define/boundary-conditions/wall wall,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
/define/boundary-conditions/wall baffle,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
/define/boundary-conditions/wall cleaner,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
/define/boundary-conditions/wall collar_1,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
/define/boundary-conditions/wall collar_2,,,,,,,,,, 0.8,,,,,,,,,,,,, 1 ,,
Computational Fluid Dynamics Based Models for Assessing UV Reactor Design and Installation

```
/define/boundary-conditions/wall collar_3 ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall pipe_wall ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_1_body ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_1_face ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_2_body ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_2_face ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_3_body ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
/define/boundary-conditions/wall sensor_3_face ,,,,,,,,,, , 0.8 ,,,,,,,,,, ,, 1 ,,  
;
/solve/patch fluid () temperature 1 
/solve/set/equations  
disco yes  
temperature no  
flow no  
ke no  
g g g  
/iterate 20  
/file/write-case-data ,yes  
;
/define/user-defined/compiled-functions load "libudf"  
/define/models/dpm/user-defined "none" "none" "uv_output::libudf" "uv_dosage::libudf" "none" 1  
/define/models/dpm/numerics/tracking-parameters 100000 ,,,  
/define/injections/set-injection-properties no_drw ,,,, "Calgon_15000.inj" ,, ,  
/define/injections/set-injection-properties drw ,,,, "Calgon_15000.inj" yes yes 1 ,,,  
/report/dpm-sample "drw" () "outlet" () () no  
!mv outlet.dpm outlet_Cal_61calib_ie0.8_test95_drw_1.dpm  
/report/dpm-sample "drw" () "outlet" () () no  
!mv outlet.dpm outlet_Cal_61calib_ie0.8_test95_drw_2.dpm  
/report/dpm-sample "drw" () "outlet" () () no  
!mv outlet.dpm outlet_Cal_61calib_ie0.8_test95_drw_3.dpm  
/file/write-case-data ,yes  
;
```
APPENDIX E
IMPACT OF DRW INPUT PARAMETERS AT LOW AND HIGH FLOW RATES

The turbulent dispersion of particles in Fluent using the discrete random walk (DRW) model in Fluent is controlled by two user inputs:

- An integral time-scale constant, $C_L$, that governs how much time a particle is allowed to interact with a turbulent eddy. The recommended value for $C_L$ in Fluent is 0.15 for the $k$-$\varepsilon$ turbulence model and its variants and 0.3 for the Reynolds stress model (we used 0.15 in all of our simulations). Munoz et al. (2007) performed a sensitivity study and found that a decrease in $C_L$ from 0.30 to 0.15 resulted in a slight reduction in the predicted RED (1.2%), but that the change was “practically unimportant.”
- Choice of “Random Eddy Lifetime” or constant eddy lifetime. The eddy lifetime is proportional to the product of the time-scale constant, $C_L$, and local turbulent parameters (ratio of the turbulent kinetic energy, $k$, to the turbulent energy dissipation, $\varepsilon$). If random eddy lifetime is selected, the eddy lifetime is a random variation about the constant eddy lifetime. In the periodic report, we performed a sensitivity analysis, and the choice of random or constant eddy lifetime did not significantly affect our predictions of RED.

The following figures show the results of individual particle tracks colored by cumulative dose (J/m²) with and without DRW released from the same point (stream ID = 7700) in the Calgon Sentinel simulation for a relatively low flow rate (Figures E.1 through E.5) and the high flow rate (Figures E.6 through E.9). For the particle tracks with DRW, 3 tries were performed at $C_L$ values of 0.01, 0.15 (recommended), 0.3, and 0.6. The range of $C_L$ values that Munoz et al. (2007) found in the literature was from 0.06 to 0.63. For each value of $C_L$, simulations were performed with both random and constant eddy lifetime. It should be noted that because the DRW particle tracks are randomly influenced by local turbulent conditions, the particles can take different paths, and the cumulative dose for a particular particle track cannot be directly compared to the same particle track from a different simulation.

The results show that the time-scale constant, $C_L$, has the most significant impact on the movement of the DRW particle tracks when the flow rate is low (Re ~ 100,000). The choice of random vs. constant eddy lifetime does not appear to influence the particle path significantly. At low values of $C_L$ ($C_L = 0.01$) the particle interaction time with the turbulent eddies is small and the paths look fairly smooth. At higher values of $C_L$, the paths become more erratic and “jumpy” since the particles are influenced more by the turbulent eddies.

At the high flow rate (Re ~ 800,000), all the particle paths are smoother due to the increased mean velocity magnitude relative to the turbulent fluctuating velocity components. Thus the impact of the time-constant value and choice of DRW vs. no-DRW in the particle tracking model is more significant at lower flow rates (lower Reynolds number) in the turbulent regime.

