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

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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
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

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

**Research Models (used for benchmarking)**
- P1 + WSGG model (gas & particles)
- P1 + WSGG model & gray particles

**Industrial Model (main application)**
- P1 + Gray gas & particle model (neglect all spectral variations)
- P1 + gray constant (neglect all spectral and spatial variations)

**Usable in MFIX-TFM and MFIX-DEM!**

**Model uncertainty**

"Basic Model"
2. Project Update

We have received a 1 year, no cost extension

<table>
<thead>
<tr>
<th>Tasks</th>
<th>Year 1</th>
<th>Year 2</th>
<th>Year 3</th>
<th>Year 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10/17</td>
<td>01/18</td>
<td>04/18</td>
<td>07/18</td>
</tr>
<tr>
<td>T-1: Project Management and Planning</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>10/18</td>
<td>01/19</td>
<td>04/19</td>
<td>07/19</td>
</tr>
<tr>
<td>T-2: Testing of the previously developed MFIX-RAD Radiation Model Plug-In</td>
<td></td>
<td>07/19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T-3: Implementing basic radiation model within MFIX-DEM</td>
<td></td>
<td></td>
<td>07/19</td>
<td></td>
</tr>
<tr>
<td>T-4: Implementation and Verification of Industrial Models</td>
<td>10/19</td>
<td>01/20</td>
<td>04/20</td>
<td>07/20</td>
</tr>
<tr>
<td>T-5: Industrial Model Application and Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T-6: Development of High-End Research Models</td>
<td></td>
<td></td>
<td>07/20</td>
<td></td>
</tr>
<tr>
<td>T-7: Comprehensive Validation and Benchmark</td>
<td></td>
<td></td>
<td></td>
<td>01/21</td>
</tr>
</tbody>
</table>

Near completion!

Done!
2. Project Update

Modeling approach

Energy equations for MFiX-TFM

Gas

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

Solids

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

Single particle/parcel Energy equation for MFiX-DEM or MFiX-PIC

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

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

Modeling approach

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

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

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
2. Project Update

Modeling approach

Gray P1 model assumptions

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

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

Spatially varying coefficients

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)

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

Gas phase absorption

$$ \Gamma = \frac{1}{3(a_g + a_s + \sigma_s) - C\sigma_s} $$

Solid phase absorption

Gas phase emission

Solid phases emission
2. Project Update

Modeling approach

Distributing the source terms with P1

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

Continuous phase

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

Dispersed phase m (M total)

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

Spectral models for \( a_g \)

- “gray constant” \( a_g = const \) (user input)
- “gray” => Planck mean absorption using \( CO_2 \) and \( H_2O \)
- “gray and non-gray” WSGG based on \( CO_2 \) and \( H_2O \)

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

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

### Modeling approach

#### Weighted Sum of Gray Gas (WSGG) model

- Derived by fitting model coefficients such that total emissivity in a 1-d slab of gas matches full spectral result
- Typically 4-5 gray gases are sufficient

**Gray WSGG model**

The mean absorption coefficient is

\[
\alpha_g = \frac{\ln(1 - \varepsilon)}{L}
\]

The total emissivity of a H$_2$O/CO$_2$ mixture is

\[
\varepsilon = \sum_{i=0}^{N_g} k_i (1 - e^{-a_i P (X_{H2O}+X_{CO2})L})
\]

Path length either defined as \( L = \frac{3.6V}{A} \) (mean beam length) or as \( L = V_{cell}^{1/3} \) (results are mesh dependent!)

#### Non-gray WSGG model

Solve \( N_g \) “gray-gas” equations i.e. for the \( i \)th gray gas

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

The weighting factors are given by

\[
k_i = \sum_{j=0}^{N_k} b_{i,j} T^j
\]

The source terms are then given by

\[
-\nabla \cdot q_{rg} = \sum_{i=0}^{N_g} a_i G_i - 4a_i k_i \sigma T^4
\]

L is not needed!!!
2. Project Update
Modeling overview

Start
- Initialize computations
- Decompose the domain
- Compute various terms/fluxes in equations for the fluid phase
- Apply BC and solve the system of equations for fluid variables

TFM
- Compute various terms/fluxes in equations for solid phases
- Apply BC and solve the system of equations for solid phase variables

DEM
- Output

PIC
- Calculate $S_r$, the source/sink term due to thermal radiation

PMC
- RTE
- P1
- Planck mean absorption

Continuous phase
- Constant-Gray
- Gray
- Gray-WSGG
- NonGray-WSGG

WSGG models
- Taylor
- Smith
- Johansson
- Kangwanpongpan
- Krishnamoorthy
- Yin
- Dorigon
- Bordbar
- Guo
- Shan

Dispersed phase
- Constant-Gray
- Gray
- Gray-WSGG
- NonGray-WSGG

Buckius-Hwang correlation

Stop
- Finished time steps
2. Project Update

T4: Implementation and Verification of Industrial Models

- 3D Steady, single phase, gray
- Radiation model: P1, WSGG – SMITH82
- $L = 1.44$ (3.6 $V/A$, based on domain) optical thickness = 0.49
- $X_{H_2O} = 0.2$; $X_{CO_2} = 0.1$; $p = 1.0$ atm
- Mesh: 17x17x34

Verification of gray-WSGG implementation by comparison with ANSYUS-FLUENT results

Verification of non-gray WSGG implementation by comparison with results reported in Literature
Gray and non-gray WSGG models implemented correctly, which one should we use as “Industrial Model”? Problems with the gray-WSGG

- Results strongly depend on the choice for $L$
- Results differ from non-gray result

We prefer the non-gray version as our “Industrial Model” since it does not require arbitrary choice for $L$!

