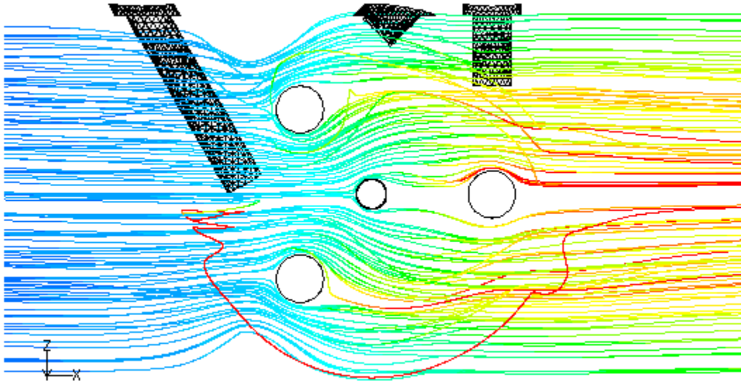
February 28, 2009

Radiation Dose Modeling in FLUENT®

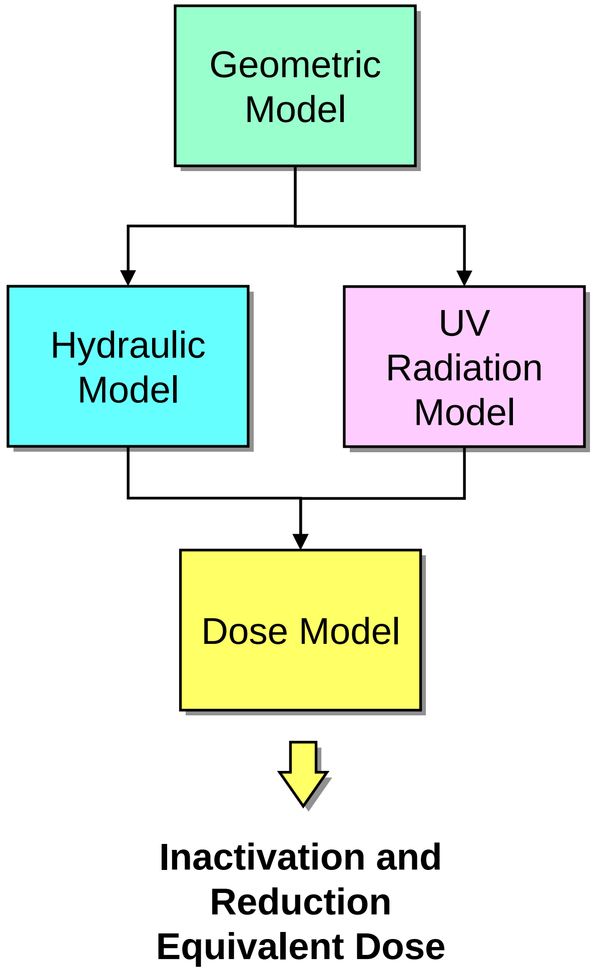


Clifford K. Ho

Sandia National Laboratories
Albuquerque, NM

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.

Modeling Approach



Overview

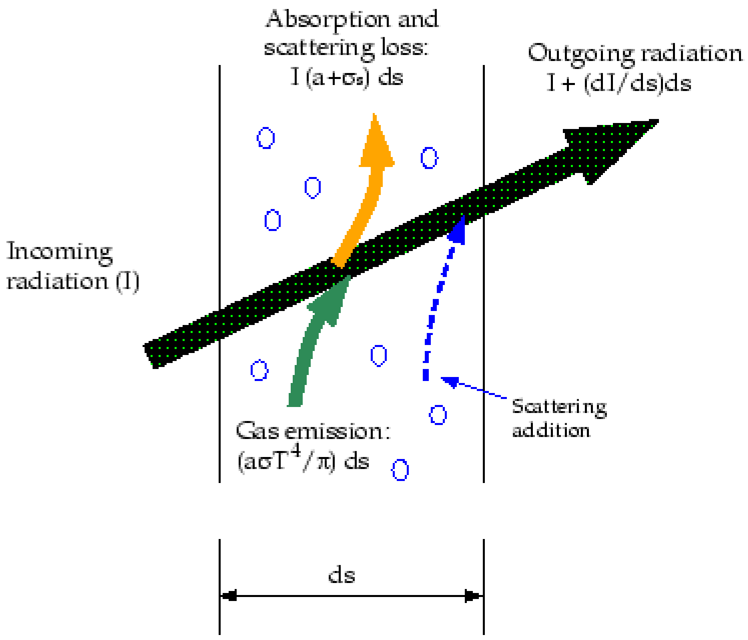
Radiation Dose Modeling in FLUENT®

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

Sandia National Laboratories

Discrete Ordinates Radiation Model

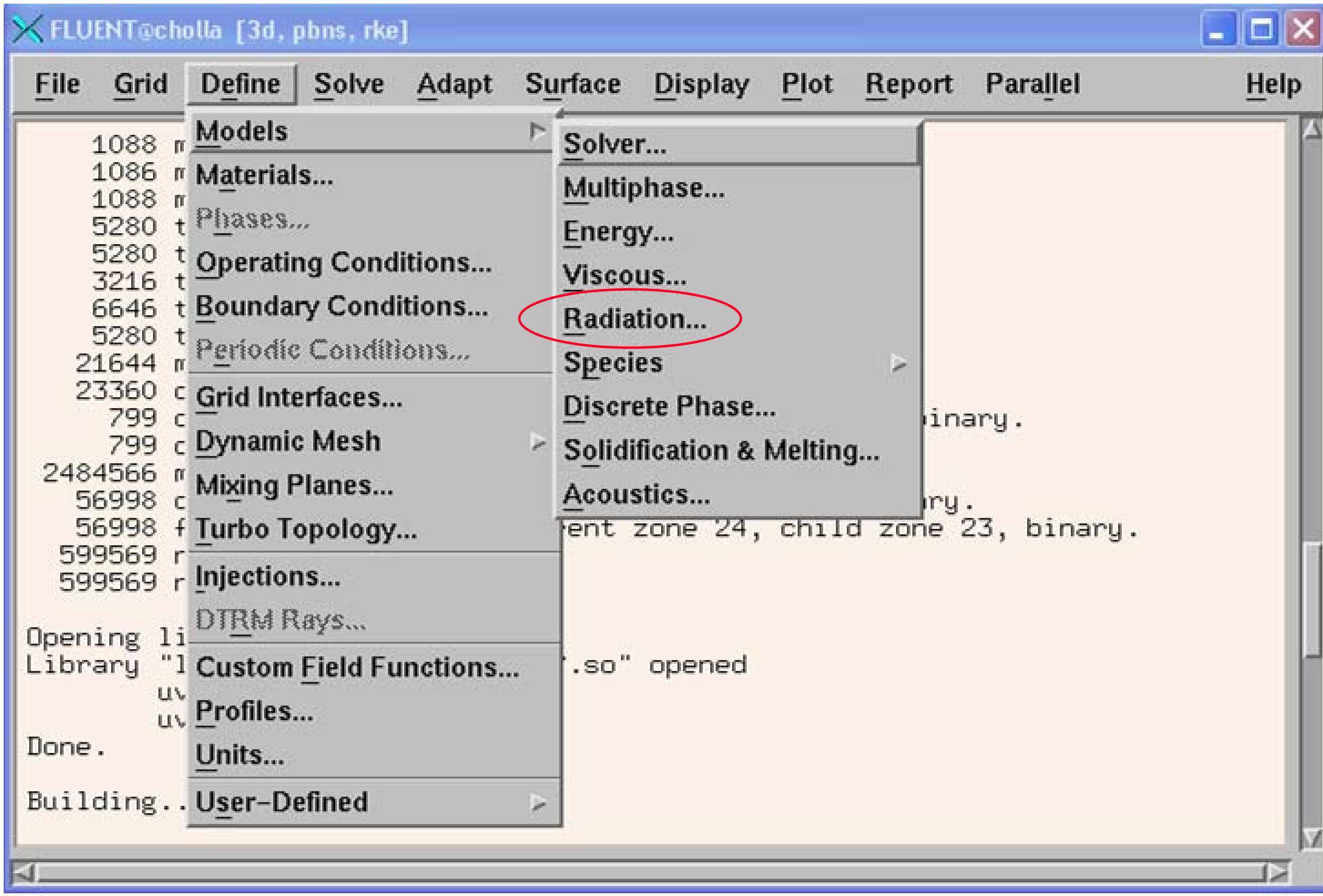
- **Solves the radiative transfer equation over a domain of discrete solid angles**
- **Calculates radiation intensity as a function of absorption, scattering, reflection, and emission**
- **Integrated within FLUENT CFD/hydraulic model**
  - **Impacts of geometry within the reactor (shadowing, reflection)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



