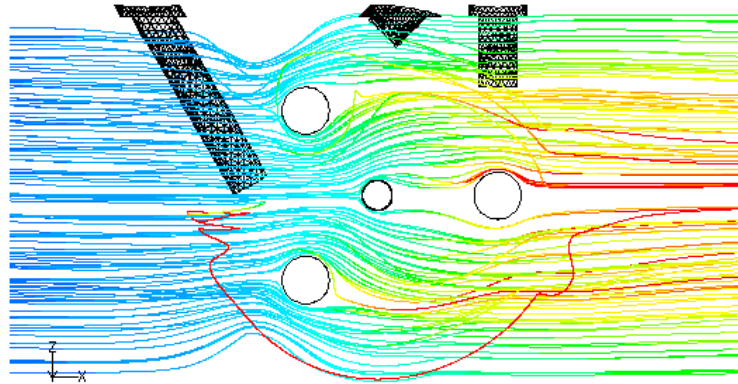


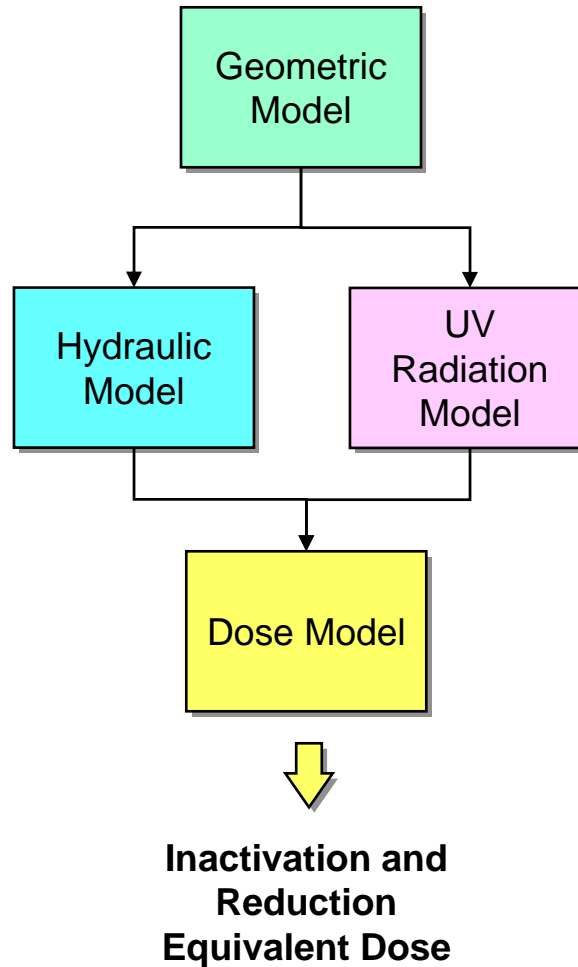
# Radiation Dose Modeling in FLUENT®



**Clifford K. Ho**

***Sandia National Laboratories  
Albuquerque, NM***

# Modeling Approach





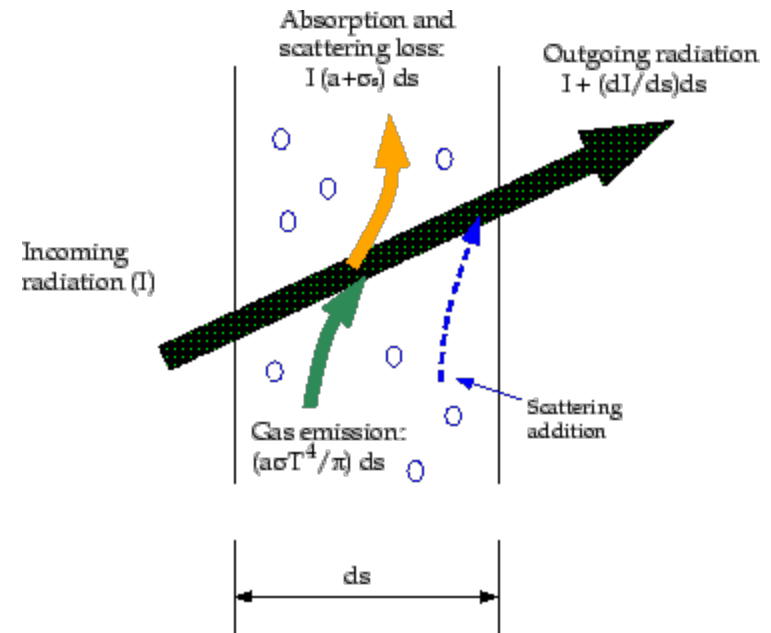
# Overview

## Radiation Dose Modeling in FLUENT®

- **Discrete Ordinates Radiation Model**
- **Particle Tracking and Dose**
- **Calculation of RED**

# Discrete Ordinates Radiation Model

- Solves the radiative transfer equation over a domain of discrete solid angles
- Calculates radiation intensity as a function of absorption, scattering, reflection, and emission
- Integrated within FLUENT CFD/hydraulic model
  - Impacts of geometry within the reactor (shadowing, reflection) readily implemented