As discussed in “RED Simulations of Calgon Reactor Using Fluent DO Radiation Model” in Chapter 3, the impact of these particle-tracking parameters at lower flow rates may also be due to large simulated turbulent kinetic energies and viscosities, which impact the turbulent fluctuating...
velocity components that are used in the DRW model. Even though the hydraulic simulation converged using the default convergence criteria (0.001), the simulated turbulent viscosity (and, hence, turbulent kinetic energy) was still very large. An additional 1000 iterations were run following the initial convergence, and results showed that the impact of DRW vs. no-DRW on the simulated RED was much smaller (2%). In addition, the particle paths resulting from the DRW simulation were much more similar to the particle paths of the no-DRW simulation (see Figure E.10). Thus, the erratic particle paths displayed in the previous figures can also be due to excessive simulated turbulent viscosity ratios that impact the turbulent velocity components.
Figure E.2  Low flow (velocity ~ 0.3 m/s, Reynolds number ~ 1e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.01

Figure E.3  Low flow (velocity ~ 0.3 m/s, Reynolds number ~ 1e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.15
Figure E.4 Low flow (velocity ~ 0.3 m/s, Reynolds number ~ 1e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.3

Figure E.5 Low flow (velocity ~ 0.3 m/s, Reynolds number ~ 1e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.6
Appendix E: Impact of DRW Input Parameters at Low and High Flow Rates

Figure E.6 High flow (velocity ~ 2.6 m/s, Reynolds number ~ 8e5), no DRW, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj

Figure E.7 High flow (velocity ~ 2.6 m/s, Reynolds number ~ 8e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.15
Figure E.8  High flow (velocity ~ 2.6 m/s, Reynolds number ~ 8e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.3

Figure E.9  High flow (velocity ~ 2.6 m/s, Reynolds number ~ 8e5), DRW, 3 tries, 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime (left), constant eddy lifetime (right), time scale constant = 0.6
Figure E.10 Low flow (velocity ~ 0.3 m/s, Reynolds number ~ 1e5), 1 injection (Stream ID = 7700), injection file = Calgon_15000.inj, random eddy lifetime, time scale constant = 0.15, no-DRW (left); DRW, 3 tries (right)
REFERENCES


# ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
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<tbody>
<tr>
<td>AIAA</td>
<td>American Institute of Aeronautics and Astronautics</td>
</tr>
<tr>
<td>AwwaRF</td>
<td>Awwa Research Foundation (now Water Research Foundation)</td>
</tr>
<tr>
<td>B. subtilis</td>
<td><em>Bacillus subtilis</em> bacterium</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
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<tr>
<td>DENARD</td>
<td>Degremont North American Research and Development</td>
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<tr>
<td>DO</td>
<td>discrete ordinates</td>
</tr>
<tr>
<td>DRW</td>
<td>discrete random walk</td>
</tr>
<tr>
<td>EPA</td>
<td>U.S. Environmental Protection Agency</td>
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<tr>
<td>$\varepsilon$</td>
<td>turbulent dissipation rate ([m^2/s^3])</td>
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<td>i</td>
<td>particle number</td>
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<tr>
<td>IDI</td>
<td>Infilco Degremont Inc.</td>
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<tr>
<td>$k$</td>
<td>turbulent kinetic energy ([m^2/s^2])</td>
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<td>LES</td>
<td>large eddy simulation</td>
</tr>
<tr>
<td>LP</td>
<td>low pressure mercury lamp</td>
</tr>
<tr>
<td>LT2ESWTR</td>
<td>Long-Term 2 Enhanced Surface Water Treatment Rule</td>
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<tr>
<td>MP</td>
<td>medium pressure mercury lamp</td>
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<tr>
<td>MS2</td>
<td>type of bacteriophage used to validate ultraviolet reactors</td>
</tr>
<tr>
<td>N</td>
<td>number of viable microbes remaining after exposure to ultraviolet light</td>
</tr>
<tr>
<td>$N_o$</td>
<td>number of viable microbes introduced to ultraviolet system</td>
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<tr>
<td>$n_p$</td>
<td>total number of particles simulated</td>
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<td>PAC</td>
<td>Project Advisory Committee</td>
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<td>QA/QC</td>
<td>quality assurance/quality control</td>
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<tr>
<td>$R^2$</td>
<td>coefficient of determination</td>
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<tr>
<td>RED</td>
<td>reduction equivalent dose ([J/m^2])</td>
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<td>RNG</td>
<td>renormalization group</td>
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<tr>
<td>s</td>
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