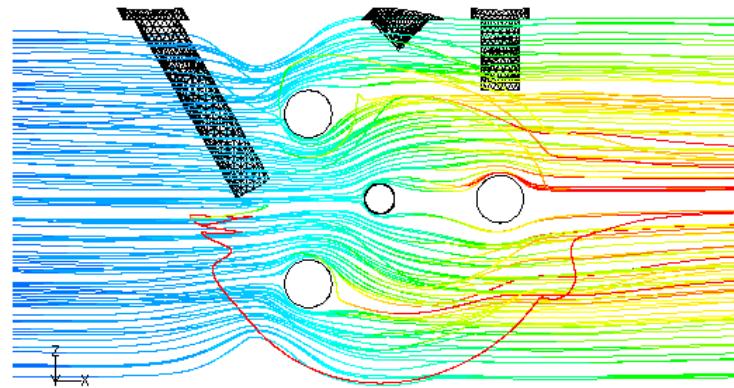


# Important Factors for Computational Modeling of UV Disinfection Systems



Clifford K. Ho,<sup>1</sup> Siri S. Khalsa,<sup>1</sup> Ed Wicklein,<sup>2</sup> and Harold Wright<sup>2</sup>

<sup>1</sup>*Sandia National Laboratories*  
<sup>2</sup>*Carollo Engineers*

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

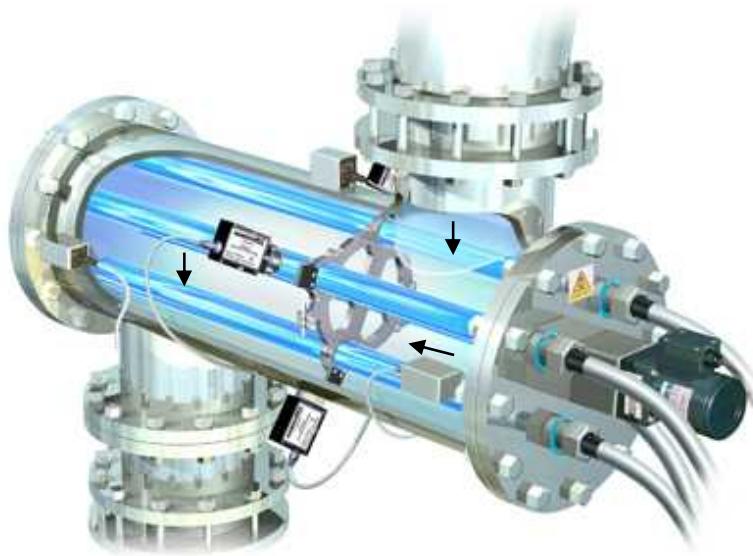


# Overview

- **Introduction**
- **Modeling Approach**
- **Sensitivity Analyses**
- **Conclusions**



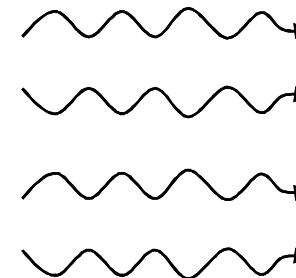
# How Does UV Disinfection Work?



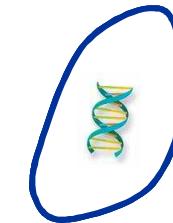
[www.aquionics.com](http://www.aquionics.com)

**Flowing water is exposed to UV light in a reactor chamber**

UV Light



Cryptosporidium

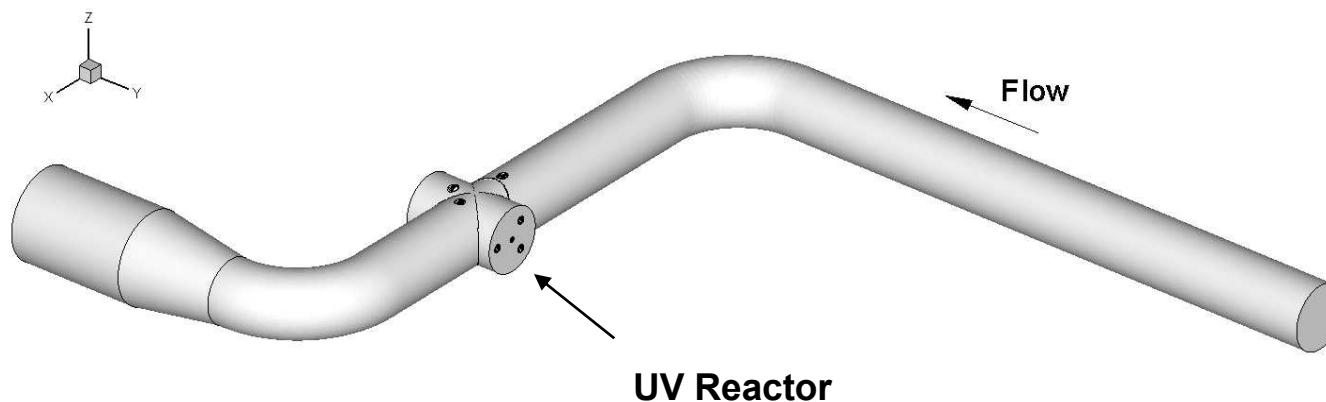


**UV light makes the pathogen non-infectious by damaging its DNA**



# Problem Statement

- **Validation of UV disinfection systems requires costly biodosimetry tests (usually off-site)**
- **Installed systems may have different piping configurations than the validated system**





# Objectives

- **Evaluate computational fluid dynamics (CFD) modeling as a means to assess performance of UV disinfection systems**
  - **Can we replace or minimize biodosimetry with CFD modeling?**
  - **Will the installed system perform at least as well as the validated system?**
  - **What processes and design features most impact performance?**
  - **What factors impact the accuracy of the modeling?**