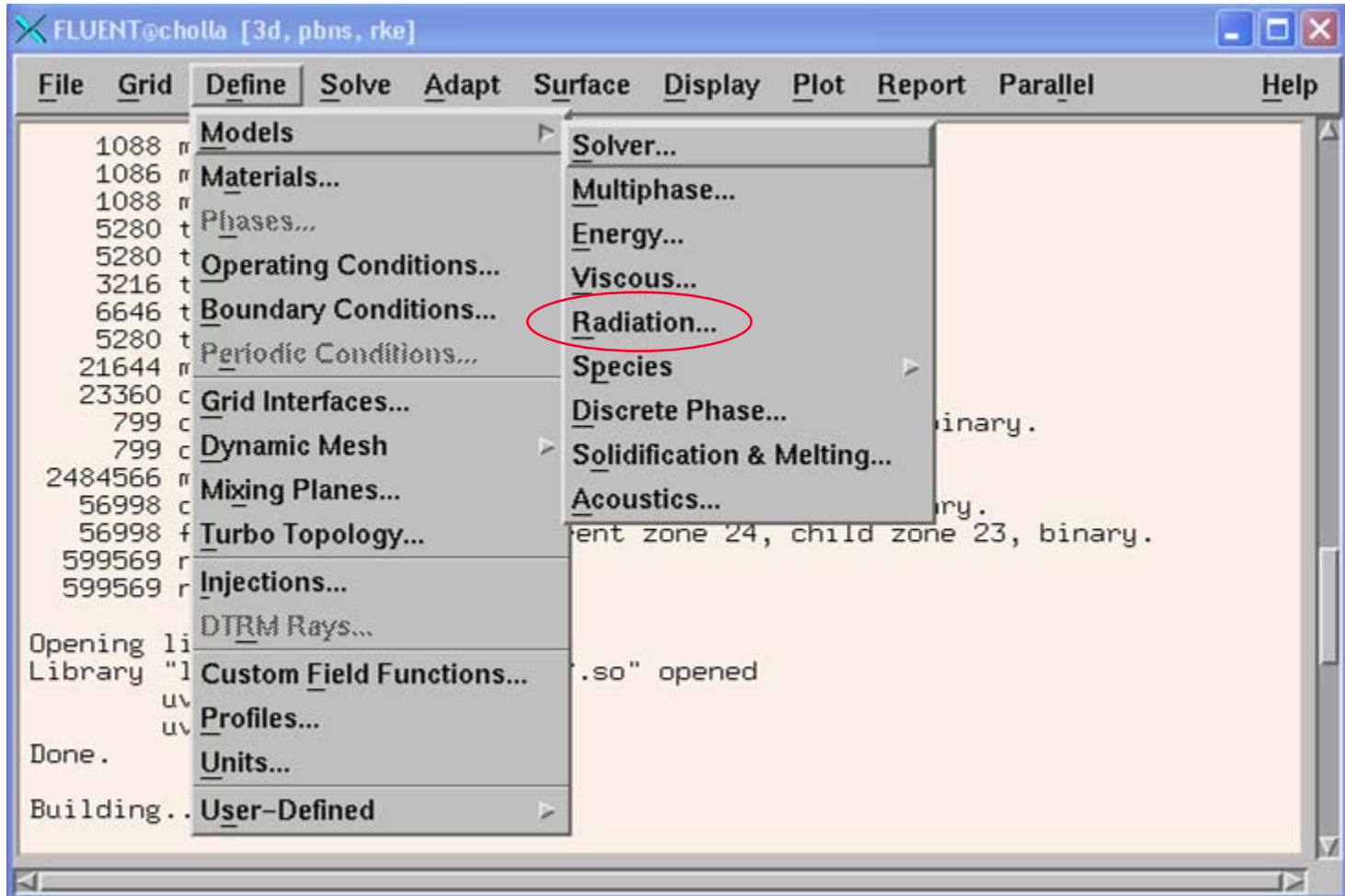




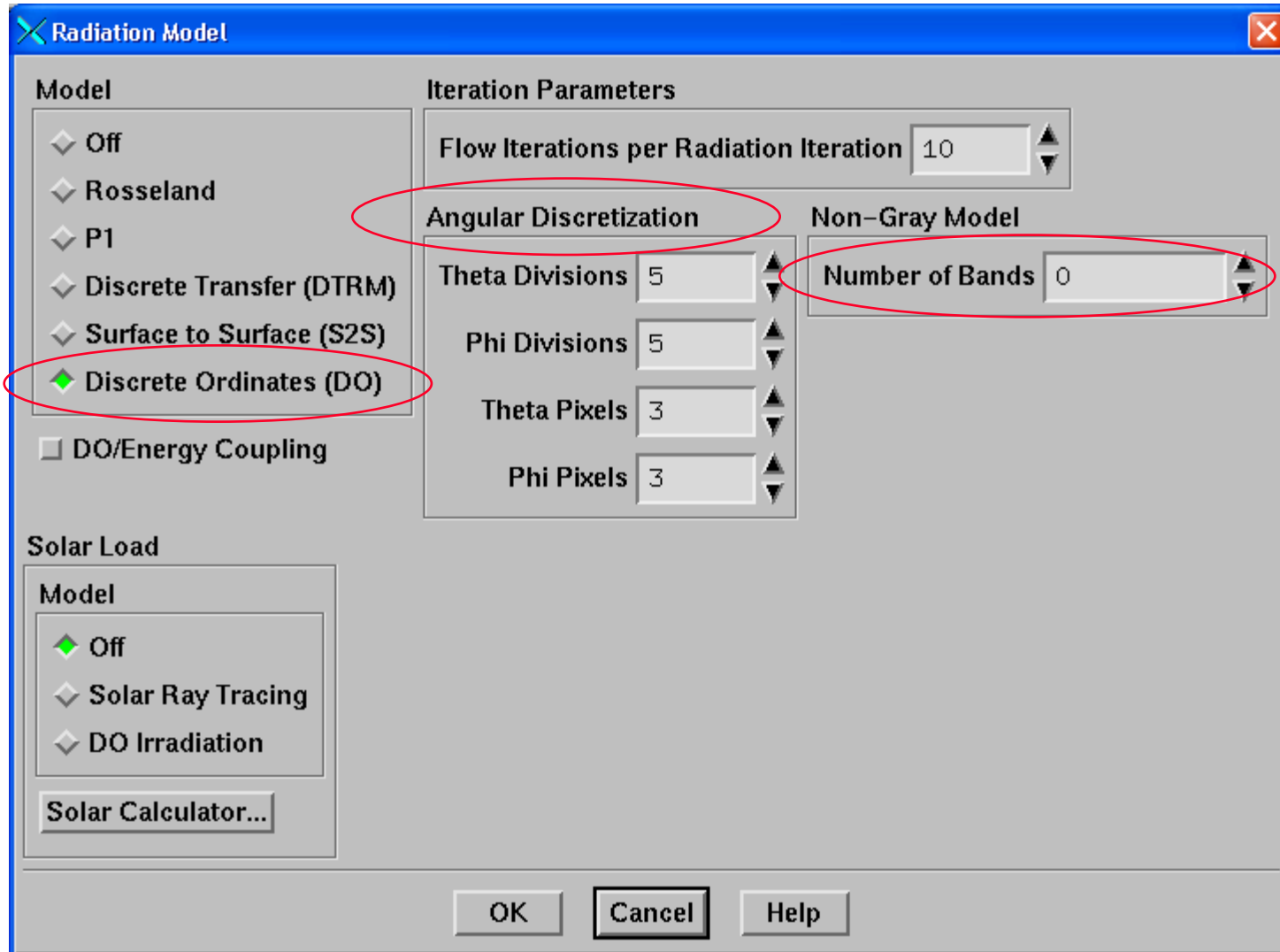
# Step-by-Step Guide

[www.sandia.gov/cfd-water](http://www.sandia.gov/cfd-water)

# Turn on Radiation Model in FLUENT

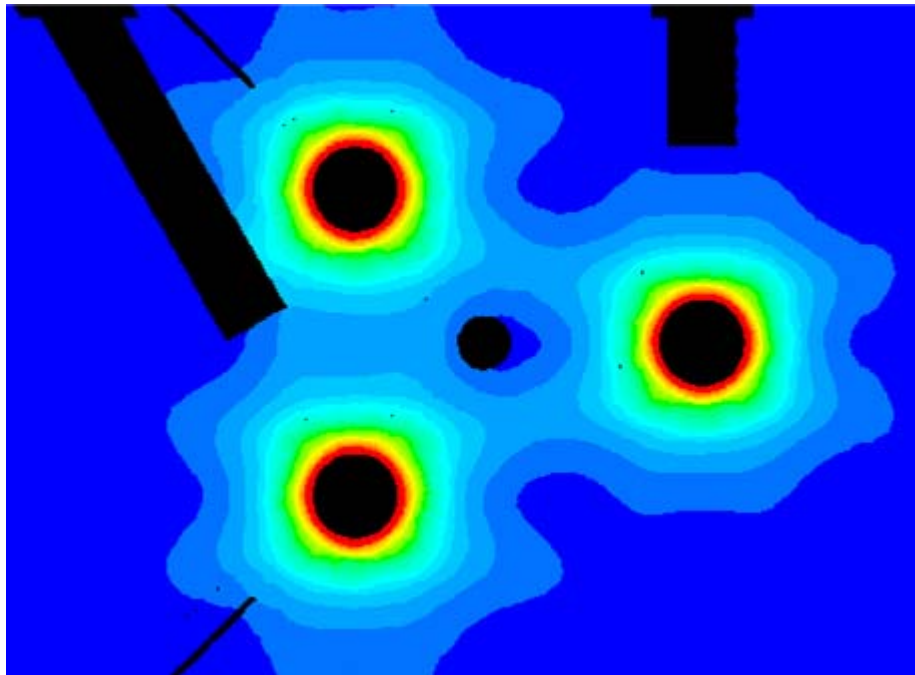


# DO Model Parameters

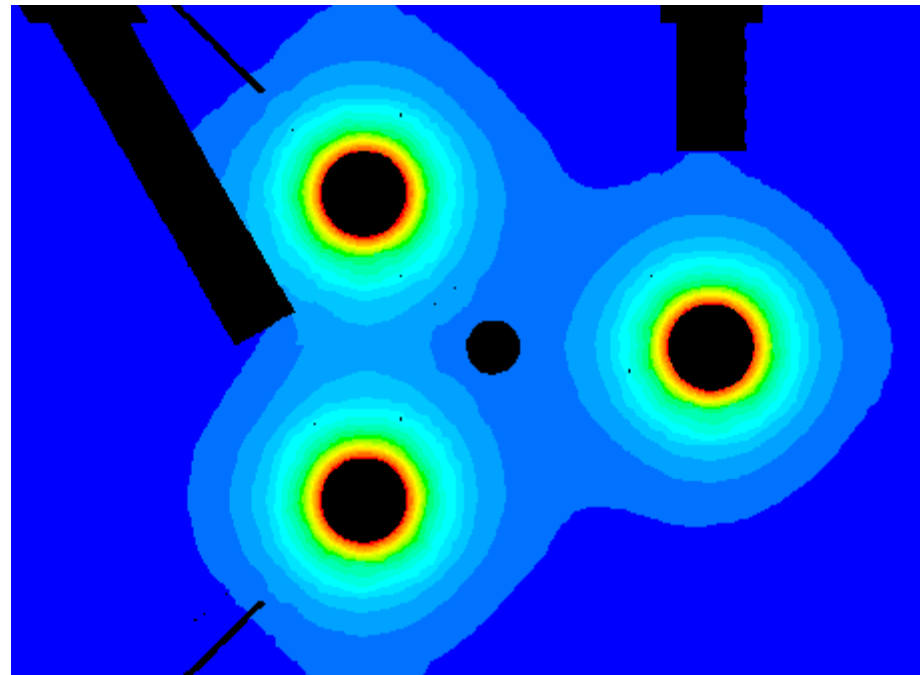


# Impact of Theta x Phi Discretization on Simulated Incident Radiation Field

theta x phi = 2 x 2



theta x phi = 5 x 5



Calgon 12" Sentinel® UV Reactor



# Specify UV Transmittance of Water

- Define > Materials...

