Radiation Dose Modeling in FLUENT®

Clifford K. Ho

Sandia National Laboratories
Albuquerque, NM

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Modeling Approach

- Geometric Model
- Hydraulic Model
- UV Radiation Model
- Dose Model

Inactivation and Reduction Equivalent Dose
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
Turn on Radiation Model in FLUENT
DO Model Parameters

**Radiation Model**

- **Model**
  - Off
  - Rosseland
  - P1
  - Discrete Transfer (DTRM)
  - Surface to Surface (S2S)
  - Discrete Ordinates (DO)

- **Iteration Parameters**
  - Flow Iterations per Radiation Iteration: 10
  - Angular Discretization:
    - Theta Divisions: 5
    - Phi Divisions: 5
    - Theta Pixels: 3
    - Phi Pixels: 3

- **Non-Gray Model**
  - Number of Bands: 0

- **Solar Load**
  - Model
    - Off
    - Solar Ray Tracing
    - DO Irradiation

- **Solar Calculator...**
Impact of Theta x Phi Discretization on Simulated Incident Radiation Field

\[
\text{theta x phi = 2 x 2} \quad \text{theta x phi = 5 x 5}
\]

Calgon 12” Sentinel® UV Reactor
Specify UV Transmittance of Water

- Define > Materials...

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

\[I / I_o = \text{Intensity reduction at } x = 1\text{ cm}\]

\[a = \text{Absorption coefficient (1/m)}\]
Specify UV Radiation Boundary Condition

- Define > Boundary Conditions...
Applying Wall Reflection

- Define > Boundary Conditions...
Simulated UV radiation field with and without wall reflection
(Calgan 12” Sentinel® UV Reactor)

UV Intensity (W/m^2)

With Wall Reflection

No Wall Reflection

UVT = 88%

UVT=88%
Overview
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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...
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

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
  – 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/m²) = Incident radiation (W/m²) x 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/m²) are contained in this file
  - Can be read by Excel
View Dose Histogram

- Report > Discrete Phase > Histogram
Overview
Radiation Dose Modeling in FLUENT®

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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

\[ \log \text{Inactivation} = \log \left( \frac{N_0}{N} \right) \]

\( N_0 = \) 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](http://www.sandia.gov/cfd-water)
  – (1) Windows-based executable and source file
  – (2) Excel spreadsheet

<table>
<thead>
<tr>
<th>Realization, Particles, log_Inactivation(log(No/N)), RED</th>
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</thead>
<tbody>
<tr>
<td>1, 781, 9.2072E-01, 1.6130E+01</td>
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<tr>
<td>2, 782, 9.5080E-01, 1.6719E+01</td>
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<tr>
<td>3, 780, 9.5016E-01, 1.6706E+01</td>
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<tr>
<td>4, 780, 9.4099E-01, 1.6526E+01</td>
</tr>
<tr>
<td>5, 780, 9.5880E-01, 1.6876E+01</td>
</tr>
</tbody>
</table>

Output from FluentRED.exe

Number of realizations = 5
\text{t-value} = 2.770
Mean RED = 1.6591E+01 \text{mJ/cm}^2\text{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

\[ y = 0.9535x \]

\[ R^2 = 0.9279 \]
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
FluentUV

- Wizard-like template for generating models and grids of UV reactors and piping in FLUENT

- Muhammad.Sami @ansys.com
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