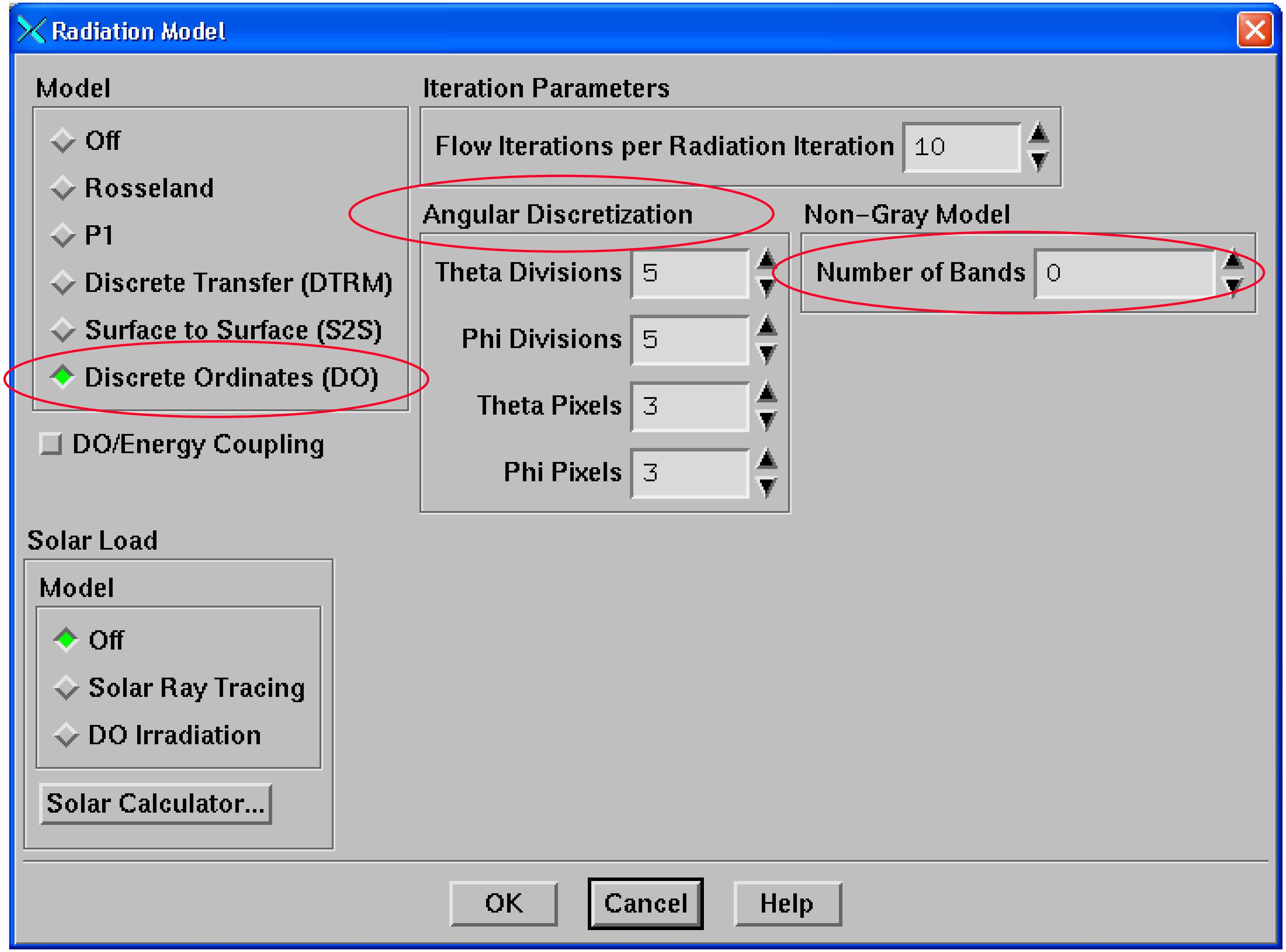
Step-by-Step Guide

www.sandia.gov/cfd-water

Turn on Radiation Model in FLUENT



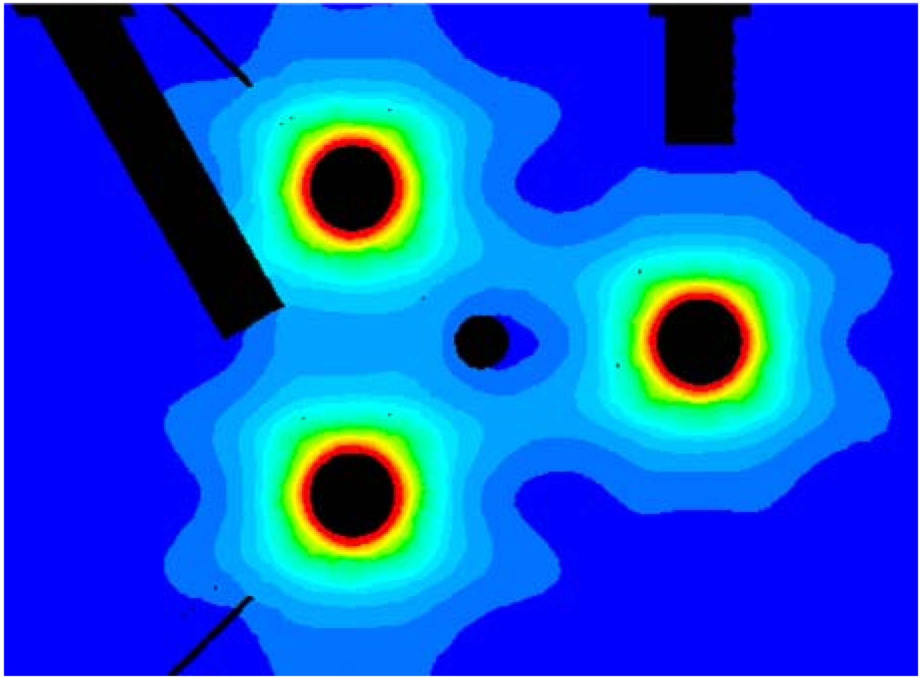
DO Model Parameters



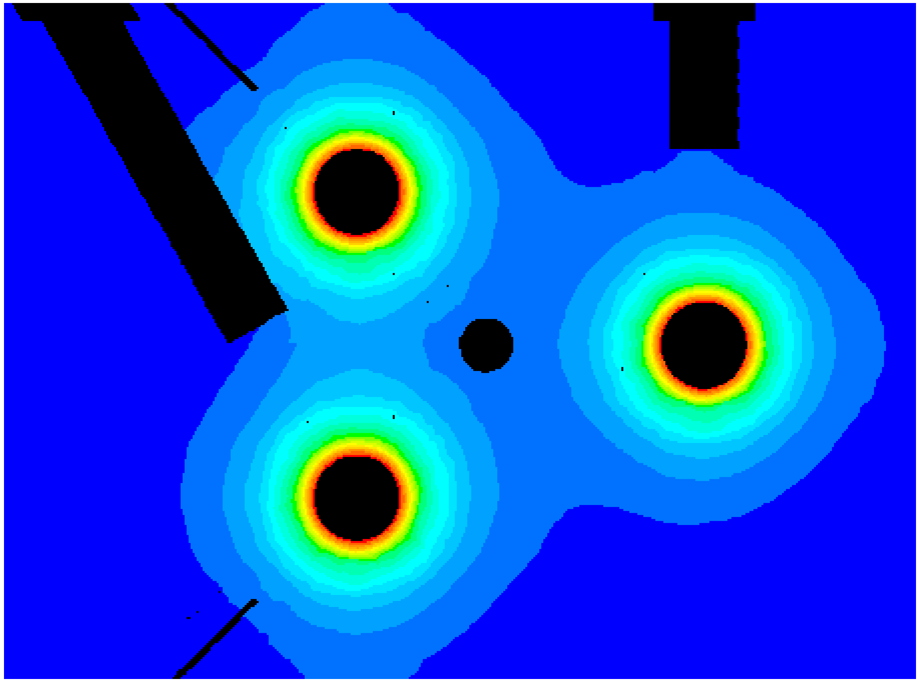
Sandia National Laboratories

Impact of Theta x Phi Discretization on Simulated Incident Radiation Field

theta x phi = 2 x 2



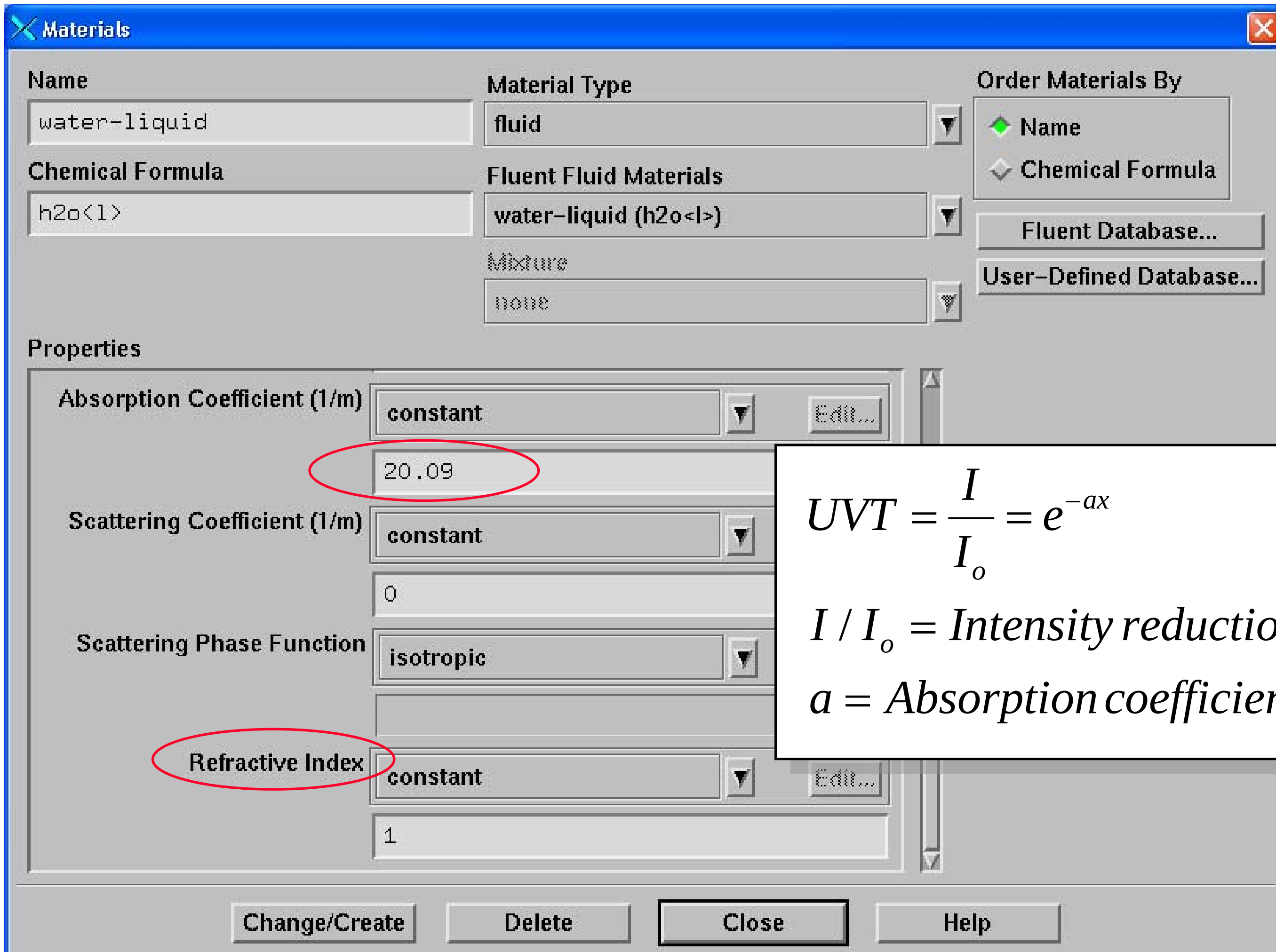
theta x phi = 5 x 5



Calgon 12” Sentinel® UV Reactor

Specify UV Transmittance of Water

- **Define > Materials...**



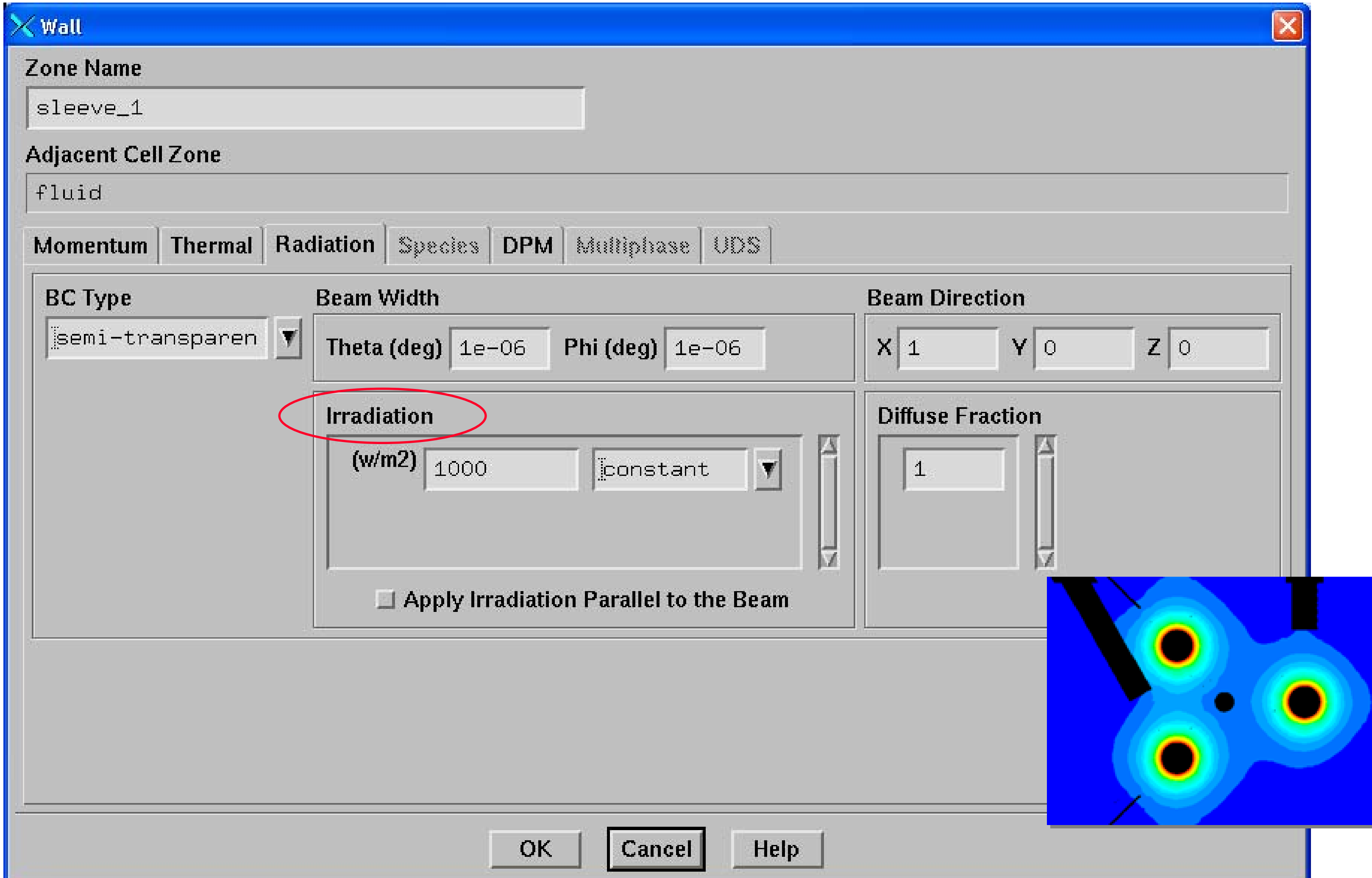