**Materials**

Name: water-liquid

Material Type: fluid

Order Materials By: Name

Chemical Formula: h2o<l>

Fluent Fluid Materials: water-liquid (h2o<l>)

Mixture: none

Fluent Database...

User-Defined Database...

**Properties**

Absorption Coefficient (1/m): constant, 20.09

Scattering Coefficient (1/m): constant, 0

Scattering Phase Function: isotropic

Refractive Index: constant, 1

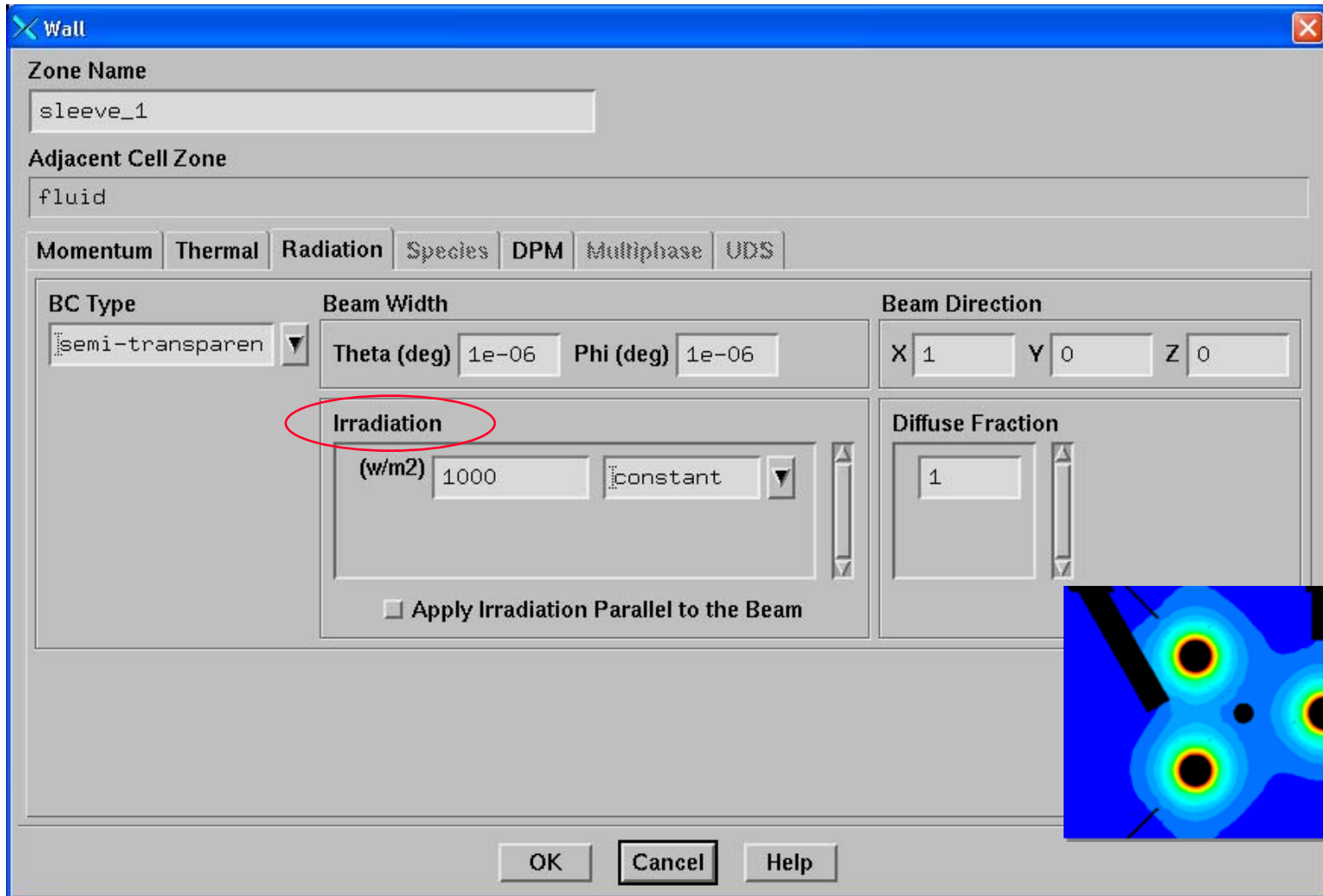
Change/Create Delete Close Help

$$UVT = \frac{I}{I_o} = e^{-ax}$$

$I / I_o$  = Intensity reduction at  $x = 1 \text{ cm}$   
 $a$  = Absorption coefficient (1/m)

# Specify UV Radiation Boundary Condition

- Define > Boundary Conditions...



Wall

Zone Name  
sleeve\_1

Adjacent Cell Zone  
fluid

Momentum Thermal **Radiation** Species DPM Multiphase UDS

BC Type  
semi-transparent

Beam Width  
Theta (deg) 1e-06 Phi (deg) 1e-06

Beam Direction  
X 1 Y 0 Z 0

**Irradiation**  
(w/m<sup>2</sup>) 1000 constant

Diffuse Fraction  
1

Apply Irradiation Parallel to the Beam

OK Cancel Help

# Applying Wall Reflection

- Define > Boundary Conditions...

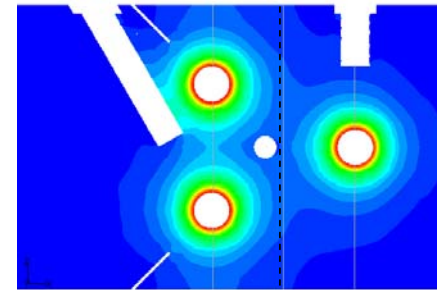
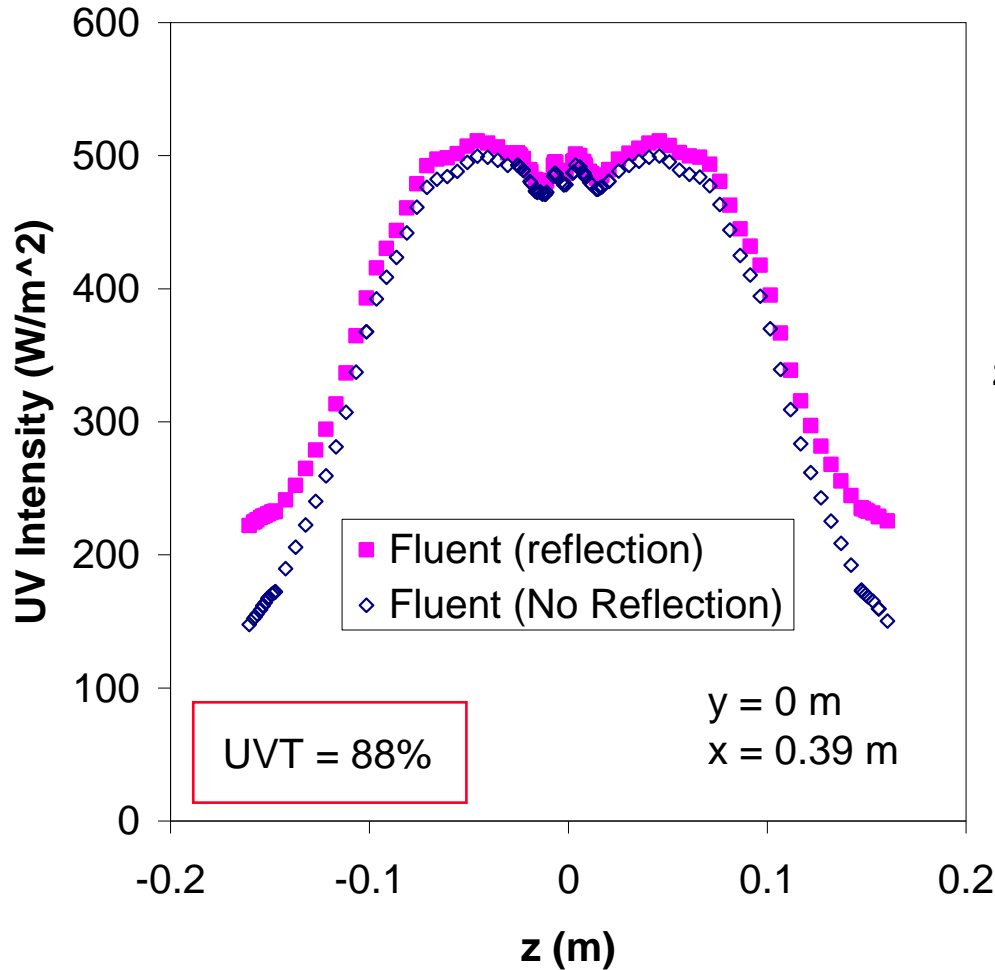
The screenshot shows the 'Wall' dialog box with the following settings:

- Zone Name: reactor\_body
- Adjacent Cell Zone: fluid
- Thermal Conditions:
  - Heat Flux (w/m2): 0, constant
  - Internal Emissivity: 0.8** (circled in red), constant
  - Wall Thickness (m): 0
  - Heat Generation Rate (w/m3): 0, constant
- Material Name: aluminum
- Shell Conduction:

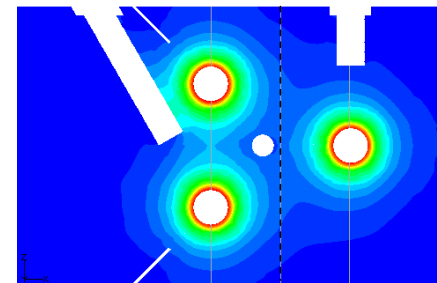
Buttons: OK, Cancel, Help

# Incident Radiation Fields

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



z With Wall Reflection  
x



No Wall Reflection

UVT=88%



# Overview

## Radiation Dose Modeling in FLUENT®

- Discrete Ordinates Radiation Model
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# Particle Tracking and Dose

- **Define injection points**
- **Define particle tracking model**
- **Define user-defined function to accumulate dose for each particle**

# Define Injections and Particle Tracking Model

- Define > Injections...

**Set Injection Properties**

Injection Name: drw

Injection Type: file

Particle Type:  Inert  Droplet  Combusting  Multicomponent  Custom

Material: anthracite | Diameter Distribution: linear | Oxidizing Species:

Evaporating Species: | Devolatilizing Species: | Product Species:

Point Properties | **Turbulent Dispersion** | Wet Combustion | Components | UDF | Multiple Reactions

**Stochastic Tracking**

Discrete Random Walk Model  
 Random Eddy Lifetime  
Number of Tries: 3  
Time Scale Constant: 0.15

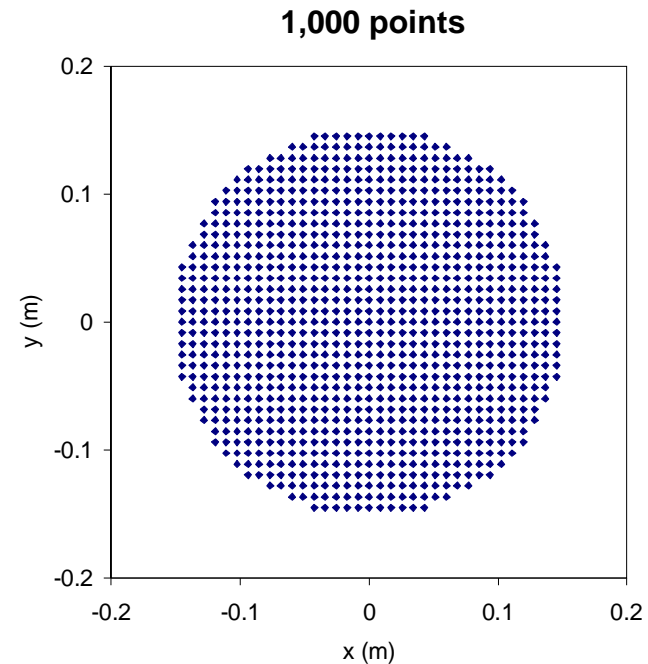
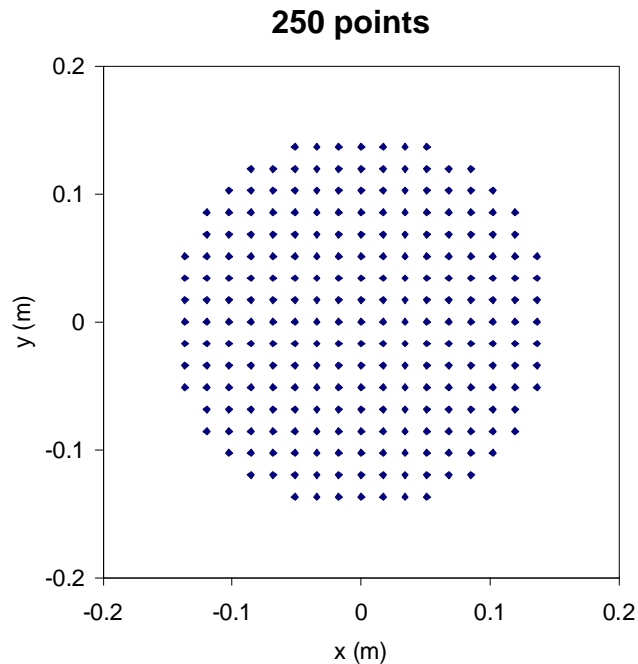
Cloud Tracking

Cloud Model  
Min. Cloud Diameter (m): 0  
Max. Cloud Diameter (m): 100000

OK File... Cancel Help

# Injection Pre-Processor

- Defines arbitrary number of injection points in a circular region (e.g., pipe inlet) and writes to a file for FLUENT
  - [www.sandia.gov/cfd-water](http://www.sandia.gov/cfd-water)

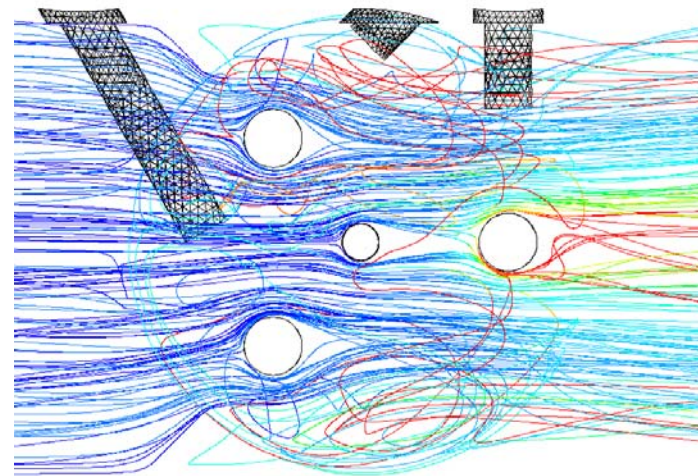
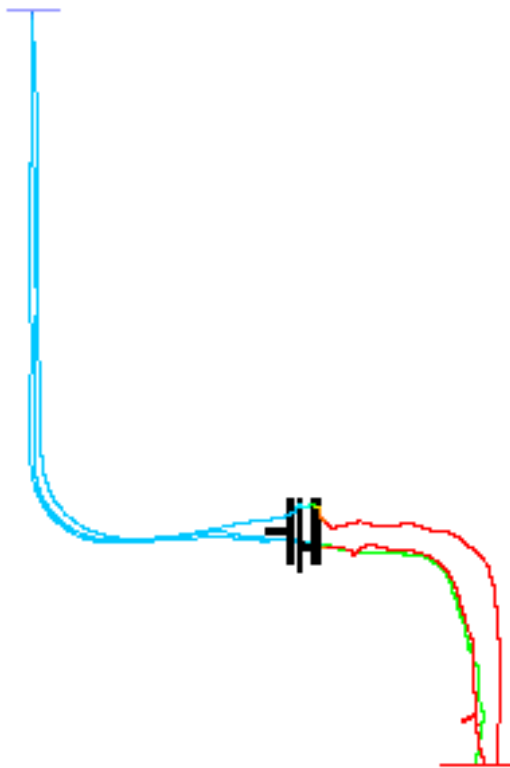