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See talk by Wicklein, Wright, and Ho

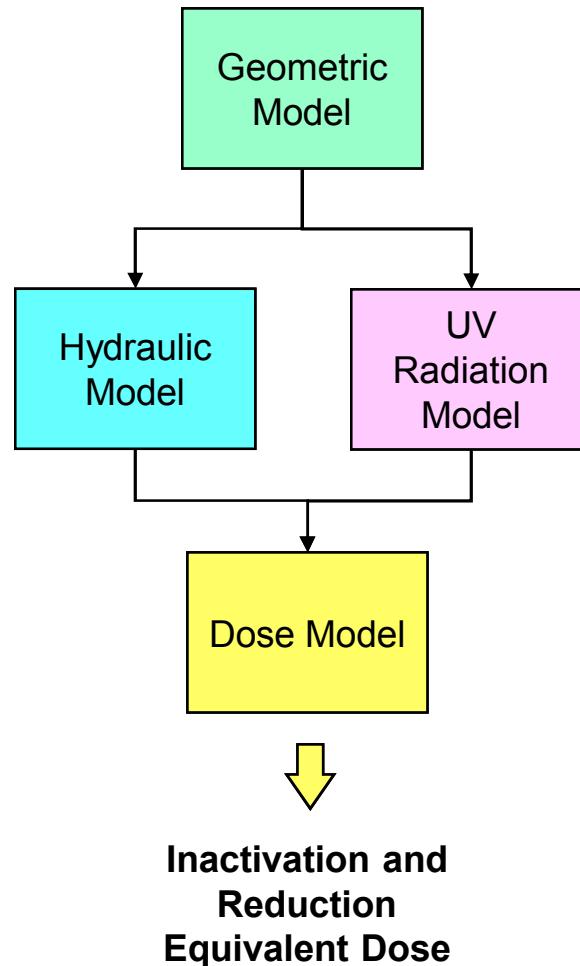
Time: Wed., 8:30 AM

Title: Computational Fluid  
Dynamics Modeling of UV  
Reactor Validation Tests

Session: UV Validation and Adenovirus

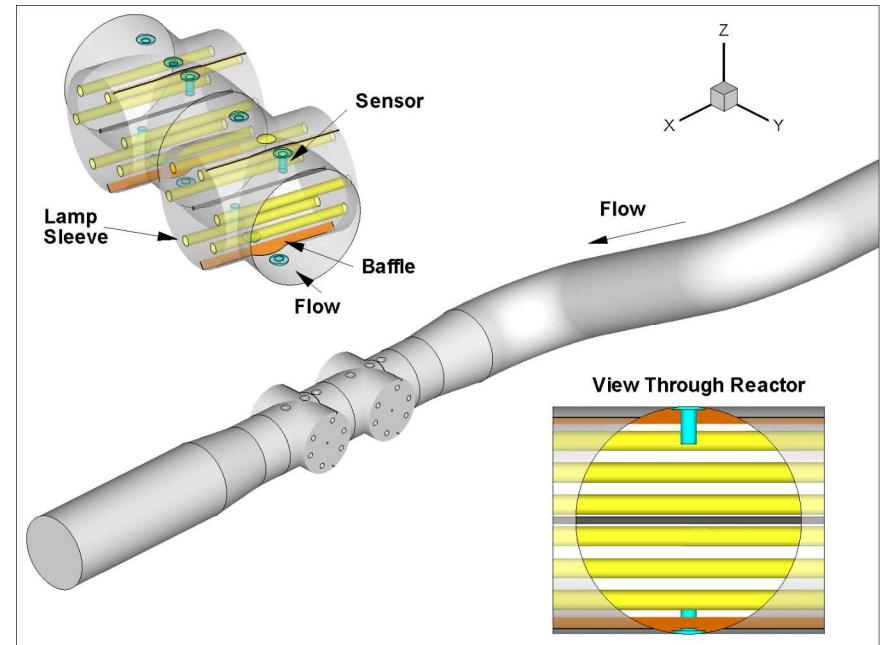


# Modeling Approach



# Hydraulic Modeling

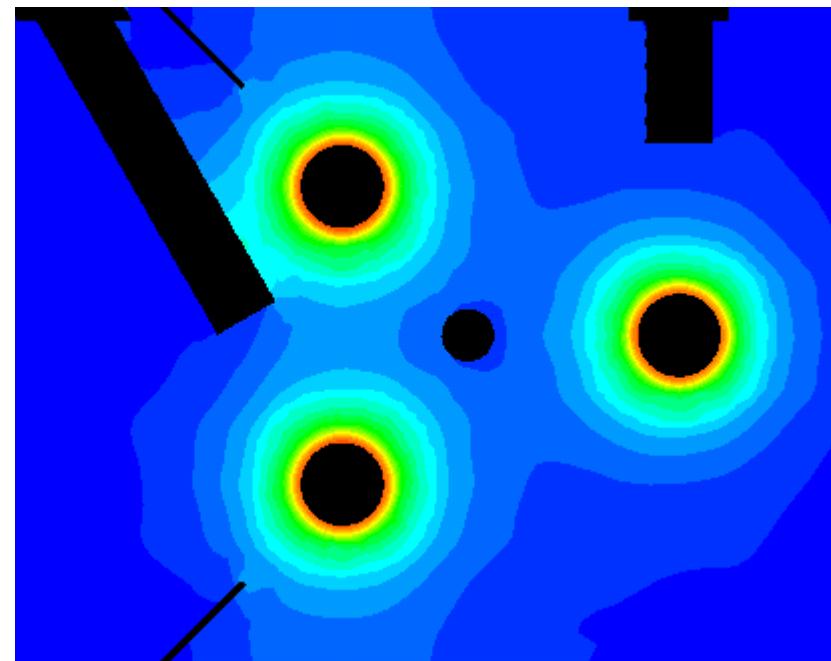
- Develop geometry and grid to represent features of UV reactor and piping
  - Ensure results are grid independent
- Apply appropriate boundary conditions
  - E.g., Inlet velocity, flow rate
- Obtain converged flow field



GAMBIT/FLUENT model of the Ozonia Aquaray® H2O reactor and piping.