$$UVT = \frac{I}{I_o} = e^{-ax}$$

$$I / I_o = Intensity\ reduction\ at\ x = 1cm$$

$$a = Absorption\ coefficient\ (1/m)$$

Specify UV Radiation Boundary Condition

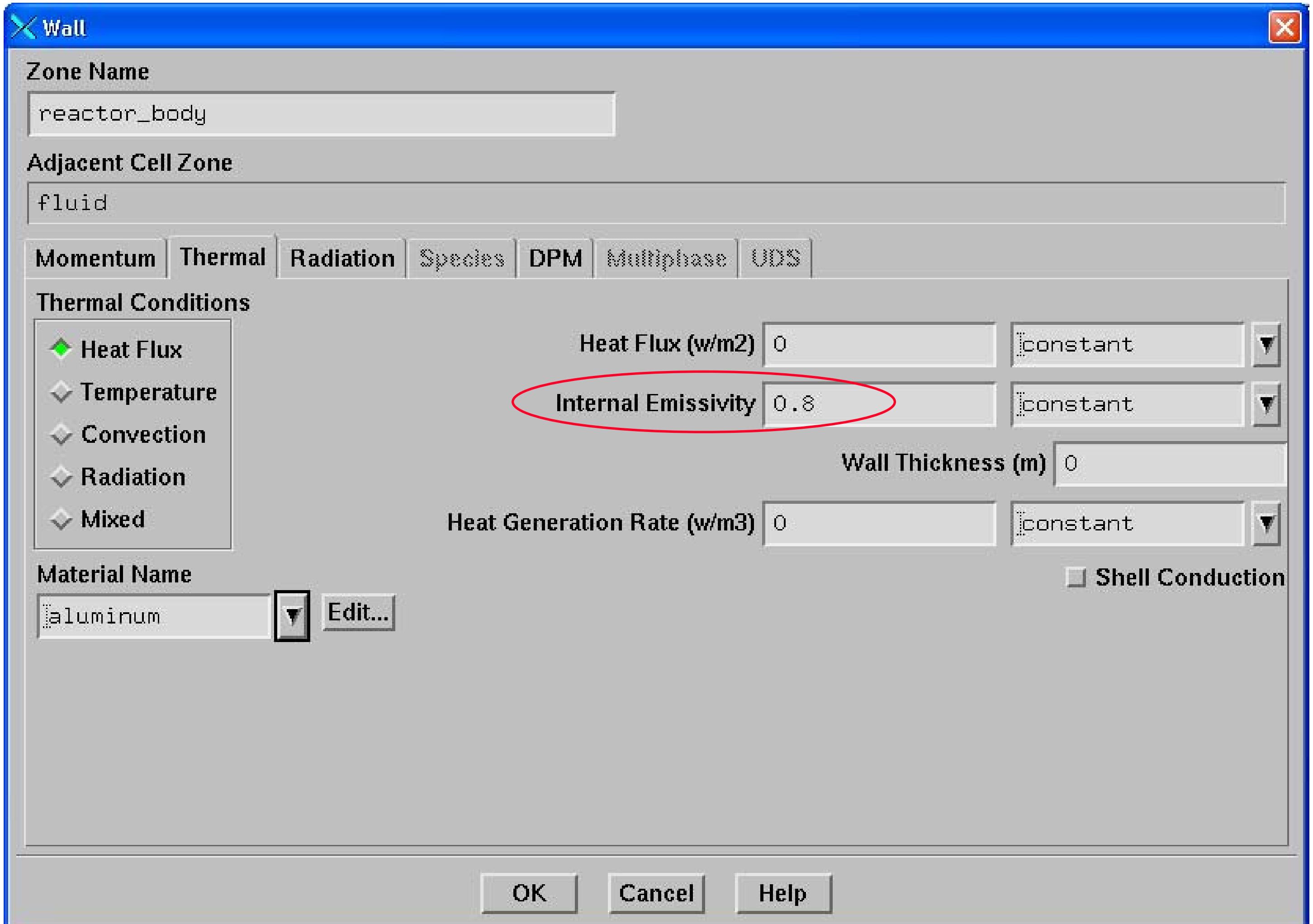
- **Define > Boundary Conditions...**



Sandia National Laboratories

Applying Wall Reflection

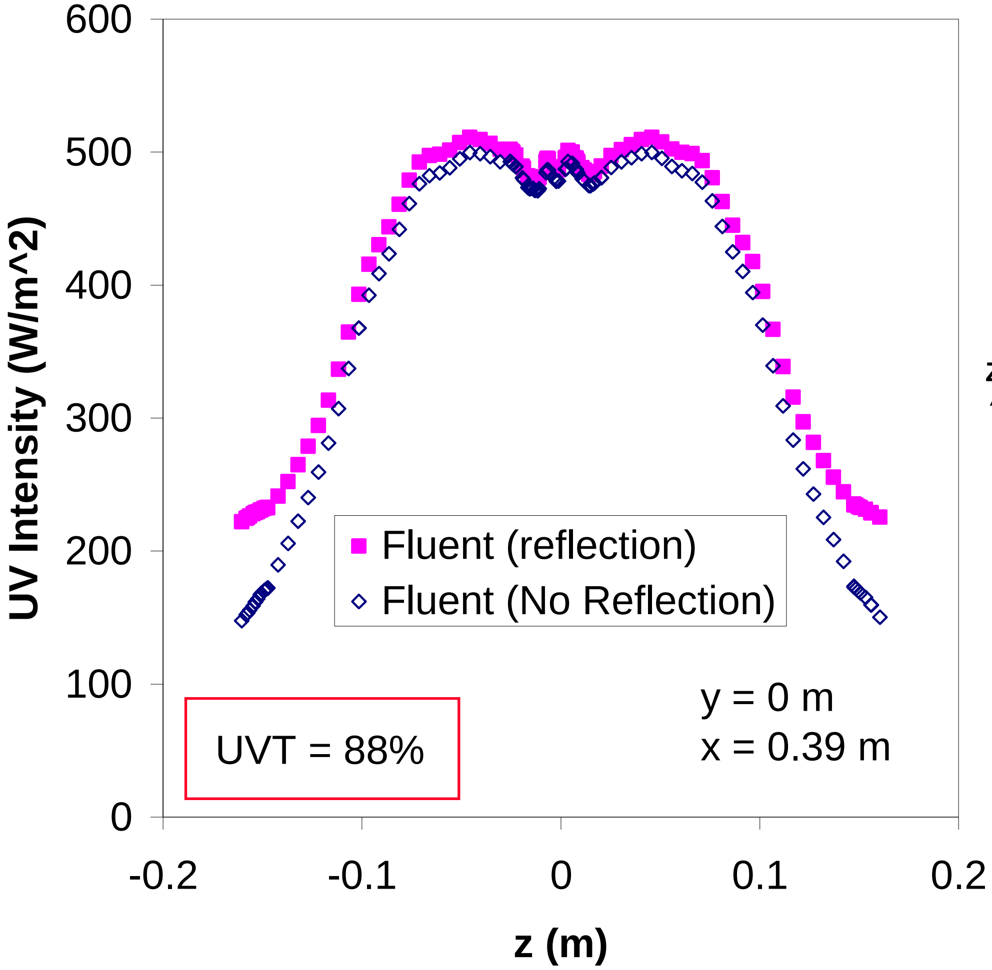
- **Define > Boundary Conditions...**

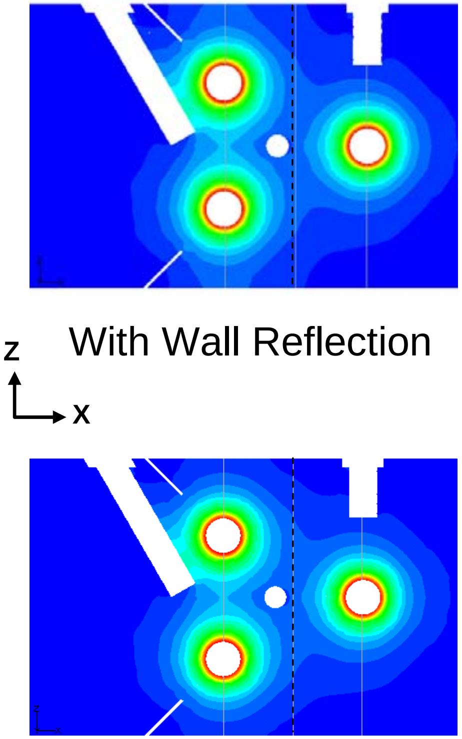


Incident Radiation Fields

Simulated UV radiation field with and without wall reflection

(Calgon 12” Sentinel® UV Reactor)