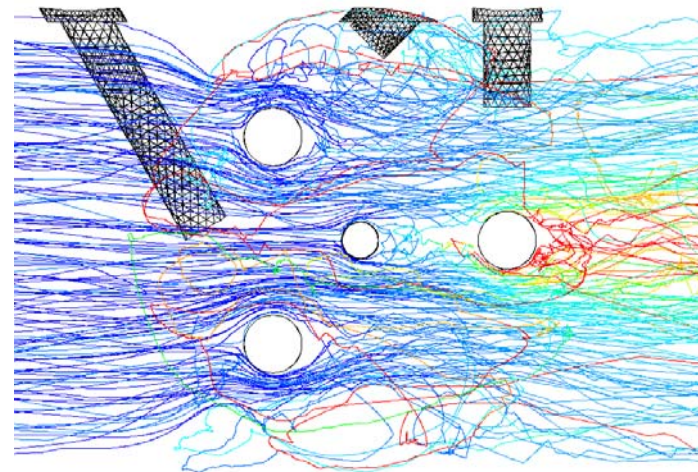


# Particle Tracking

## Discrete Random Walk model



No-DRW



DRW

Calgon 12" Sentinel® UV Reactor



# Calculating Dose from Particle Tracks



# User-Defined Function (UDF)

## Particle Dose Calculation

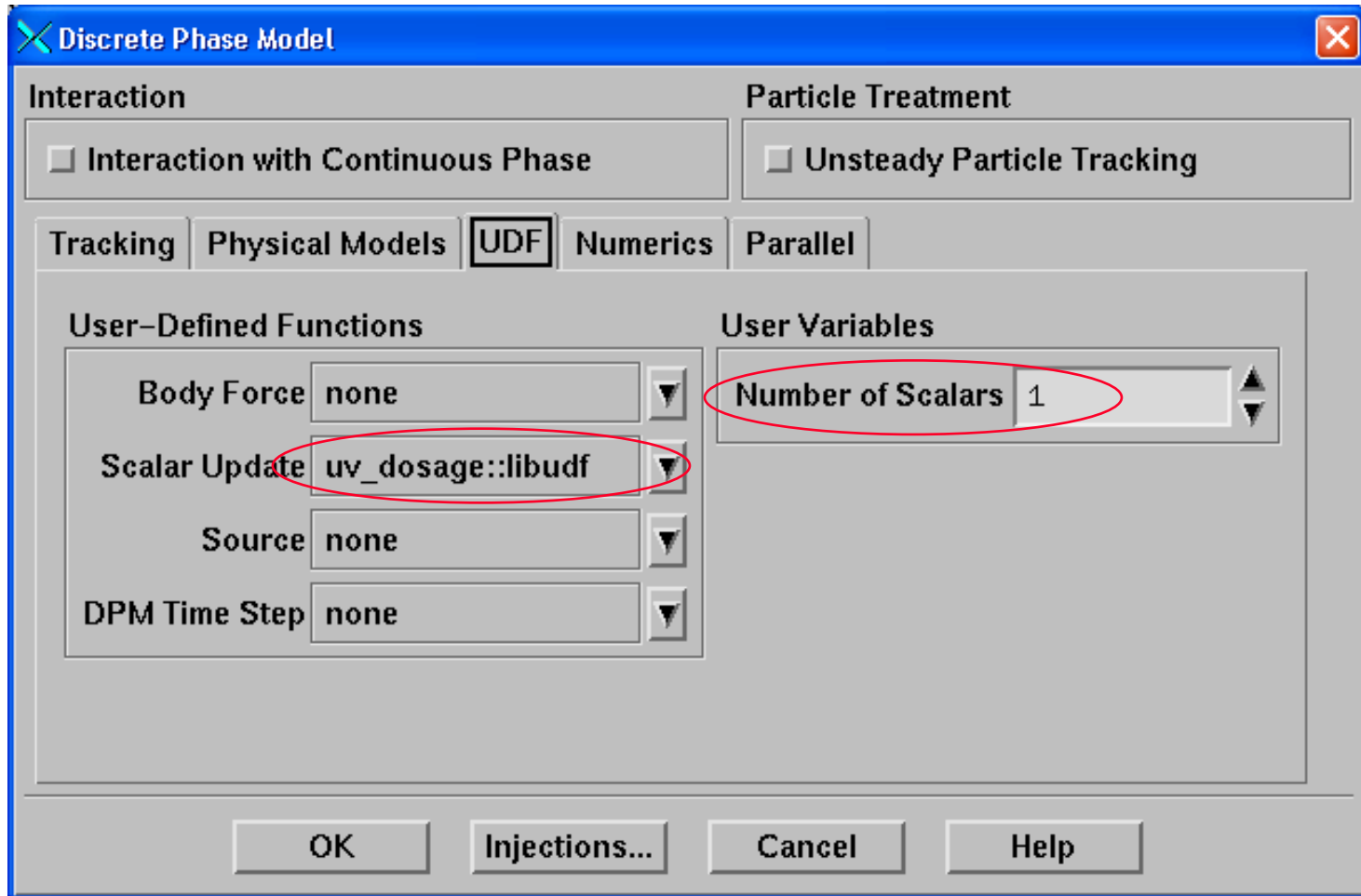
- Dose UDF (“libudf”) for Windows and Unix can be found at [www.sandia.gov/cfd-water](http://www.sandia.gov/cfd-water)
  - Extract “libudf” directory into same directory as case and data files being used in FLUENT
- Load the Dose UDF into FLUENT
  - Define > User-Defined > Functions > Compiled...
  - Specify “libudf” for the library name

*For each particle:*

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

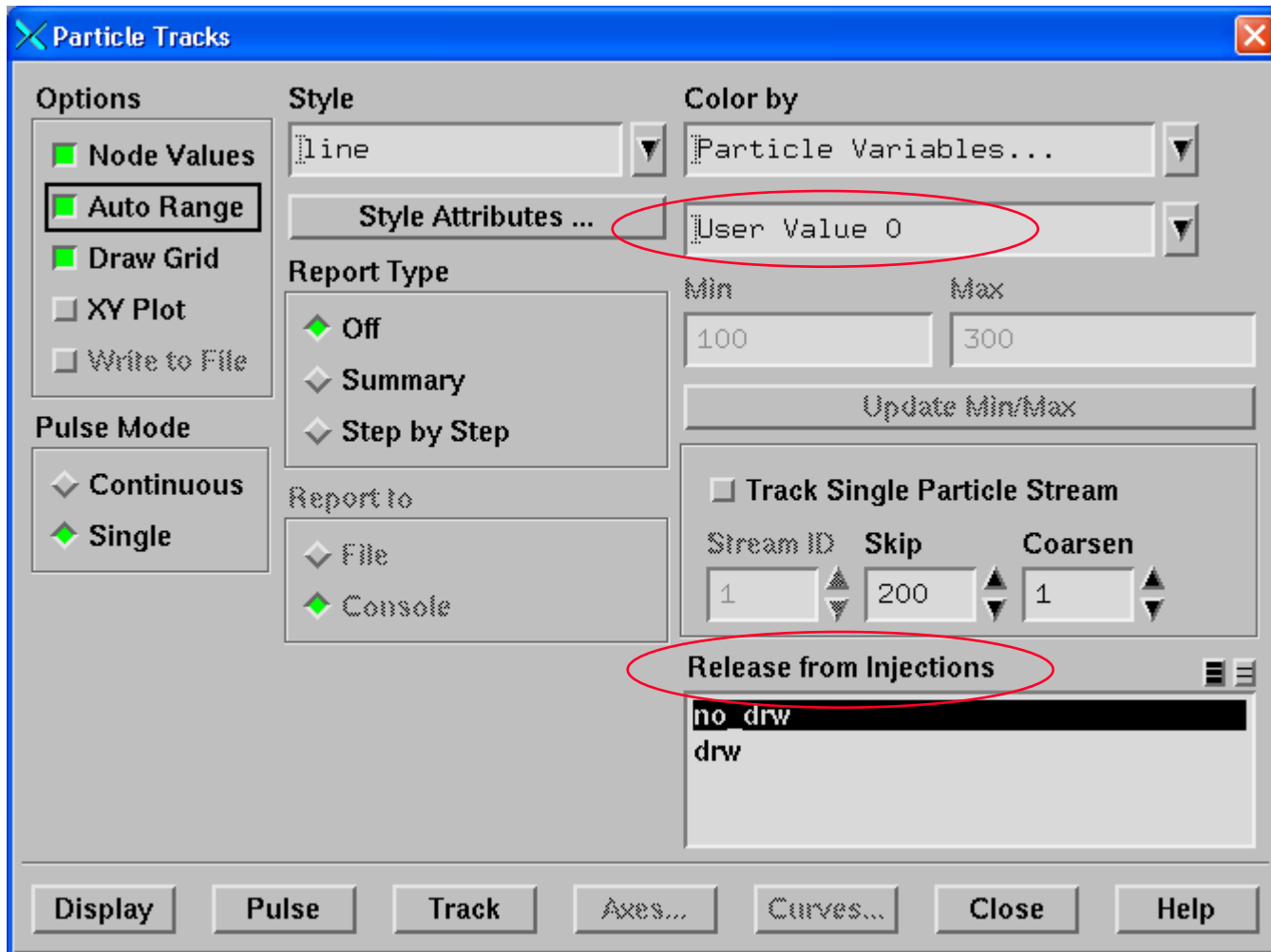
# Dose UDF Settings

- Define > Models > Discrete Phase...

