Implementing General Framework in MFiX for Radiative Heat Transfer in Gas–Solid Reacting Flows DE-FE0030485

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Outline

1. Project Description and Objectives
2. Project Update
3. Preparing Project for Next Steps
4. Concluding Remarks
1. Project Description and Objectives

NETL’s MFiX — Multiphase Flow with Interphase eXchange

• Central to the laboratory’s multiphase flow reactor modeling efforts

• Provides support to achieve DOE’s goals
  1. Cost of Energy and Carbon Dioxide (CO2) Capture from Advanced Power Systems
  2. Power Plant Efficiency Improvements

• Built with varying levels of fidelity/computational cost
  ▪ Lower fidelity models for large scale reactor design
  ▪ High fidelity models to support the development of lower fidelity models

Solution time

Model uncertainty

DNS
Direct Numerical Simulation: Very fine scale, accurate simulations for very limited size domain

MFiX DEM
Discrete Element Method: Track individual particles and resolve collisions

MFiX Hybrid
Hybrid: Continuum and discrete solids coexist

MFiX TFM
Two-Fluid Model: Gas and solids form an interpenetrating continuum

MFiX PIC
Particle-in-Cell: Track parcels of particles and approximate collisions

ROM
Reduced Order Models: Simplify models with limited application
1. Project Description and Objectives

Status of the beginning of the project

High-end validation study:
- Fine grid with 1.3M cells
- Two solid phases (coal and recycled ash)
- Detailed gasification chemical kinetic (17 gas species, 4 solid species)

What was missing the in the model?
No real radiative heat transfer modeling available in MFiX!

Driving Question/Motivation
Enhance MFiX capabilities by including models for radiative heat transfer following MFiX’s multi-fidelity approach

Results from: “Fluidized Beds – recent applications”, W. Rogers, 215 IWTU Fluidization Workshop
1. Project Description and Objectives

Technology benchmarking: comparing three popular CFD packages

<table>
<thead>
<tr>
<th>Capability</th>
<th>MFiX</th>
<th>OpenFOAM (open source)</th>
<th>ANSYS-FLUENT (commercial)</th>
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<tbody>
<tr>
<td>TFM reacting</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>DEM reacting</td>
<td>yes</td>
<td>no</td>
<td>no</td>
</tr>
<tr>
<td>Radiative Heat transfer</td>
<td>no</td>
<td>Gray, P1, DOM</td>
<td>Gray, simple WSGG, P1, DOM</td>
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</table>
1. Project Description and Objectives

MFIX-RAD development plan

"Research Models"

- PMC + Line-by-line model (full spectral resolution ~10 million lines) -> model error free
- PMC + Weighted Sum of Gray Gases (WSGG) model

"Industrial Model"

- P1 + WSGG model (gas & particles)
- P1 + WSGG model & gray particles
- P1 + Gray gas & particle model (neglect all spectral variations)
- P1 + gray constant (neglect all spectral and spatial variations)

"Basic Model"

Usable in MFIX-TFM and MFIX-DEM!
## 2. Project Update

We have received a 1 year, no cost extension

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<th>Tasks</th>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
<th>Year 4</th>
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<td>T-1: Project Management and Planning</td>
<td>10/17</td>
<td>01/18</td>
<td>04/18</td>
<td>07/18</td>
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<td>T-2: Testing of the previously developed MFIX-RAD Radiation Model Plug-In</td>
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<td>T-7: Comprehensive Validation and Benchmark</td>
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</table>

We have received a 1 year, no cost extension.

- **T-1: Project Management and Planning**
  - **Done!**

- **T-2: Testing of the previously developed MFIX-RAD Radiation Model Plug-In**
  - **Ongoing**

- **T-3: Implementing basic radiation model within MFIX-DEM**
  - **Early stage work (MS student)**

- **T-4: Implementation and Verification of Industrial Models**

- **T-5: Industrial Model Application and Analysis**

- **T-6: Development of High-End Research Models**

- **T-7: Comprehensive Validation and Benchmark**

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**University of Wyoming**
2. Project Update

Modeling approach

Energy equations for MFiX-TFM

Gas
\[ \varepsilon_g \rho_g c_{pg} \left( \frac{\partial T_g}{\partial t} + u_g \cdot \Delta T_g \right) = \nabla q_g + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rg} + H_{wall} (T_{wall} - T_g) - \nabla \cdot \tilde{q}_{rg} \]