With Wall Reflection

No Wall Reflection

UVT=88%

Overview

Radiation Dose Modeling in FLUENT®

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

Sandia National Laboratories

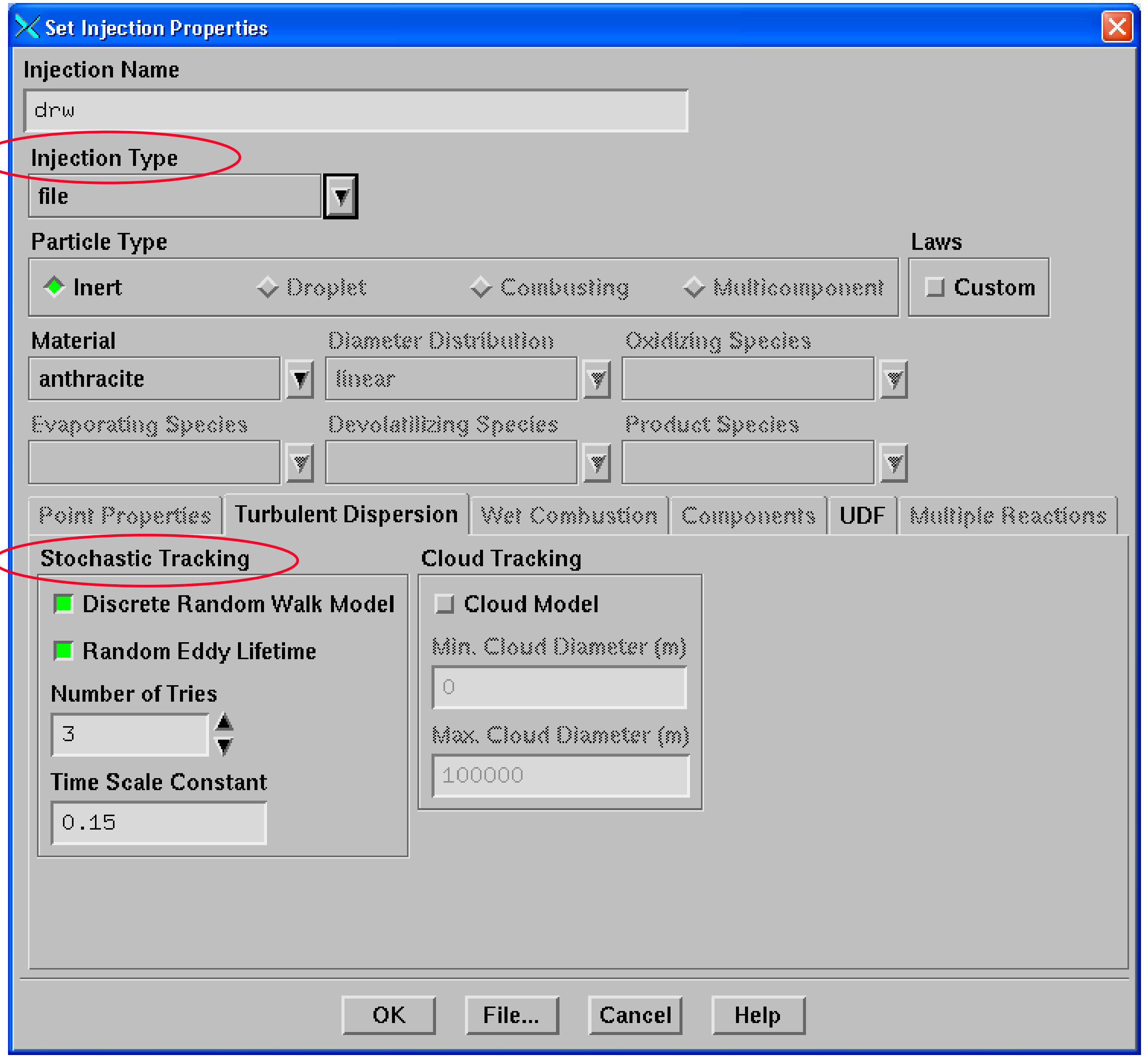
Particle Tracking and Dose

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

Sandia National Laboratories

Define Injections and Particle Tracking Model

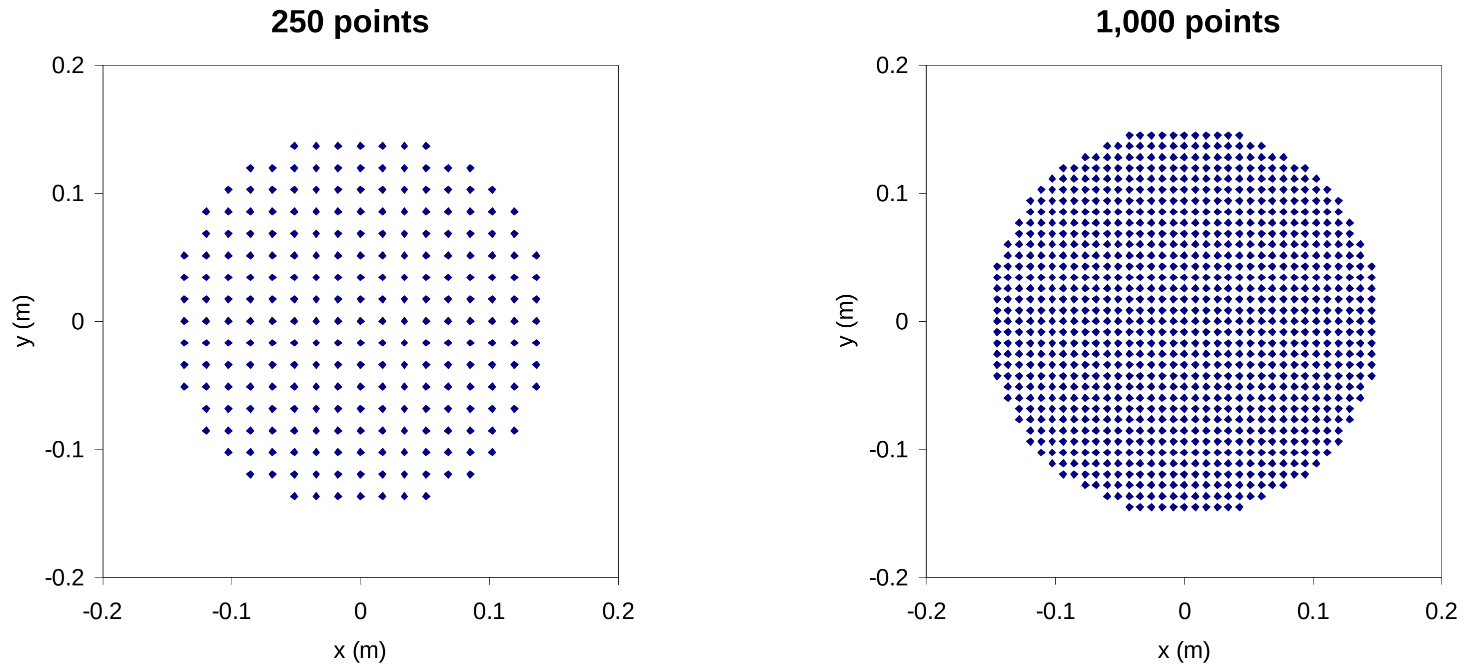
- **Define > Injections...**



Sandia National Laboratories

Injection Pre-Processor

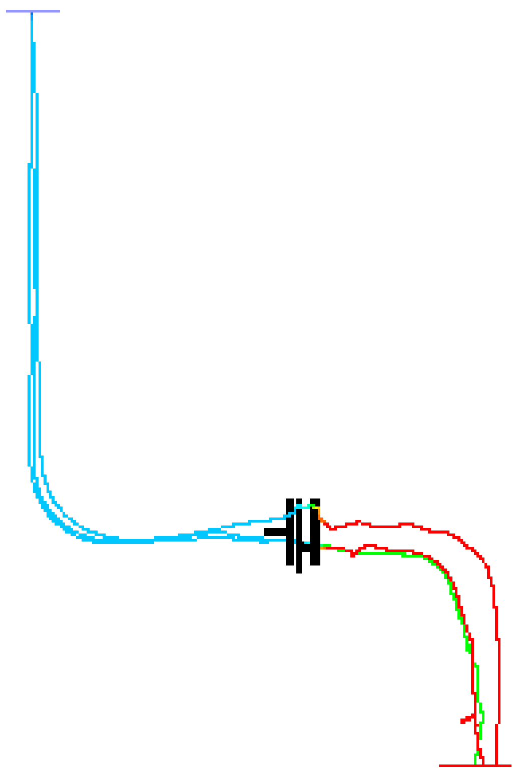