# Implement UV Radiation Model

- **Implement appropriate UV radiation model**
  - Lamp orientation and features
  - Sensor orientation and features
  - Spectral dependencies
  - Directional dependencies
  - Refraction through quartz sleeve
  - Wall reflection
- **Liu et al. (2004) provides evaluation of alternative models**
  - Line source integration, multiple point source summation, discrete ordinates, etc.



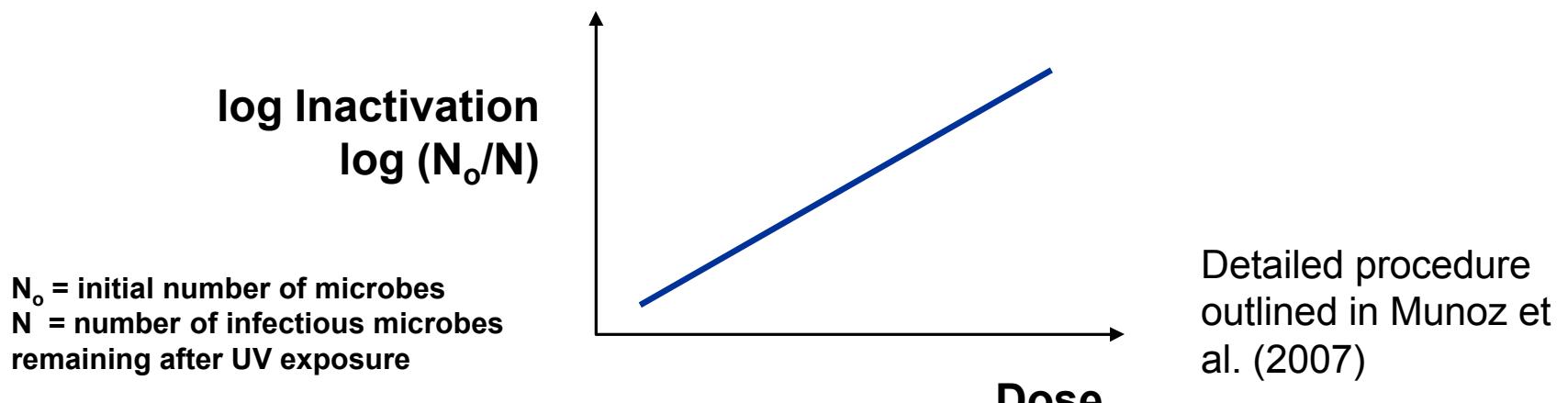
Simulated UV Intensity Field  
(Calgon 12" Sentinel® UV Reactor)

# Calculate Microbial Inactivation and Equivalent Dose

- Perform particle tracking in UV radiation field to obtain particle dose distribution

$$\text{Dose (J/m}^2\text{)} = \text{Incident radiation (W/m}^2\text{)} \times \text{Exposure time (s)}$$

- Calculate microbial inactivation and equivalent dose (RED) using dose-response curve





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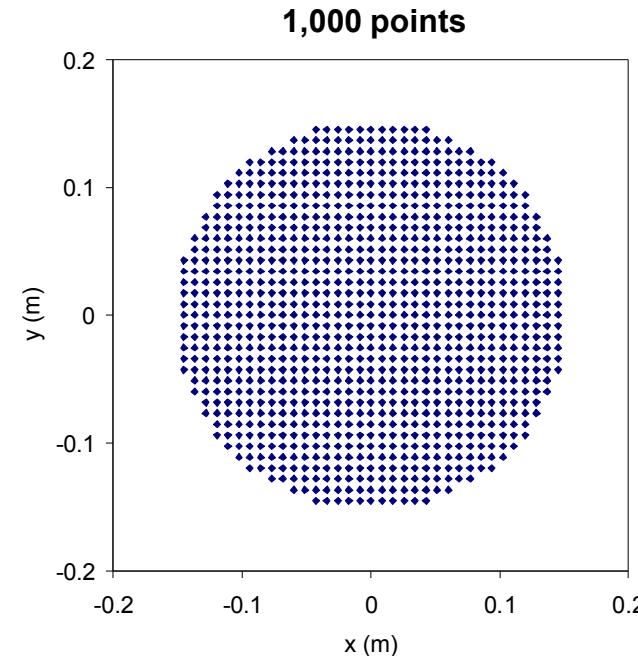
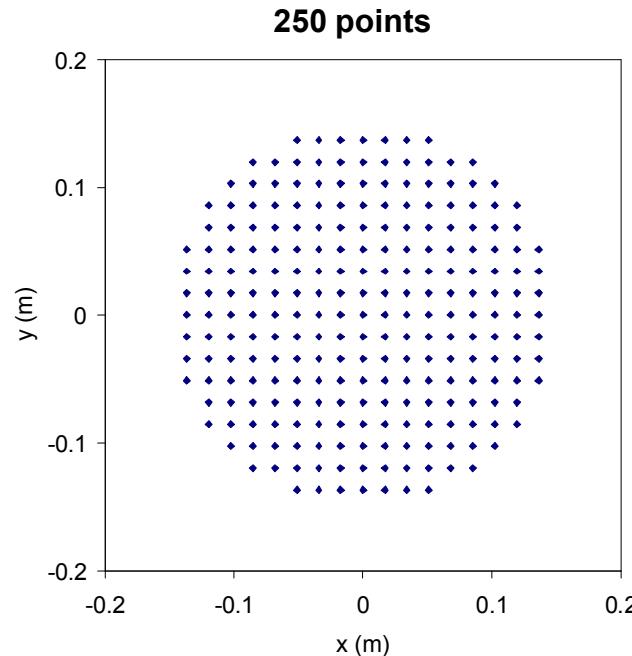