Solids
\[ \varepsilon_{sm} \rho_{sm} c_{psm} \left( \frac{\partial T_{sm}}{\partial t} + u_{sm} \cdot \Delta T_{sm} \right) = \nabla q_{sm} + \sum_{m=1}^{M} H_{gsm} - \Delta H_{rs} - \nabla \cdot \tilde{q}_{rs} \]

Single particle Energy equation for MFiX-DEM

\[ m_i c_{p,i} \frac{dT_i}{dt} = \sum_{n=1}^{N_i} q_{i,j} + q_{i,f} + q_{i,rad} + q_{i,wall} \]

Source/Sink Terms are obtained from the thermal radiation model!
2. Project Update

\[ \frac{dI_\eta}{ds} = \vec{s} \cdot \nabla I_\eta = a_\eta I_{b_\eta} - a_\eta I_\eta - \sigma g \eta I_\eta + \frac{\sigma s_\eta}{4\pi} \int I_\eta(\vec{s}') \Phi_\eta(\vec{s}, \vec{s}') d\Omega \]

The RTE is an integro-differential equation for the spectral intensity \( I_\eta(x, y, z, \phi, \psi, \eta) \) (a function of 6 variables!)

**Source term in the energy equation:**

\[ S_{rad} = \nabla \cdot \vec{q}_{rad} = \int_{0}^{\infty} a_\eta \left( 4\pi I_{b_\eta} - \int_{4\pi} I_\eta d\Omega \right) d\eta \]

**Solution approach:**

- 3 spatial dimensions \( \vec{r}(x, y, z) \): CFD discretization
- 2 directional dimensions \( \vec{s}(\phi, \psi) \): RTE solvers
- 1 spectral dimension \( \eta \): spectral models

\( G_\eta \) spectral incident radiation
2. Project Update

Gray P1 model assumptions

1) Gray participating medium (gas and solids) -> no dependence on wavenumber $\eta$

2) Use a “Fourier series” ansatz $I(\vec{r}, \vec{s}) = \sum_{l=0}^{\infty} \sum_{-l}^{l} I_l(\vec{r}) \cdot Y_l(\vec{s})$  

3) Keeping only the first term $l = 0$ leads to the P1 approximation

4) Solve a “combined” (including all phases) P1 equation for $G$ (Helmholtz type)

$$\nabla \cdot (\Gamma \nabla G) + 4\pi \left( a_g \frac{\sigma T^4}{\pi} + E_g \right) - (a_g + a_s)G = 0$$
2. Project Update

“Distributing the source terms”

\[ \nabla \cdot (\Gamma \nabla G) + 4 \pi \left( a_g \frac{\sigma T^4}{\pi} + E_s \right) - (a_g + a_s) G = 0 \]

Continuous phase

\[ -\nabla \cdot q_{rg} = a_g G - 4a_g \sigma T^4 \]

Dispersed phase \( m \) (M total)

\[ a_s = \sum_{m=1}^{M} a_{s,m} \quad E_s = \sum_{m=1}^{M} E_{s,m} = \sum_{m=1}^{M} a_{s,m} \frac{\sigma T^4_{s,m}}{\pi} \]

\[ -\nabla \cdot q_{rs} = \sum_{m=1}^{M} a_{s,m} G - 4\pi \sum_{m=1}^{M} a_{s,m} \frac{\sigma T^4_{s,m}}{\pi} = \sum_{m=1}^{M} \left( a_{s,m} G - 4a_{s,m} \sigma T^4_{s,m} \right) = \sum_{m=1}^{M} -\nabla \cdot q_{rs,m} \]

\[ -\nabla \cdot q_{rs,m} = a_{s,m} (G - 4\sigma T^4_{s,m}) \]

Gray models for \( a_g \)

- “gray constant” \( a_g = \text{const} \) (user input)
- “gray” => Planck mean absorption using \( CO_2 \) and \( H_2O \)

Gray models for \( a_{s,m} \)

- “gray constant” based on constant emissivity and diameter of particles
- “gray” based on Buckius-Hwang correlation (depends on refractive index, mean particle size, void fraction and temperature)
2. Project Update

Basic Verification of the P1 implementation

- 2D Steady, single phase
- Heat transfer via radiation (P1, $a_g = 0.01 \text{m}^{-1}$) and diffusion
- Mesh: 30x200
- Use Ansys-Fluent solver for verification