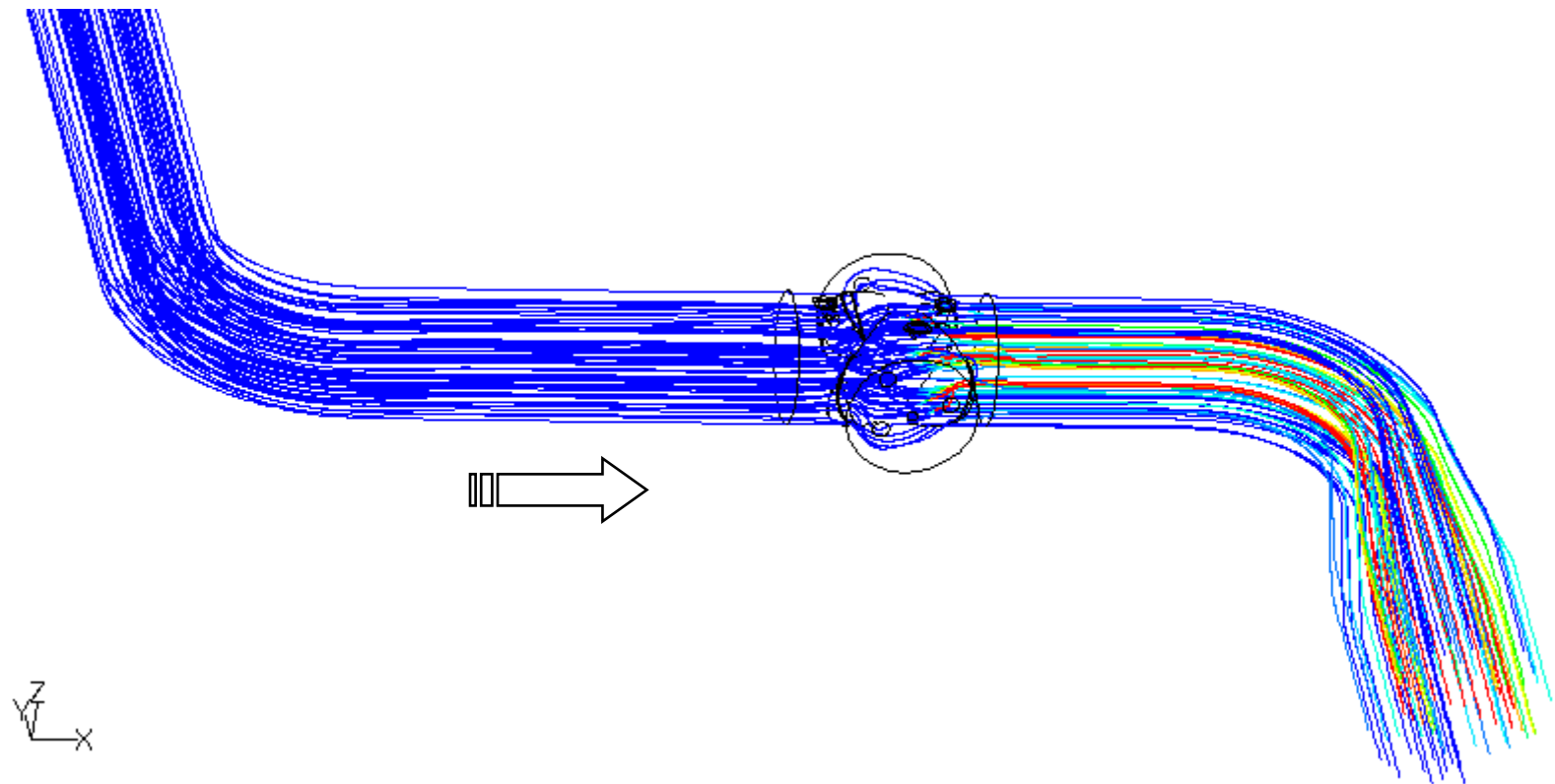


# Display Particle Tracks

- Display > Particle Tracks...