# Sensitivity of Simulated RED to Particle Tracking Parameters

- Number of particles injected
- Discrete Random Walk vs. No Random Walk
- Dependence on Flow Rate

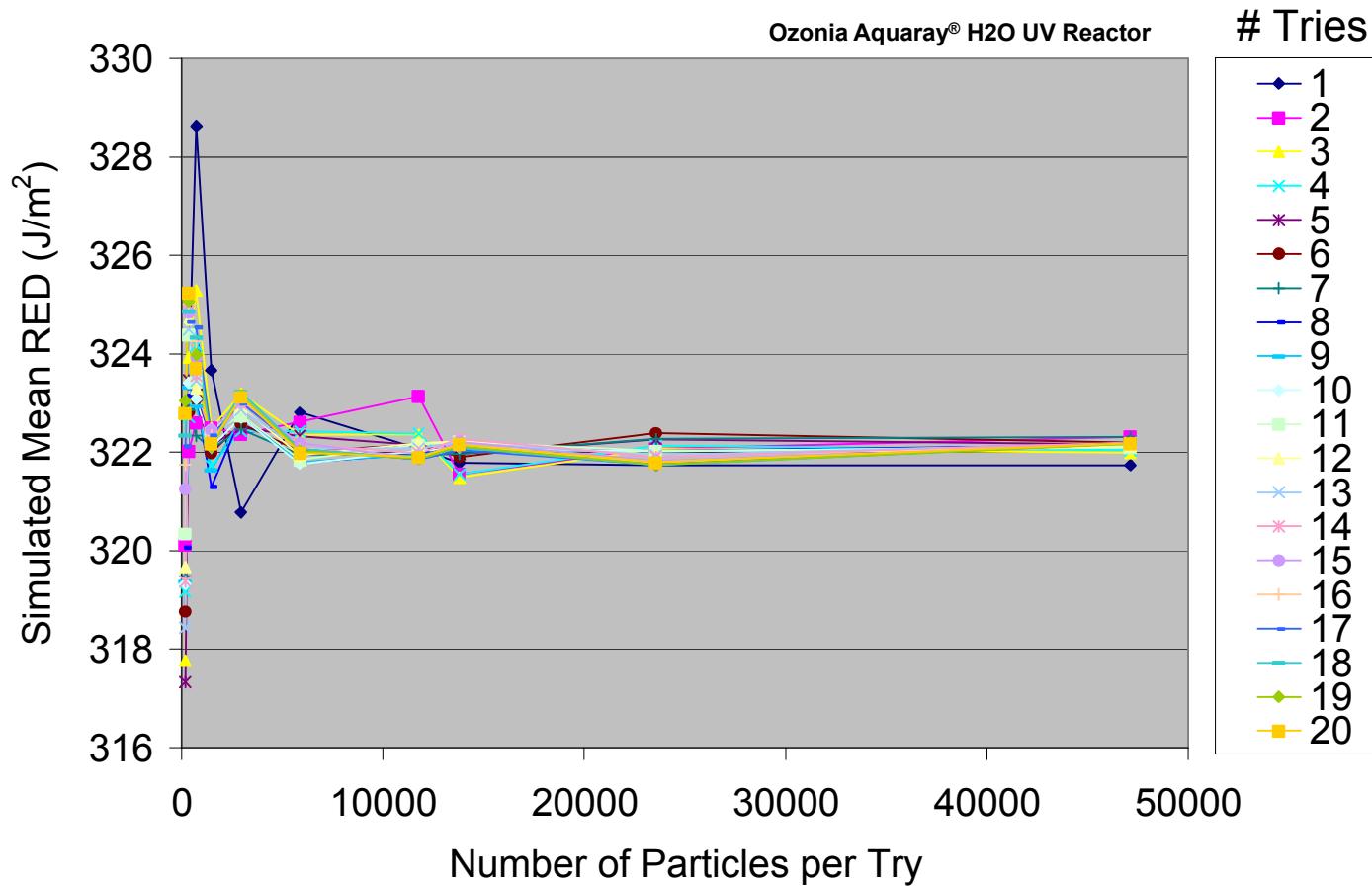
# Particle Tracking Analysis

- Ozonia Aquaray® H2O UV reactor
- Number of particles injected: 200 - 50,000
  - Number of tries using discrete random walk model: up to 20