Further analysis of this choice will be provided in Task 7!
13MW Power Systems Development Facility (PSDF) gasifier

- Mesh with 4M cells
- Chemistry based on 17 gas species, 4 solid species

Outlet
x = 0.5, y = [7.5, 8.0], z = [0.1, 0.4]
155683.6 Pa, 1227 K

Inlet
Gas: 0.035 kg/s, 300K (N₂)
234225.0 Pa

Coal: 0.3522 kg/s, 300K (Char, volatiles, Moisture, ash)
Gas: 0.18157 kg/s, 300K (N₂)

Char & ash: 3.746 kg/s, 1190K
Gas: 0.2935 kg/s, 1190K (CO, CO₂, CH₄, H₂, H₂O, N₂),
234225.0 Pa

Inlet
Gas: 0.035 kg/s, 300K (N₂)
234225.0 Pa, 482 K (N₂, O₂, H₂O), 0.342 kg/s
2. Project Update

T-5: Industrial Model Application and Analysis

(i) No radiation
(ii) Gray
(iii) Gray-wsgg
(iv) Nongray-wsgg

\( y = 6m, z = 0.25m, t = 20s \)

**Significant difference \( \Delta T > 120K \) observed!**
2. Project Update

T6: Development of High-End Research Models

Photon Monte-Carlo Method (PMC)

- PMC is essentially a Monte Carlo Integration of the RTE
- If it is coupled with a spectral database, this leads to a “model error free” solution of the RTE (numerical errors still present though)
- Work mostly done by MS student David Tobin (graduated in August)

Development approach

- Defined a basic interface to MFIX
- David coded the serial PMC method as a stand-alone Fortran program using data structures following “MFIX”
- After testing, the PMC solver was fully integrated into MFIX-RAD with the help of Dr. Kotteda
- Dr. Kotteda finished the parallel implementation of the PMC solver

Integrate RTE along a given path length (Beer’s Law)

\[ I_\lambda(S) = I_\lambda(0)e^{-\int_0^S \alpha_\lambda s^* ds^*} \approx I_\lambda(0)e^{-\alpha_\lambda S} \]

Fraction of ray’s energy absorbed in the cell

\[ F_{absorb} = 1 - e^{\alpha D_{cell}} \]
2. Project Update
T6: Development of High-End Research Models

Verification of stand-alone PMC solver by comparison with highly resolved DOM (32x16 rays)

- 3D Steady, single phase, **constant gray**
- Constant absorption coefficient = 0.1, no-scattering
- Varying wall emissivity
- Mesh: 17x17x34, tracked \( N = 10^9 \) rays

Wall heat flux along front wall (more sensitive than source term!)

\[
\nabla \cdot \vec{q}_{\text{rad}} \, dV = \int_{d\Omega} \vec{q}_{\text{rad}} \cdot \hat{n} \, dS
\]

Check conservation of energy with divergence theorem:

Average Relative Error of PMC Results: 0.00%
Average Relative Error of DOM Results: 4.94%

PMC inherently conserves energy!
2. Project Update
T6: Development of High-End Research Models

Verification of serial and parallel MFIX-RAD implementation

MFIX serial run-time ~4min

Initial result for parallel scaling are encouraging!

Scaling will improve greatly for non-gray applications
3. Preparing Project for Next Steps

Market Benefits/Assessment

• MFiX is widely used as CFD tool for modeling/optimization of reacting multiphase flow
• MFiX currently has only minimal radiative heat transfer modeling capability
• MFiX-RAD development adds
  • P1 + non-gray WSGG as the appropriate model for industrial applications (not available in either commercial (ANSYS-Fluent) or other open source (OpenFOAM) CFD codes
  • Model error free PMC solver to produce case specific benchmark data for RTE solver and Spectral Model accuracy assessment (not available in any other CFD codes)

Technology-to-Market Path

• MFiX-RAD Plug-In at current development state is available at GitLab => every MFiX user can download and use it their process modeling!
• We are seeking industry collaborators who want to use MFiX-RAD in their applications
• The MFiX-RAD Plug-In will be replaced by a full integration into the mainstream MFiX release towards the end of the project
4. Concluding Remarks

Remaining tasks

• Non-gray MFIX PMC solver
  ➢ Stand alone version for Statistical Narrow Band Model (Elsasser SNB) already implemented (see MS thesis of David Tobin)
  ➢ Line-by-line (LBL) Spectral Database (HiTran) for benchmarking (Task 6)
  ➢ Non-Gray WSGG PMC

• Task-7 “Comprehensive Validation and Benchmark”
  • Use non-Gray WSGG PMC to analyze model errors of P1 RTE solver (industrial model) for the large gasifier => P1 sufficiently accurate or not?
  • Comparison of PMC-LBL and PMC-ngWSGG results will reveal WSGG model errors
  • Such an analysis is only possible with PMC!

• Based on Task 7 make recommendations on next development steps
  ➢ Is P1-ngWSGG “sufficiently” accurate?
  ➢ If not, do we need a better RTE solver (i.e. P4, P6, or DOM)
  ➢ If not, do we need a better spectral model (k-distribution model?)