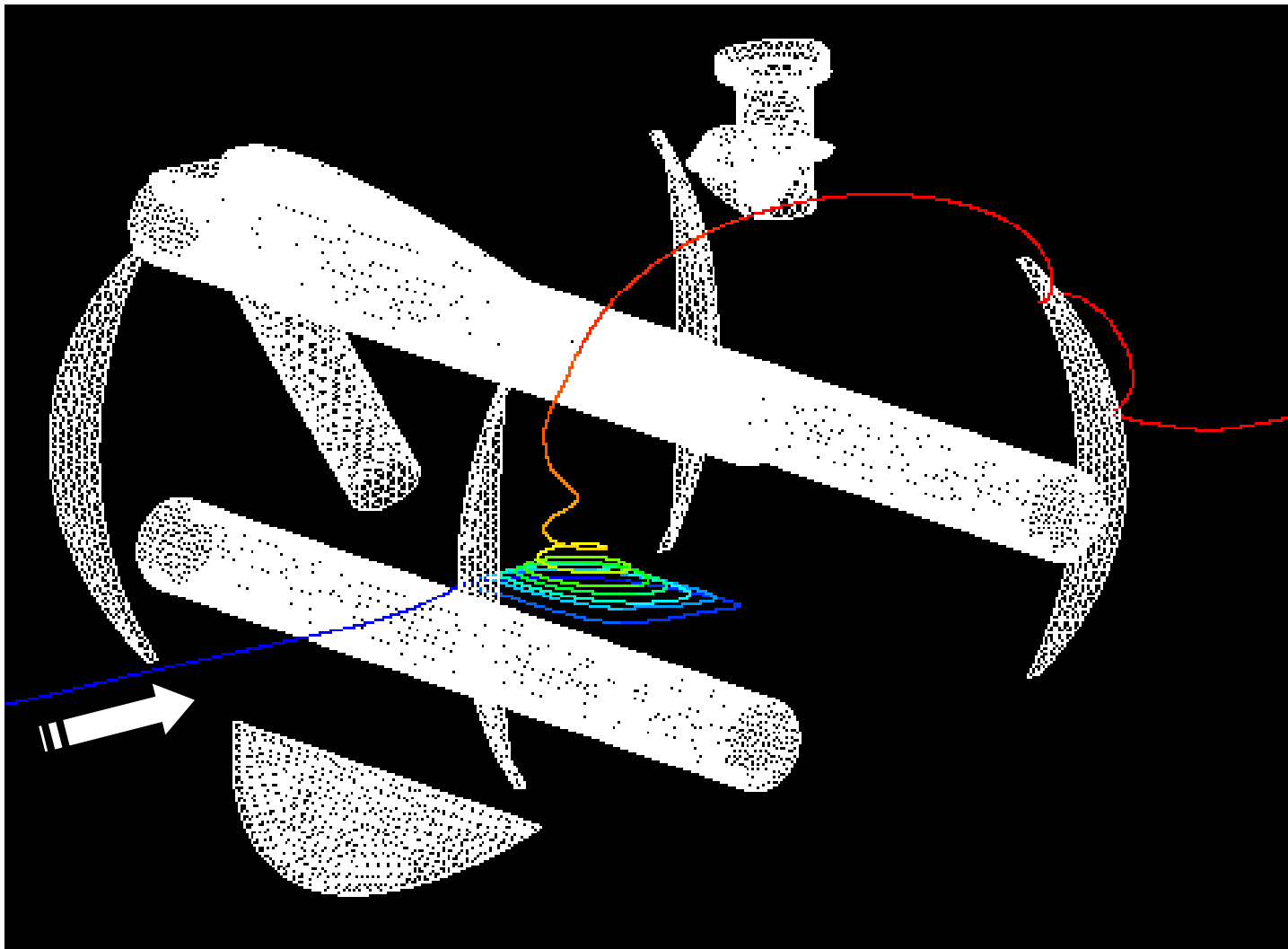


# Particle Tracks Colored by Dose



Calgon 12" Sentinel® UV Reactor

# Particle Tracks Colored by Dose

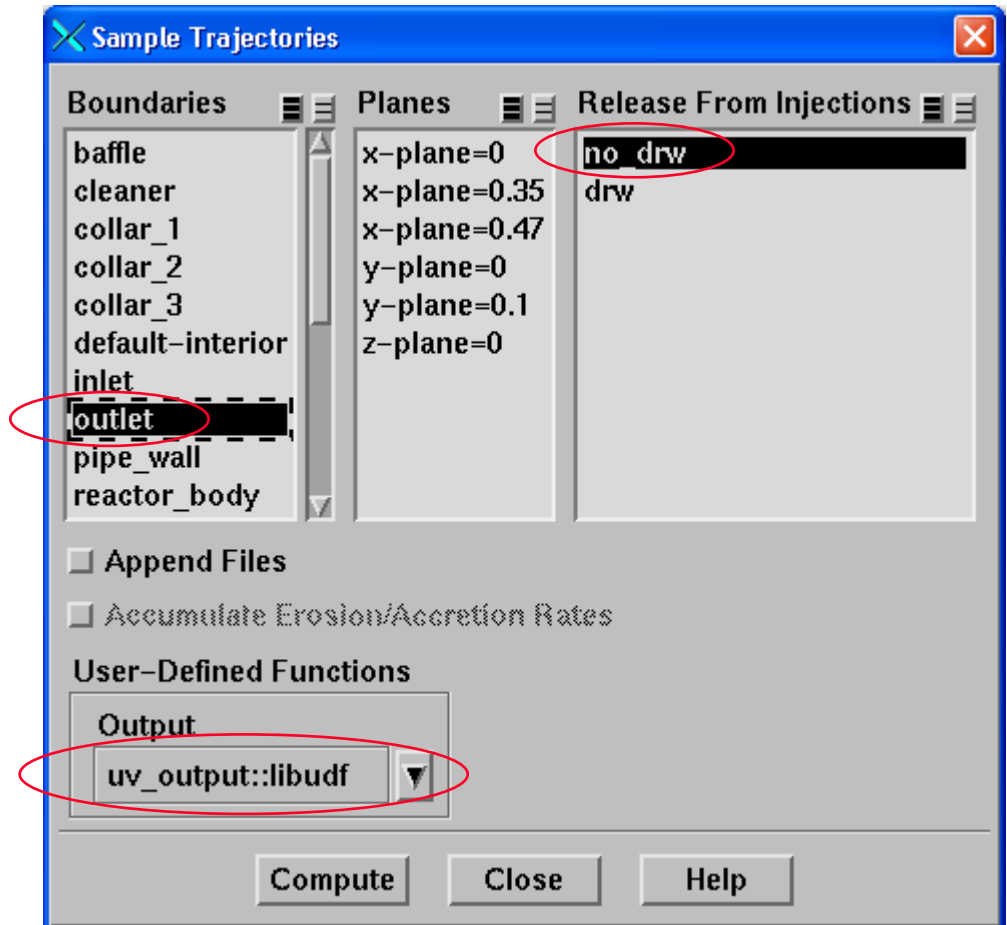


Calgon 12" Sentinel® UV Reactor

# Output Dose Results

- Report > Discrete Phase > Sample

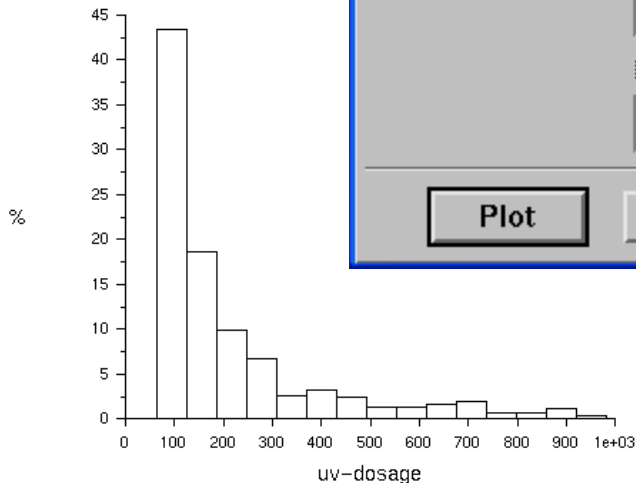
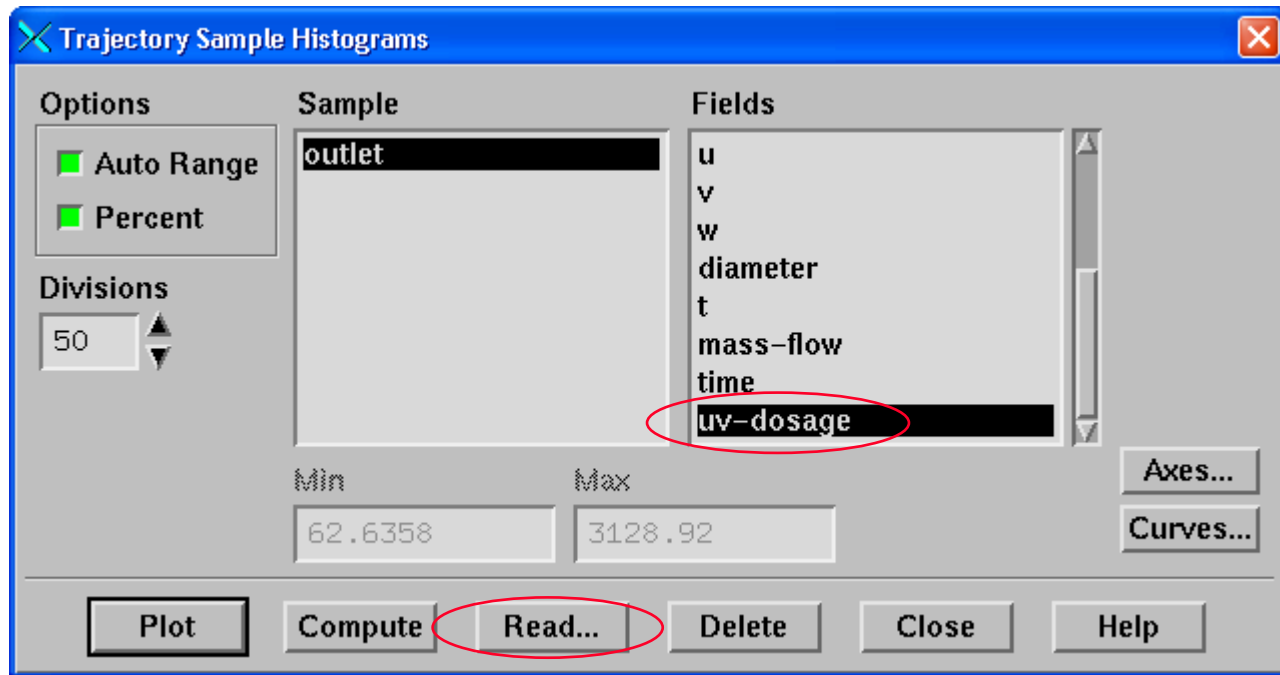
- Generates “[outlet].dpm” file
  - Cumulative particle doses ( $J/m^2$ ) are contained in this file
  - Can be read by Excel





# View Dose Histogram

- Report > Discrete Phase > Histogram





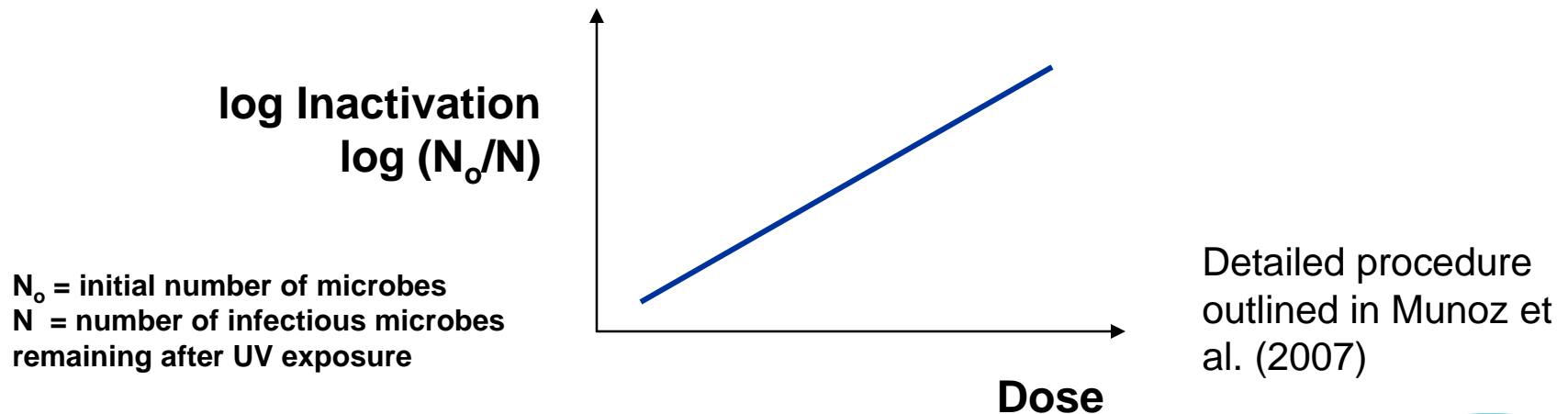
# Overview

## Radiation Dose Modeling in FLUENT®

- Discrete Ordinates Radiation Model
- Particle Tracking and Dose
- Calculation of RED