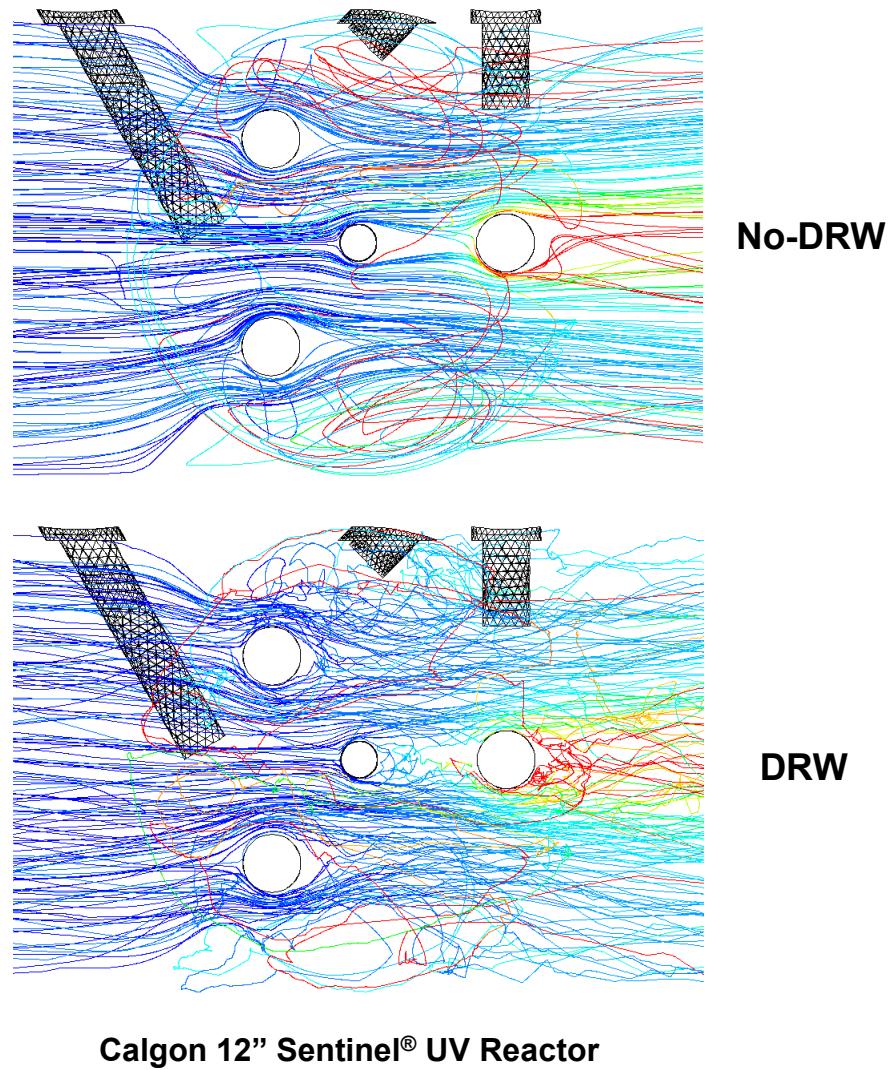
# Simulated RED as a function of particles injected

- Variability in simulated RED less than several percent with more than 5,000 – 10,000 particles for any number of tries

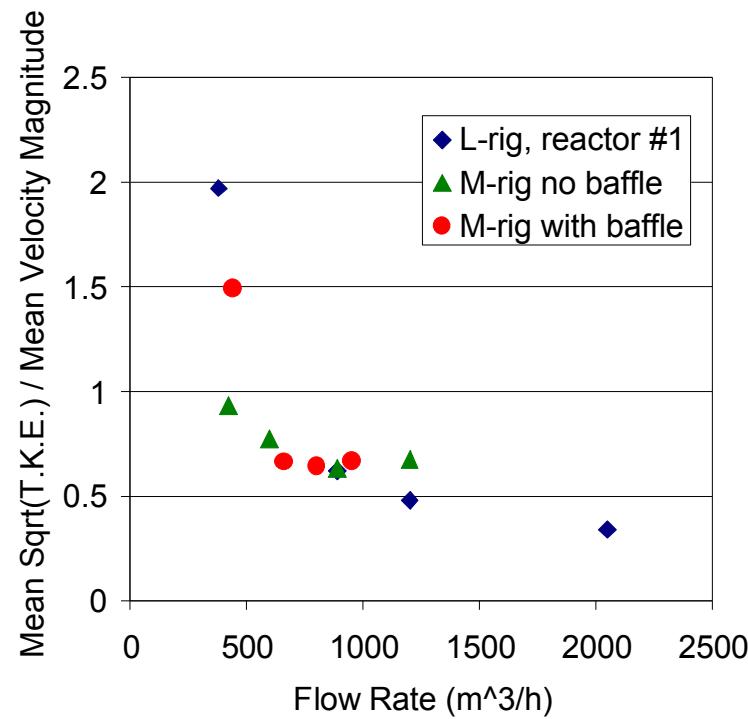
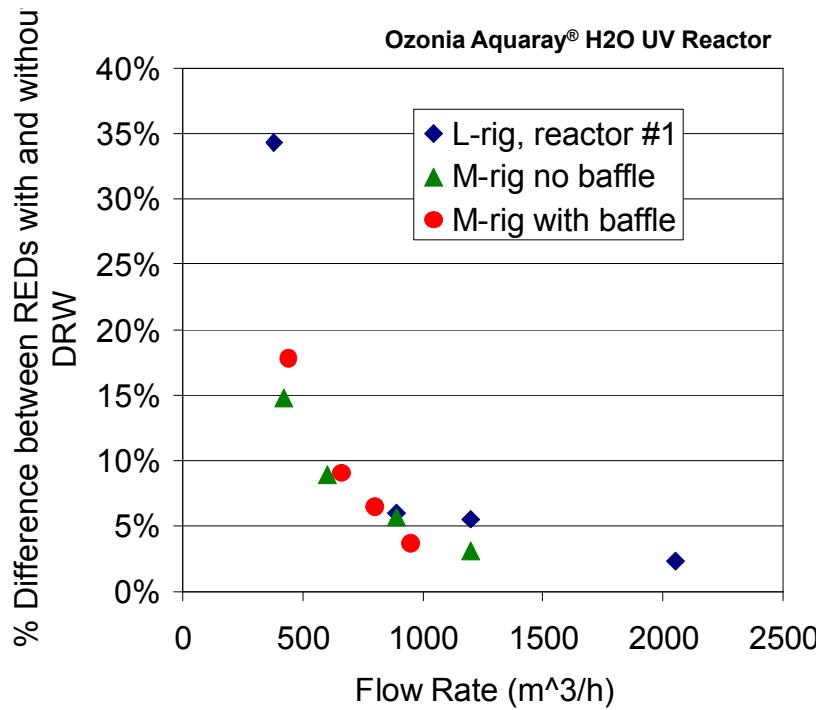