- **Defines arbitrary number of injection points in a circular region (e.g., pipe inlet) and writes to a file for FLUENT**
  - www.sandia.gov/cfd-water

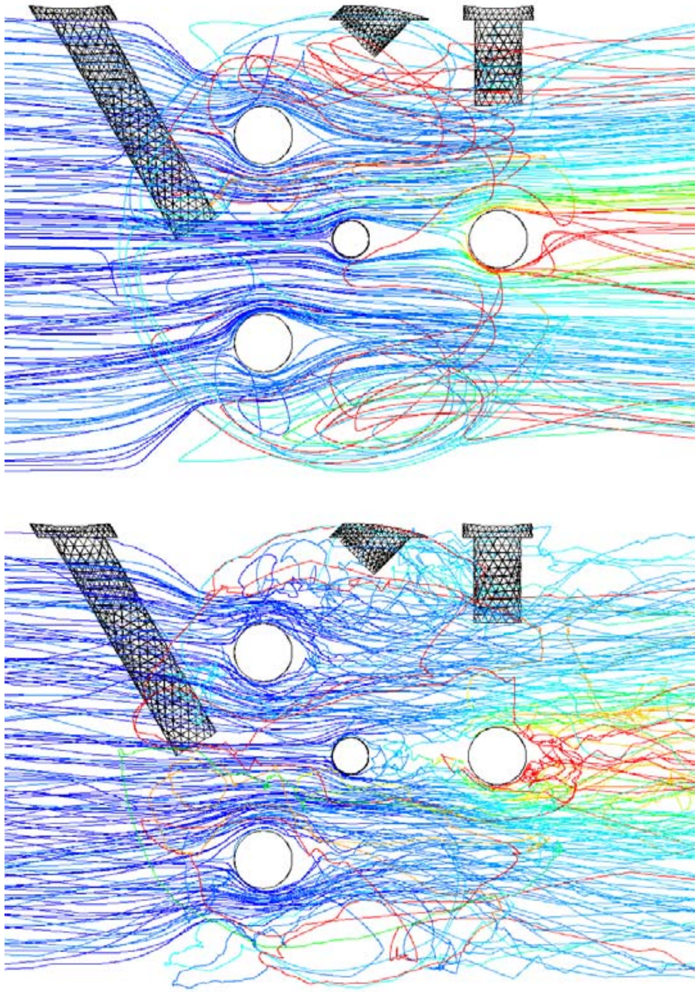


Sandia National Laboratories

Particle Tracking

Discrete Random Walk model





No-DRW

DRW

Calgon 12” Sentinel® UV Reactor

Calculating Dose from Particle Tracks

Sandia National Laboratories

User-Defined Function (UDF)

Particle Dose Calculation

- **Dose UDF (“libudf”) for Windows and Unix can be found at 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**

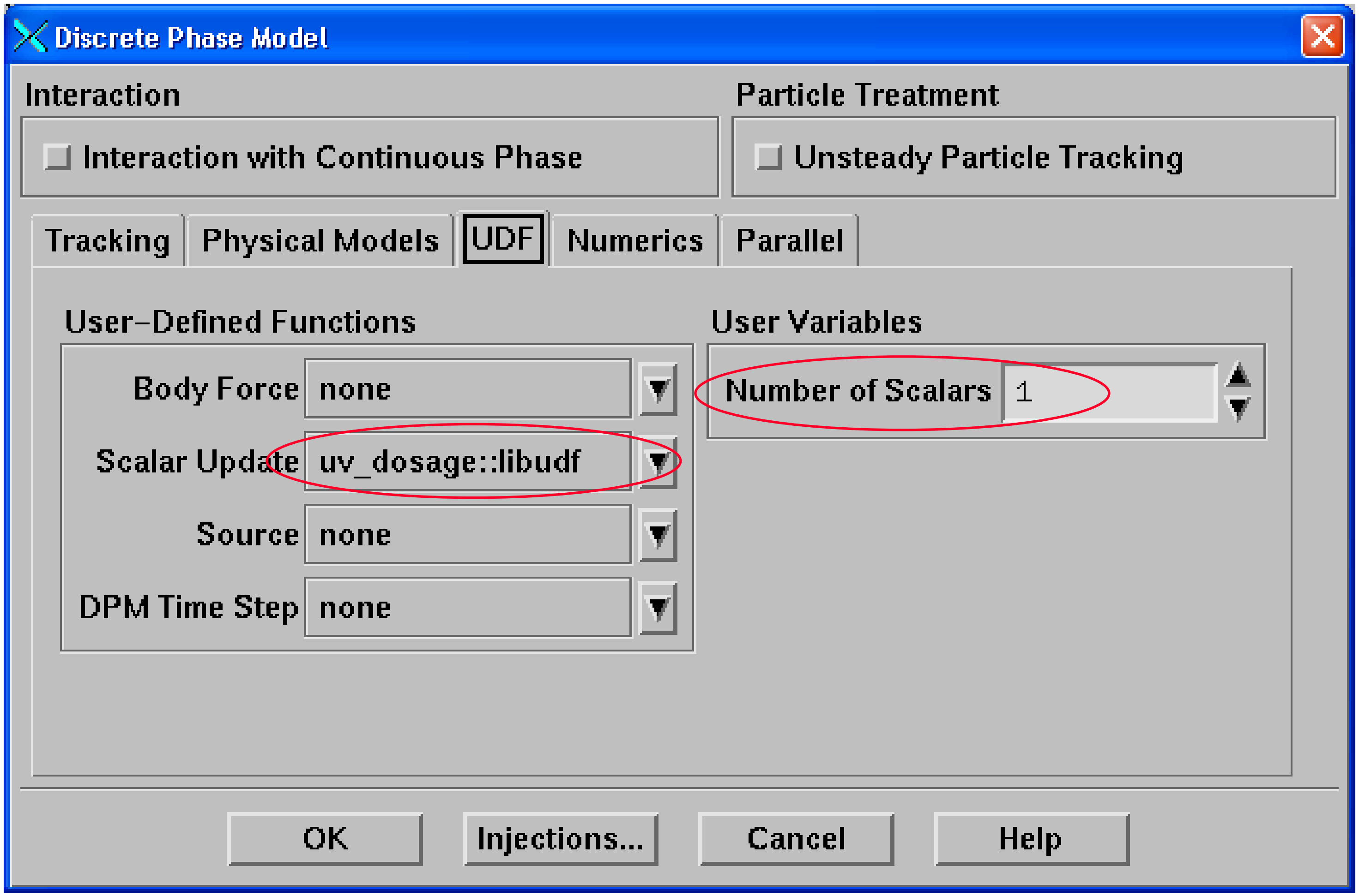
For each particle:

Dose (J/m^2) = Incident radiation (W/m^2) x Exposure time (s)

Sandia National Laboratories

Dose UDF Settings

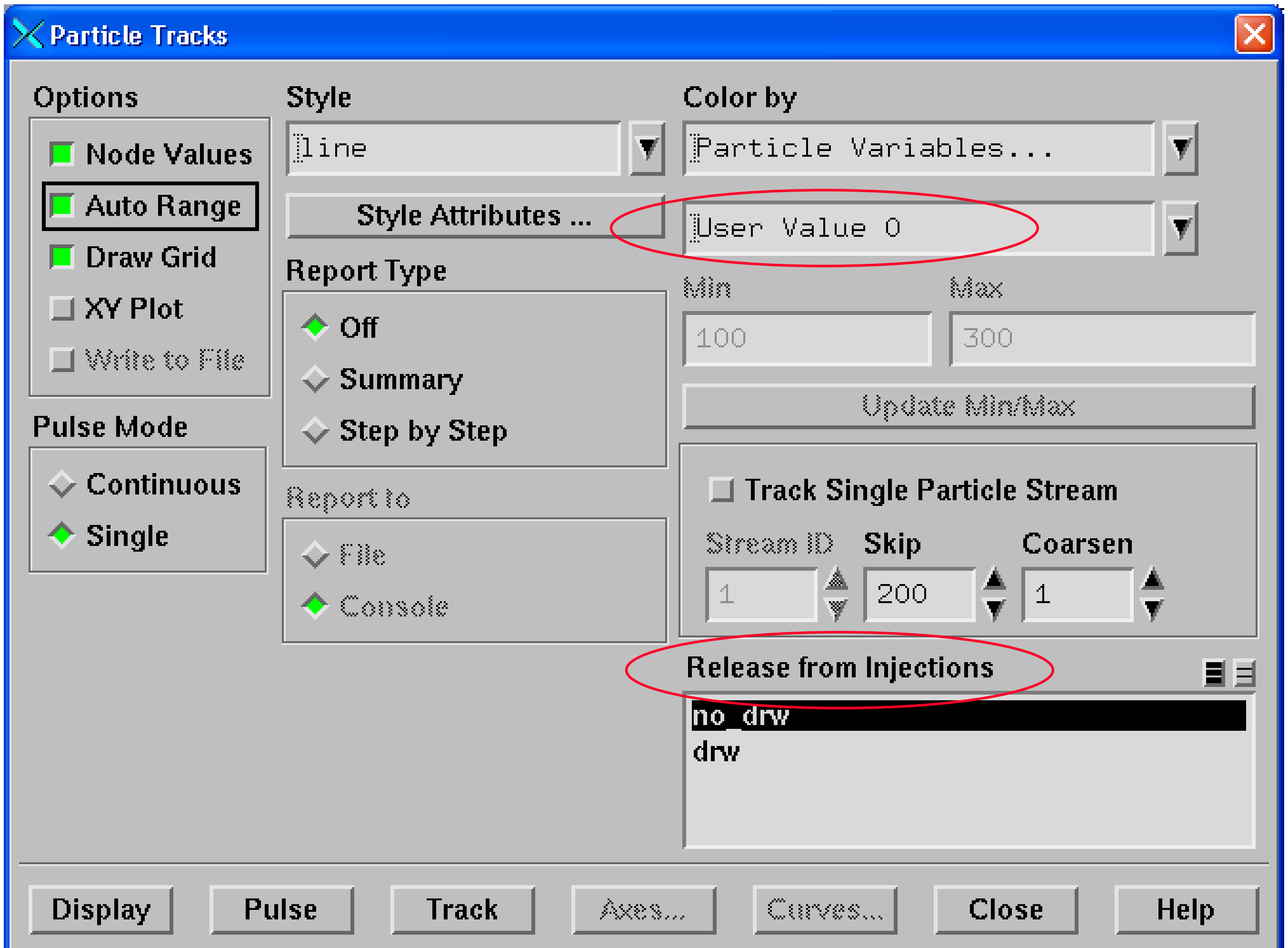
- **Define > Models > Discrete Phase...**