# Calculate Reduction Equivalent Dose (RED)

- Use appropriate dose-response curve to calculate survival ratio ( $N/N_0$ ) for each particle
- Sum particle survival ratios and divide by total number of particles to yield cumulative survival (and inactivation) ratios
- Use dose-response curve to get RED



# RED Post-Processors

- Takes data from “[outlet].dpm” and calculates RED and log inactivation
- Available at [www.sandia.gov/cfd-water](http://www.sandia.gov/cfd-water)
  - (1) Windows-based executable and source file
  - (2) Excel spreadsheet

Output from FluentRED.exe

```
Realization, Particles, log_Inactivation(log(No/N)), RED
  1,      781,    9.2072E-01,    1.6130E+01
  2,      782,    9.5080E-01,    1.6719E+01
  3,      780,    9.5016E-01,    1.6706E+01
  4,      780,    9.4099E-01,    1.6526E+01
  5,      780,    9.5880E-01,    1.6876E+01
```

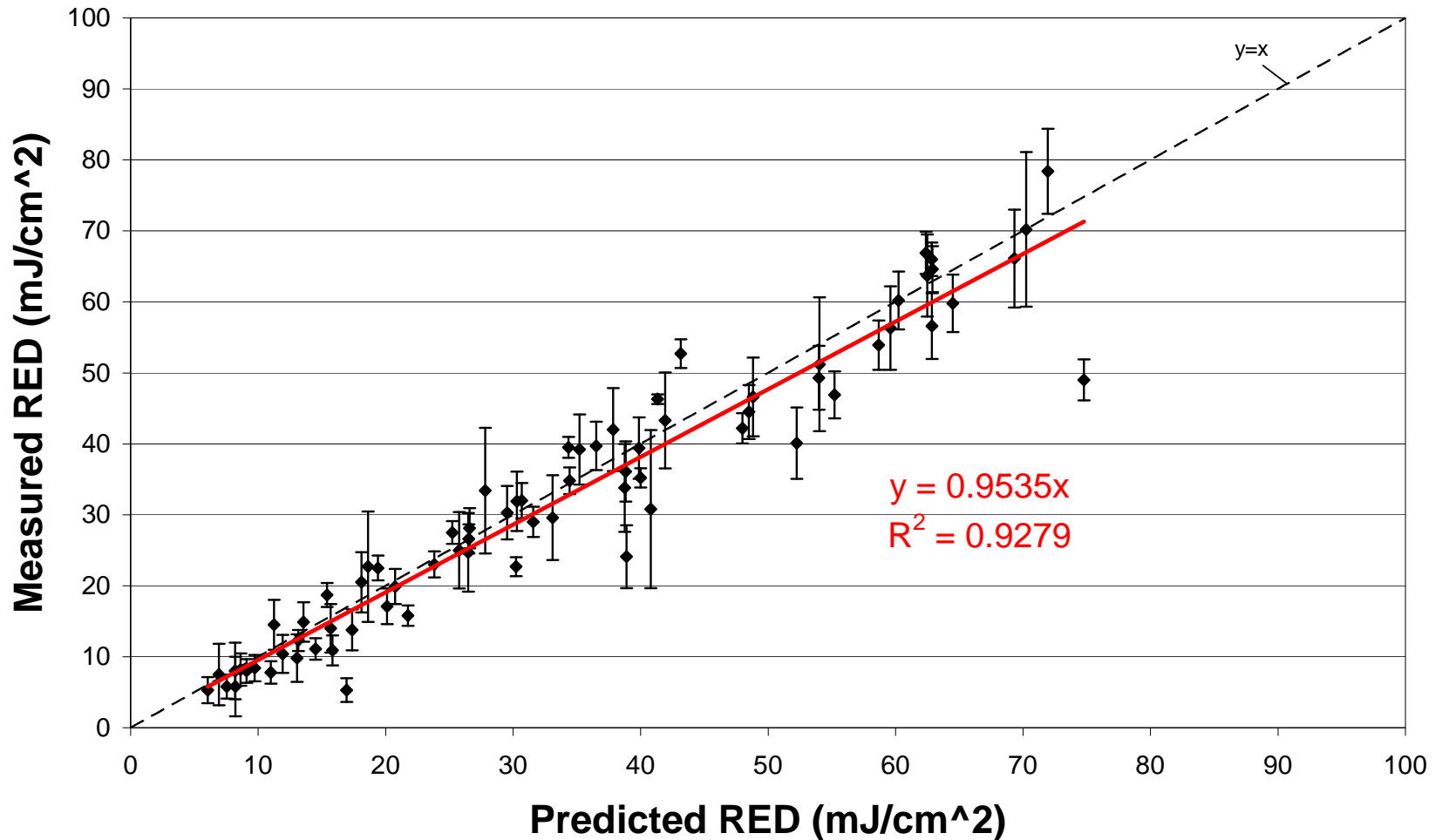
```
-----
Number of realizations =      5
t-value = 2.770
Mean RED = 1.6591E+01 mJ/cm^2
Standard Deviation of RED = 2.8613E-01
Standard Error of RED = 1.2796E-01
95% confidence interval (plus/minus) = 3.5452E-01
```



# **So now we have a simulated RED... Now what???**

- **Compare simulated RED to measured RED**
  - Evaluate the model
- **Use simulated RED as a metric to compare alternative reactor/piping designs**
  - Installed vs. validated configurations

# Measured RED vs. Simulated RED





# Summary

- **Simulating UV dose distributions in FLUENT**
  - **Discrete ordinates radiation model in FLUENT generates UV incident radiation field**
    - **Honors geometry used in hydraulic CFD simulation (e.g., shadowing, reflection)**
  - **Particle tracking yields dose distribution**
  - **Dose distribution yields RED**
- **Tutorial and tools are available at:**
  - **[www.sandia.gov/cfd-water](http://www.sandia.gov/cfd-water)**

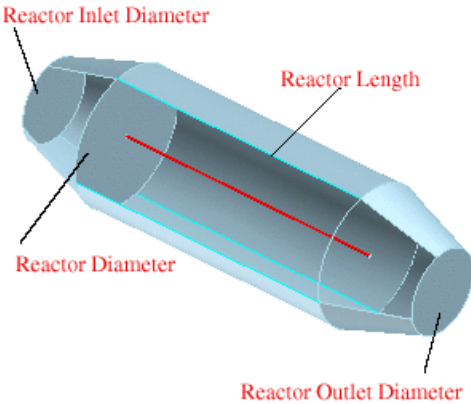
# FluentUV

- Wizard-like template for generating models and grids of UV reactors and piping in FLUENT
- Muhammad.Sami@ansys.com

**Custom Reactor: Circular Cross Section**

Length Unit Selected is:

Reactor Diameter	<input type="text" value="5"/>
Reactor Length	<input type="text" value="10"/>
Number Of Lamps	<input type="text" value="1"/>
Lamp Diameter	<input type="text" value="0.0833333"/>
Reactor Inlet Diameter	<input type="text" value="3"/>
Reactor Outlet Diameter	<input type="text" value="3"/>



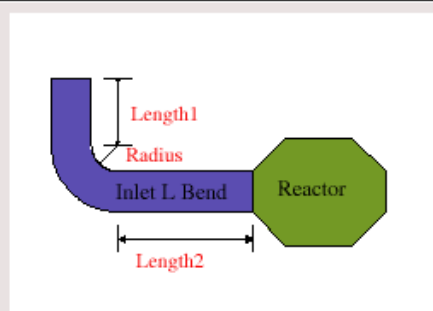
Reset to Default Values

Previous Next

**Inlet Piping**

Length Unit Selected is:

Inlet Piping



Length1	<input type="text" value="4"/>
Radius	<input type="text" value="2"/>
Length2	<input type="text" value="4"/>

Reset

Previous Next....(Outlet Piping)





# Acknowledgments

- **AwwaRF (Project #4107)**
  - **Alice Fulmer, Project Manager**
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  - **Brian Bernados, Joel Ducoste, Steve Deem, Dennis Greene, Michael Montysko**
- **Calgon Carbon Corporation**
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- **Infilco Degremont, Inc. (DENARD)**
  - **Robert Kelly and Bruno Ferran**
- **Trojan Technologies Inc.**
  - **Ted Mao**

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