# Impact of Discrete Random Walk

- Without random walk, particle motion calculated using mean velocity at each time step
- Discrete random walk model
  - Includes fluctuating velocity component at each particle time step
  - Adds more noise to particle path



# DRW vs. no-DRW Dependence on Flow Rate



- Although these runs converged with default criteria, additional iterations reduced the difference in simulated RED, even at low flow rates
- Proper initialization of kinetic energy ( $k$ ) and turbulent energy dissipation ( $\varepsilon$ ) parameters can allow improved convergence

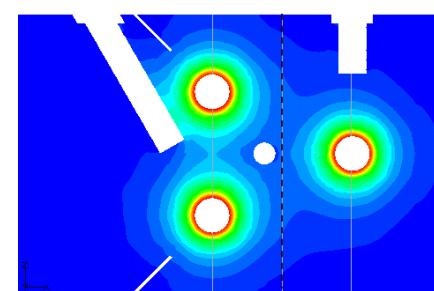
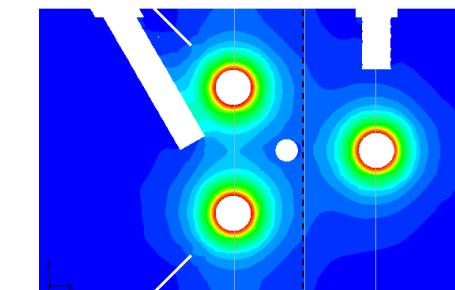
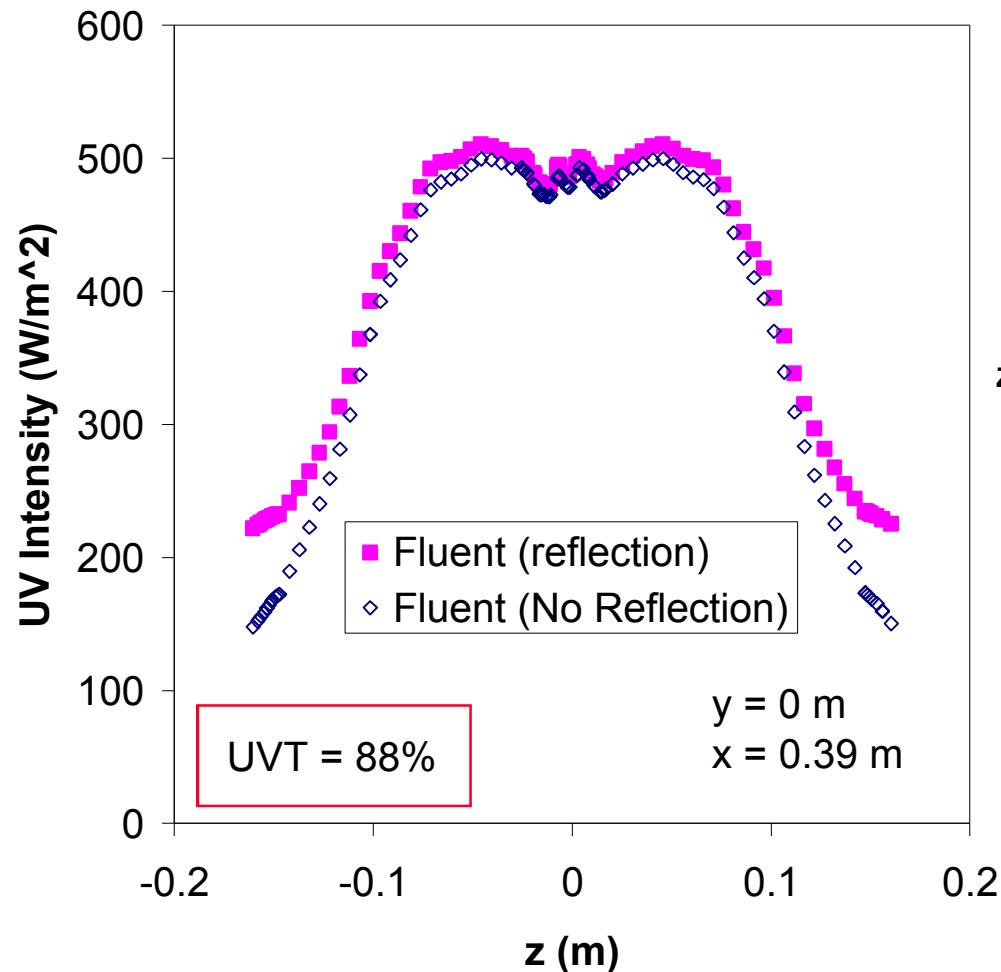


# Sensitivity to Reflection

- **Wall reflection is often neglected in UV radiation models**
- **Perform simulations with and without wall reflection to determine impact**