Incident radiation $G [\text{W/m}^2]$ fields
2. Project Update

Verification of the P1 - DEM implementation

- 2D, Radiation only (frozen “fields”), 30x90 cells
- Compare TFM and DEM results => should be identical
- Gas phase $a_g = 0.3 \, cm^{-1}$
- one particle per cell ($d_p = 1mm, \epsilon_m = 0.6 \Rightarrow a_s = 0.6 \, cm^{-1}$

Source term – gas

\[
\begin{align*}
y &= 0.11m \\
y &= 0.61m \\
y &= 0.61m
\end{align*}
\]
2. Project Update

Relevance of thermal radiation in Lab-Scale reactors (54kWth)

• Two Fluid Model
  • 2 solid phases (cold and hot char)
  • 5 gas phases ($N_2$, $O_2$, $CO$, $CO_2$, soot)
  • Neglect convective heat transfer

• Geometry
  • 2D Cylindrical
  • 20 x 60 cells

Compare results with and without radiative heat transfer!

MFIX-RAD settings in mfix.dat

```
# Radiation Model
RAD_ON = .T.
RAD_EMIS_W = 1.0 1.0 1.0 1.0
RAD_T_W = 300 300 800 800
RAD_NQUAD = 1
RAD_SKIP = 0
RAD_NRR = 10
RAD_RTE = 'P1'
RAD_SPECTRAL = 'GRAY'

Gas & solid phase reactions
2*CO --> Soot + CO2
2*CO --> Soot + CO2
CO + 0.5*O2 --> CO2
2*FC1 + O2 --> 2*CO
FC1 + CO2 --> 2*CO
2*FC2 + O2 --> 2*CO
FC2 + CO2 --> 2*CO
FC2 --> FC1
Ash2 --> Ash1
```
2. Project Update

Gas Temperature [K]  Gas volume fraction

Mass weighted average temperatures at the outlet

\[ \Delta T > 110^\circ C \]

Even in low-Temp Lab scale reactor!
2. Project Update

Relevance of thermal radiation in a Large Scale reactor (5.4 MWth)

- Same case as before but thermal power scaled up by a factor of 100
  - Include convective heat transfer to walls using average heat transfer coefficient \( h = 14 \, \text{W/m}^2\text{K} \)
- Mesh 40 x 120 cells

Mass weighted average temperature at the outlet:

\[ \Delta T > 100^\circ \text{C} \]

Even with convective heat transfer!
2. Project Update

MFiX-DEM with radiation

• Only heat transfer (no chemical reactions)
• 2D Cartesian
• Length = 0.15 m, Height = 0.90m, 15 x 45 cells
• Particle diameters 4mm, 2mm
• Particle emissivity $\epsilon_p = 0.6$
• Constant gas phase absorption coefficient $a_g = 3.0 m^{-1}$

Time = 0.1s

Gas Temperature

Solid particles location

No rad  |  p1

No rad  |  p1
3. Preparing Project for Next Steps

• Market Benefits/Assessment
  • MFiX is widely used the CFD tool for modeling/optimization of reacting multiphase flow
  • MFiX currently has no radiative heat transfer modeling capability
  • For a simple spouted bed combustor, neglecting radiative heat transfer results in temperature differences of $100^\circ C$

• Technology-to-Market Path
  • Basic MFiX-RAD Plug-In is available at GitLab => every MFiX user can download and use it their process modeling!
  • A more accurate spectral model based on WSGG is currently implemented and will be available by the end of May 2019
  • Detailed experimental data for validation is rare in Fluidized Bed Combustors/Gasifiers at larger scale
    • We will use a LBL Photon – Monte Carlo method (model error free) to validate the lower fidelity gray and WSGG models to provide uncertainty values
  • We are seeking industry collaborators who want to use MFiX-RAD in their applications
4. Concluding Remarks

• Basic radiation model (Gray, P1) has been implemented and verified for MFiX-TFM and MFiX-DEM
• First results in low-temperature spouted bed confirm that radiative heat transfer is important

Next Steps
• Extend basic radiation model to be usable in the new and improved MFIX-PIC (v19.1)
• Finish implementation and verification of industrial model (WSGG, P1)
• Implement Photon Monte Carlo solver for detailed validation of lower fidelity models
  • David Tobin (MS student) has started this task and it will be his thesis topic
4. Concluding Remarks

- We have received the detailed (1.4 M cells) MFiX case set up for the 13MW Power Systems Development Facility (PSDF) gasifier => temperature and syngas composition data available at the outlet
  - We will use this case for validation of the models in a large-scale application
  - Expect improvements compared to simulations that neglected radiative heat transfer