Sandia National Laboratories

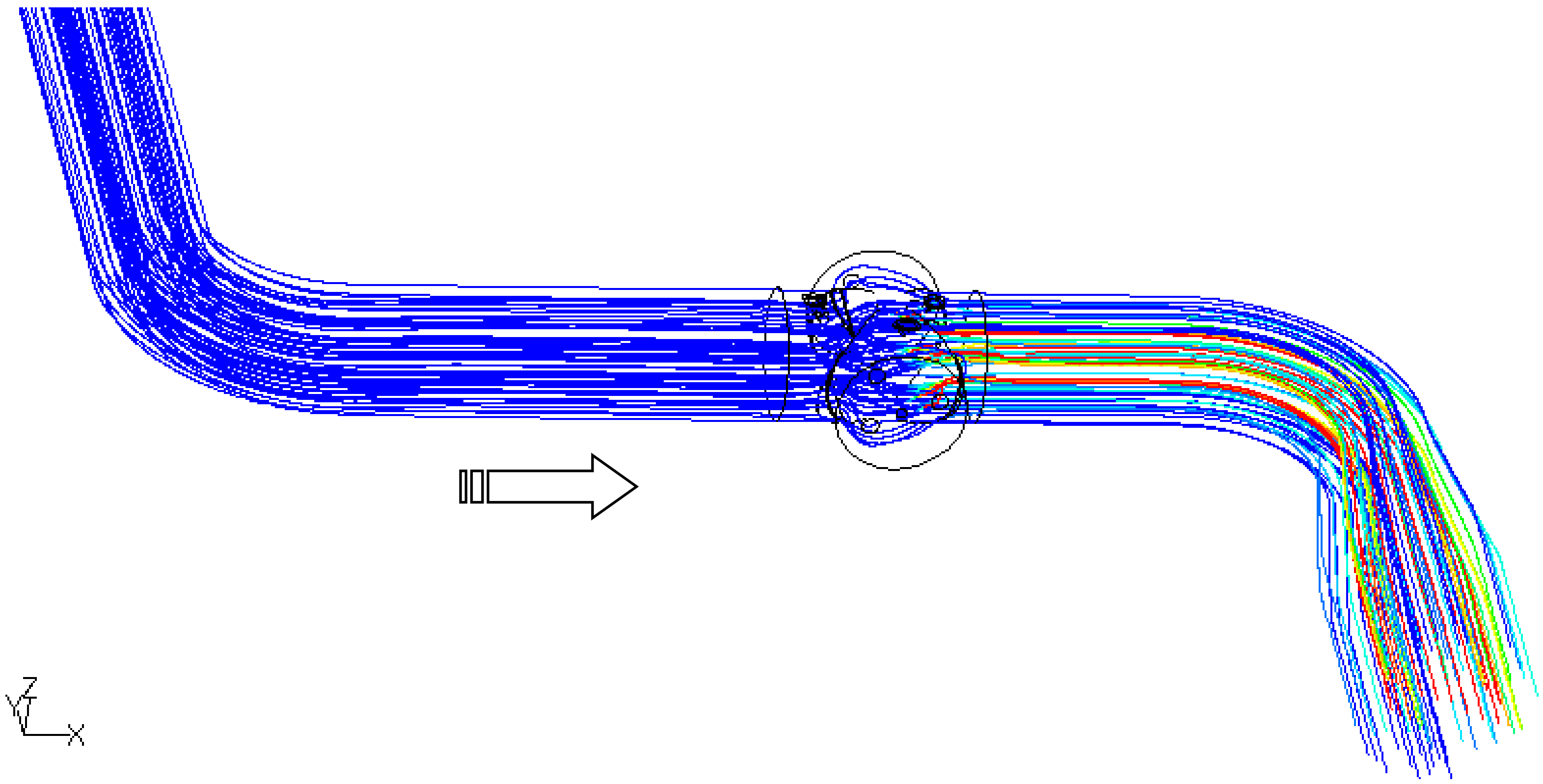
Display Particle Tracks

- **Display > Particle Tracks...**



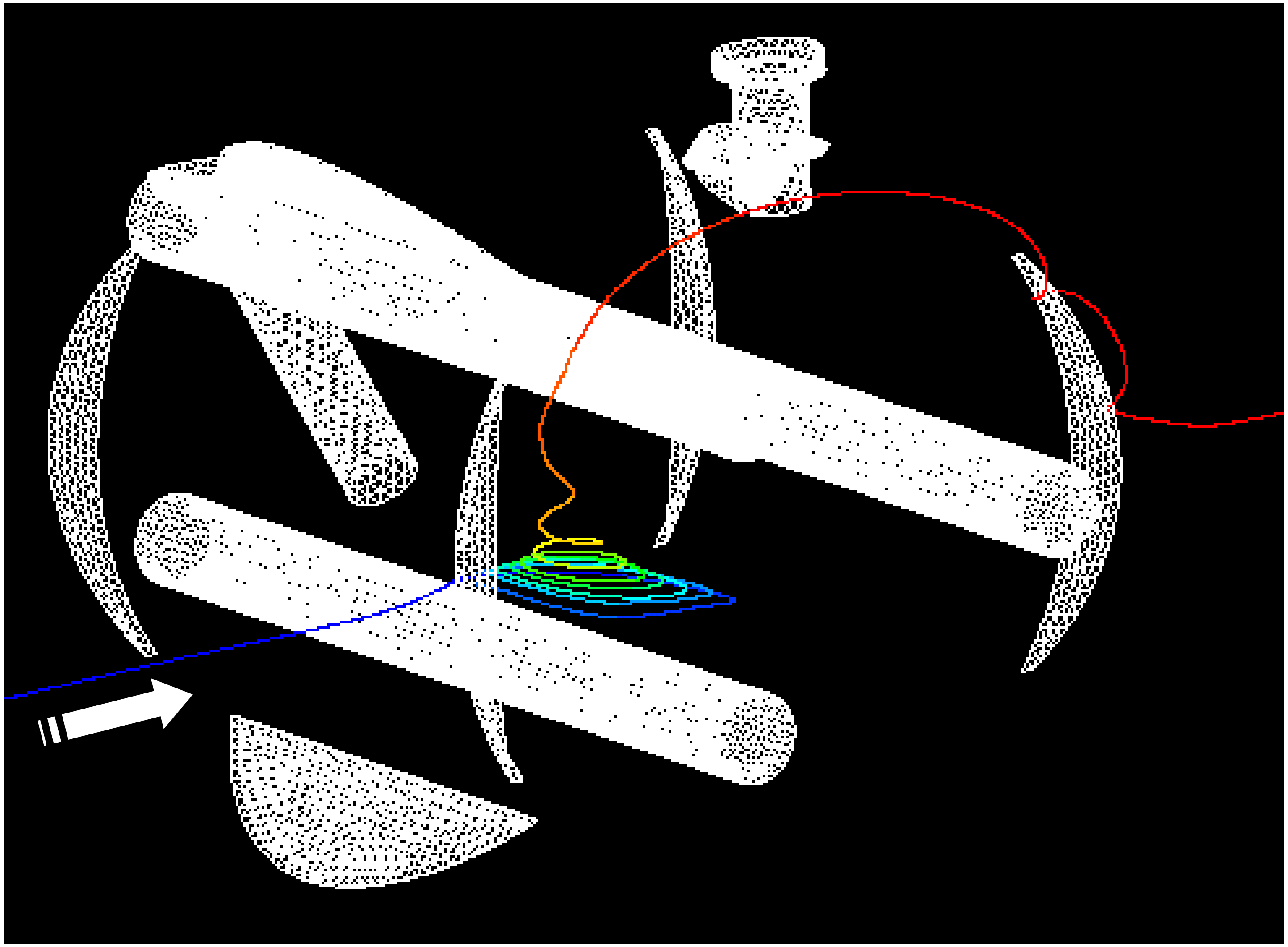
Sandia National Laboratories

Particle Tracks Colored by Dose



Calgon 12” Sentinel® UV Reactor

Particle Tracks Colored by Dose

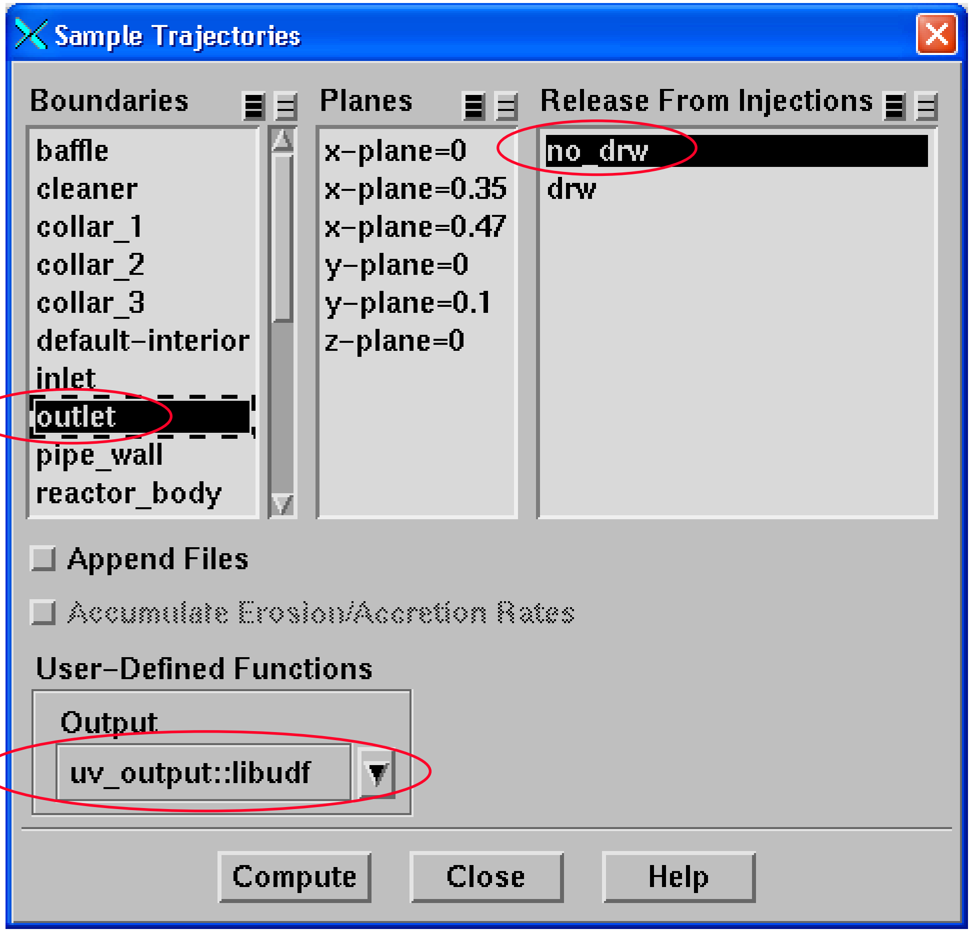


Calgon 12” Sentinel® UV Reactor

Output Dose Results

- Report > Discrete Phase > Sample

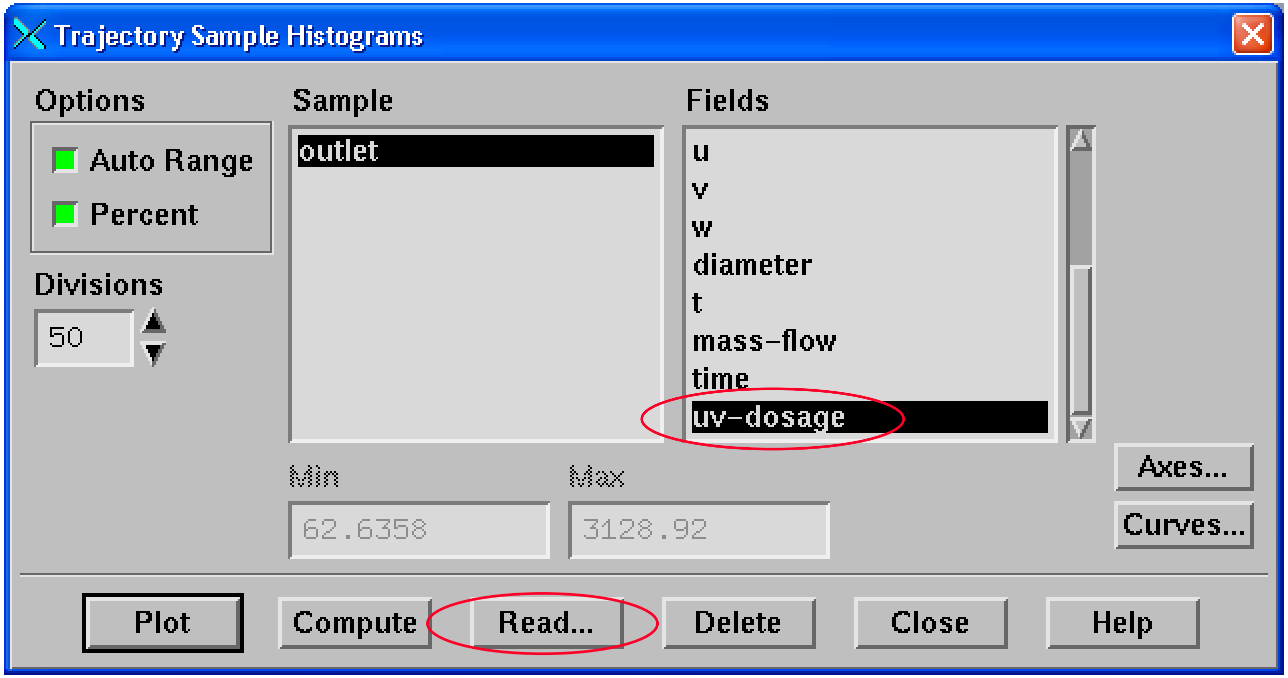
- Generates "[outlet].dpm" file
  - Cumulative particle doses (J/m^2) are contained in this file
  - Can be read by Excel