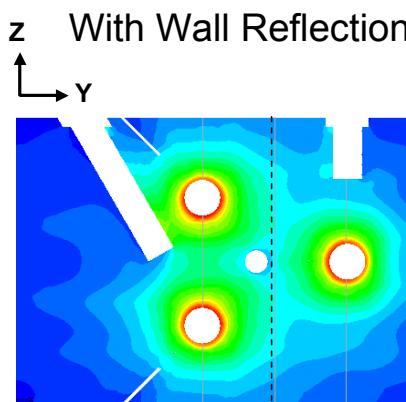
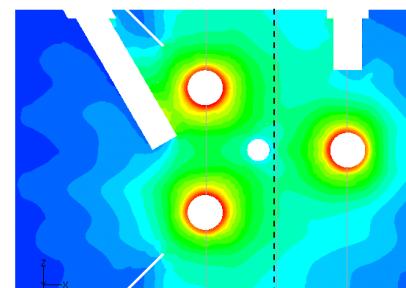
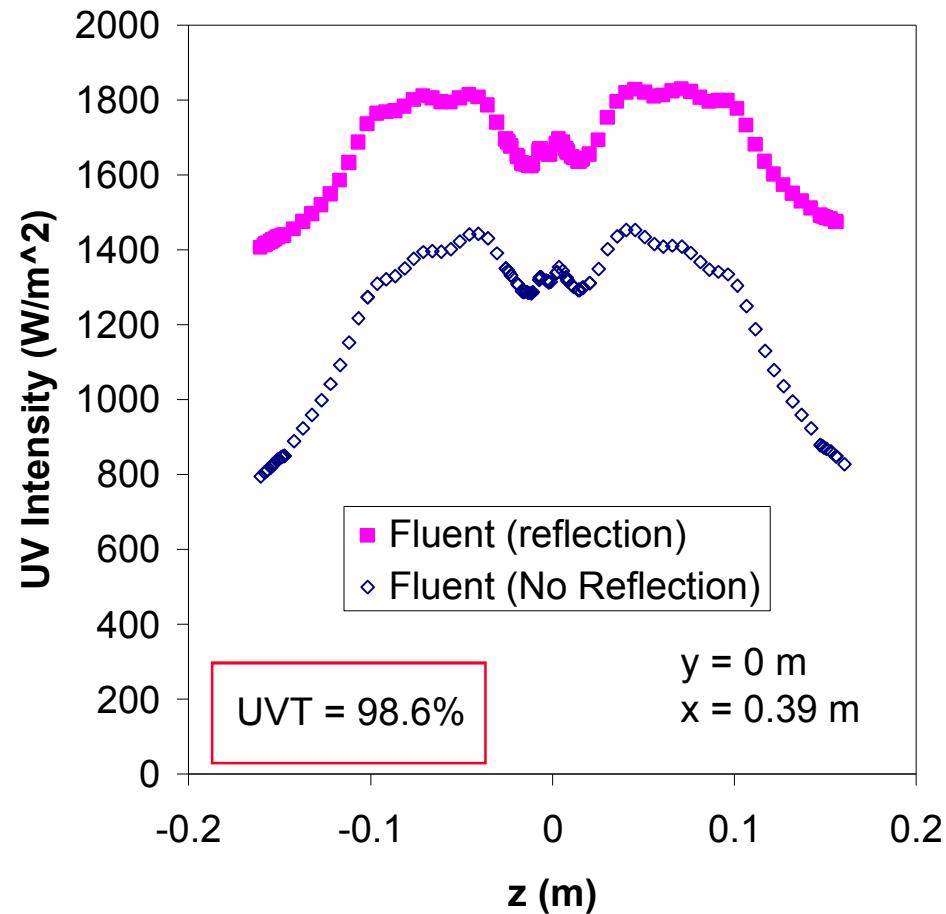
# UV Radiation Modeling

Simulated UV radiation field with and without wall reflection  
(Calgon 12" Sentinel® UV Reactor)



# UV Radiation Modeling

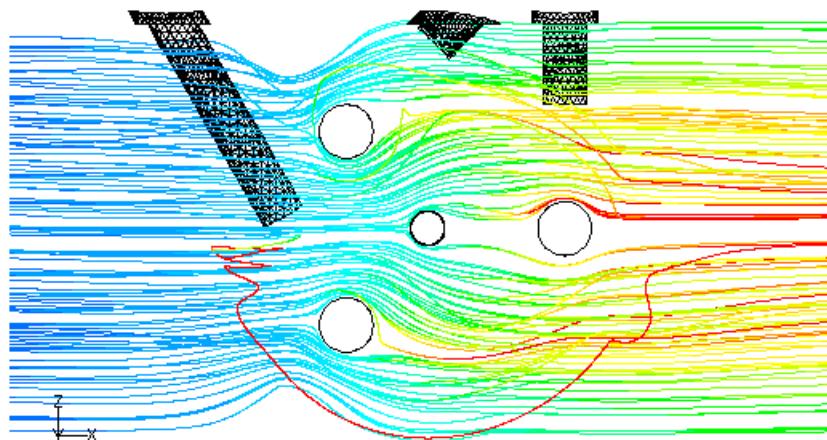
Simulated UV radiation field with and without wall reflection  
(Calgon 12" Sentinel® UV Reactor)



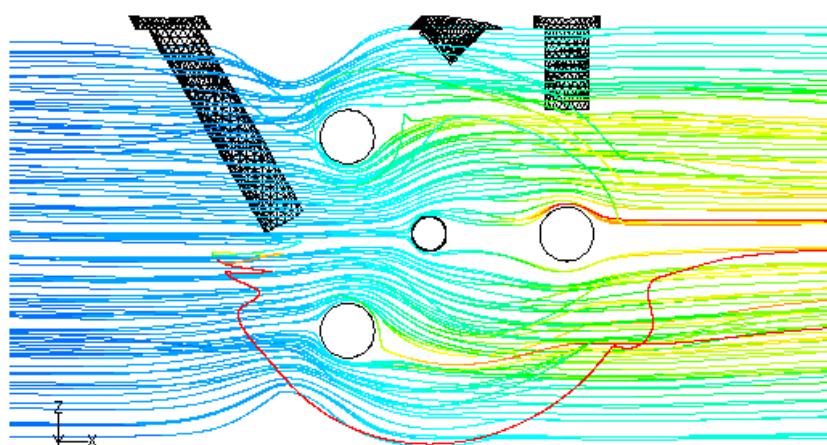


# Particle Paths Colored by Cumulative Dose

Calgon 12" Sentinel® UV Reactor

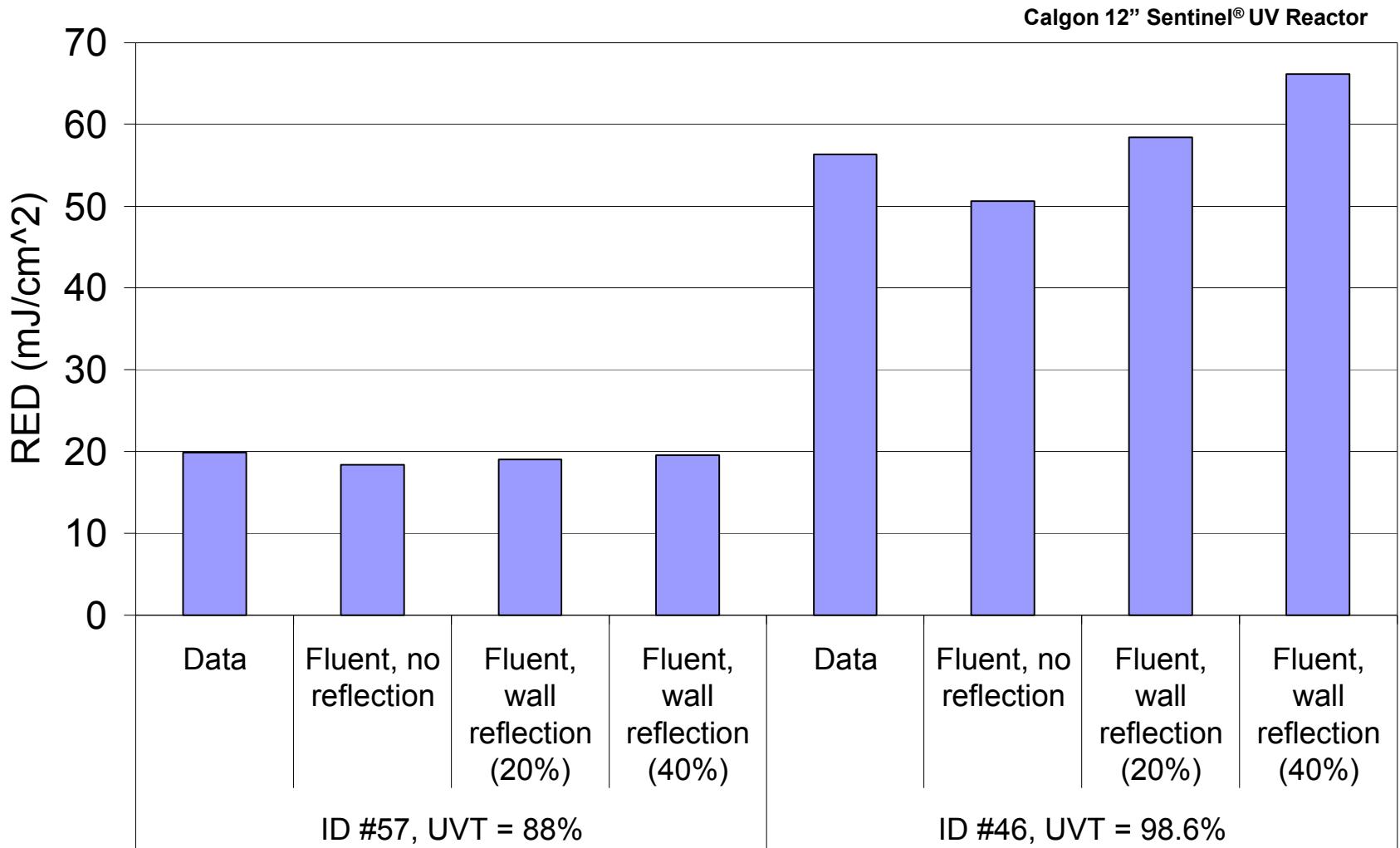


40% wall reflection



no wall reflection

# Effect of Wall Reflection on Simulated RED





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# Findings

- **Particle Tracking Sensitivity**
  - **> 5,000 – 10,000 particles produced converged RED**
  - **DRW vs. no-DRW**
    - Larger differences at lower flow rates
    - Turbulence intensity increases with lower flow rates
    - Need to ensure convergence; proper initialization of  $k$  and  $e$
- **Wall Reflection Sensitivity**
  - **Inclusion of wall reflection may be important at higher UVTs (>90%)**
  - **UV Intensity with wall reflection was more than 50% higher near wall than without**
  - **Simulated RED with wall reflection was ~15-30% higher than without wall reflection**



# Big Picture Benefits

- **CFD-based simulations of UV disinfection can be used to accurately simulated RED**
- **Performance of installed systems with different piping configurations than the validated system can be assessed using CFD**
- **Features and designs can be assessed and improved through CFD-based models**



# Acknowledgments

- **AwwaRF (Project #4107)**
  - Alice Fulmer, Project Manager
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- **Trojan Technologies Inc.**
  - Ted Mao

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