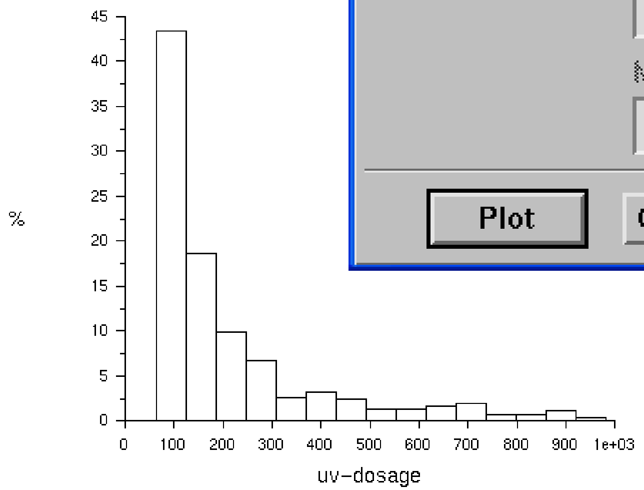


Sandia National Laboratories

View Dose Histogram

- Report > Discrete Phase > Histogram





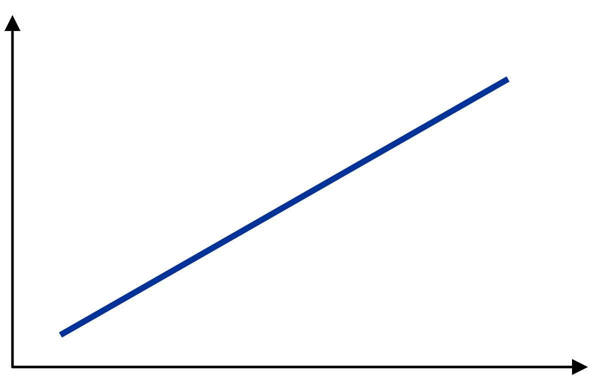
Overview

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/No) 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**



N_o = initial number of microbes
N = number of infectious microbes remaining after UV exposure

Detailed procedure outlined in Munoz et al. (2007)

RED Post-Processors

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

Output from FluentRED.exe

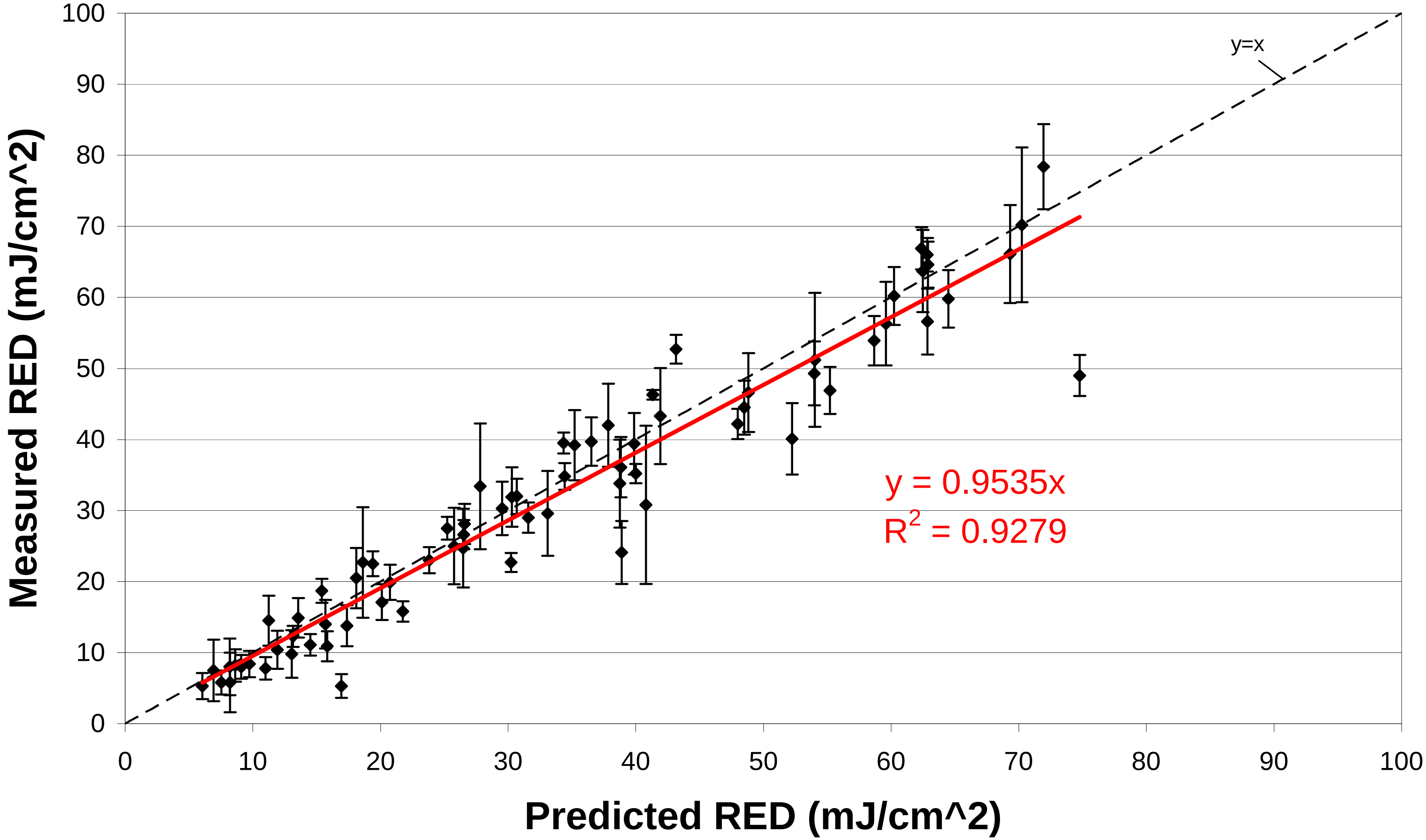
```
Realization, Particles, log_Inactivation(log(No/N)), RED
    1,     781,    9.2072E-01,    1.6130E+01
    2,     782,    9.5080E-01,    1.6719E+01
    3,     780,    9.5016E-01,    1.6706E+01
    4,     780,    9.4099E-01,    1.6526E+01
    5,     780,    9.5880E-01,    1.6876E+01
------------------------------------------------------------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

Sandia National Laboratories

Measured RED vs. Simulated RED



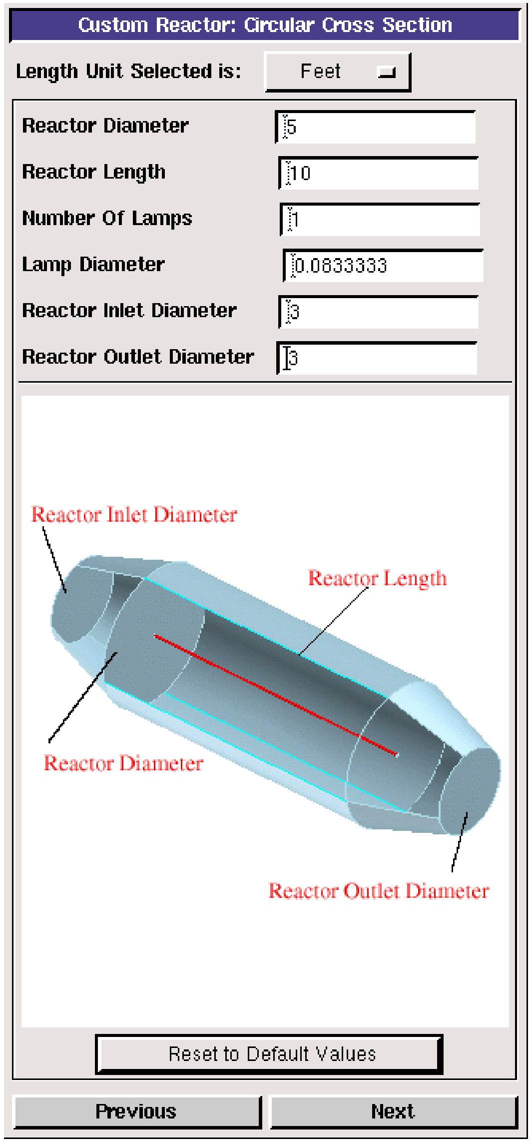
Summary

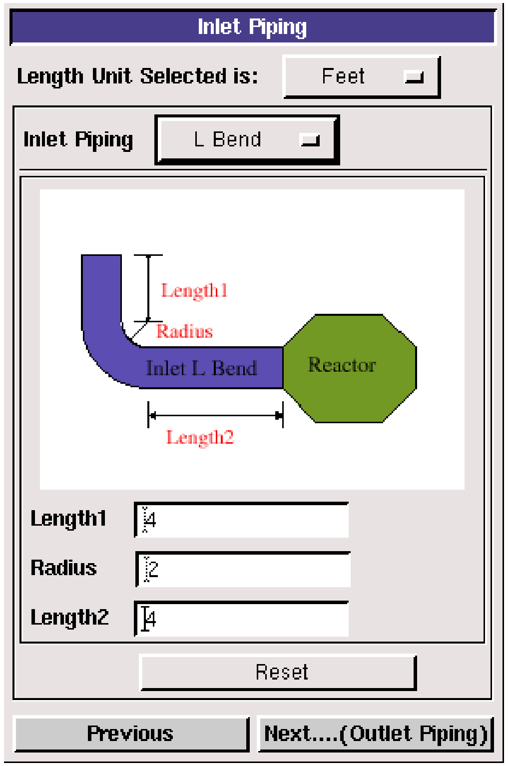
- Simulating UV dose distributions in FLUENT
  - Discrete ordinates radiation model in FLUENT generates UV incident radiation field
    - Honors geometry used in hydraulic CFD simulation (e.g., shadowing, reflection)
  - Particle tracking yields dose distribution
  - Dose distribution yields RED
- Tutorial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

Sandia National Laboratories

FluentUV

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





Sandia National Laboratories

Acknowledgments

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

Sandia Corporation gratefully acknowledges that the Awwa Research Foundation is the joint owner of the technical information upon which this manuscript is based. Sandia thanks AwwaRF for their financial, technical, and administrative assistance in funding and managing the project through which this information was discovered. The comments and views detailed herein may not necessarily reflect the views of the Awwa Research Foundation, its officers, directors, affiliates, cofunding organizations, or agents.

Sandia National Laboratories