High-Fidelity Multi-Phase Radiation Module for Modern Coal Combustion Systems

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Radiation Challenges in Multi-Phase Reacting Flows

Radiative heat transfer in high temperature combustion systems
- Thermal radiation becomes very important at elevated temperatures
- Coal and hydrocarbon fuels $C_nH_m \rightarrow H_2O, CO_2, CO, NO_x$, soot, char, ash
- CO$_2$, H$_2$O, soot, char and ash strongly emit and absorb radiative energy
  (lower temperature levels)
- Radiative effects are conveniently ignored or treated with very crude models
  - Neglecting radiation $\Rightarrow$ temperature overpredicted by several hundred °C
  - "optically-thin" or gray radiation $\Rightarrow$ temperature underpredicted by up to 100°C
  - Neglecting turbulence–radiation interactions $\Rightarrow$ temperature overpredicted by 100°C or more
- In contrast: simple vs. full chemical kinetics $\Rightarrow$ same overall heat release and similar temperature profiles
**State of the Art of Radiation Modeling**

- **Radiative Transfer Equation (RTE) Solvers**
  - DOM/FVM included in CFD codes (ray effects, poor for optically thick media, high orders expensive)
  - SHM/P–N: $P–1$ in CFD codes (cheap and powerful; poor for optically thin media); higher orders ($P–N$) complex
  - Photon Monte Carlo (very powerful; expensive, statistical scatter); ideal for stochastic turbulence models
  - $P–1$ ideal solver for optically thicker pulverized coal/fluidized beds

- **Spectral Models**
  - Full-spectrum k-distributions (very efficient; cumbersome assembly, species overlap issues)
  - Line-by-line Monte Carlo module (outstanding accuracy at small additional cost)
Research Objectives

1. Spectral radiation properties of particle clouds
   - coal, ash, lime stone, etc.,
   - varying size distributions and particle loading
   - classified, pre-evaluated and stored in appropriate databases or regression models

2. Spectral radiation models for particle clouds
   - Adapt high-fidelity spectral radiation models for combustion gases
   - Extensions to large absorbing/emitting–scattering particles in fluidized bed and pulverized coal combustors
   - New gas–particle mixing models and consideration of scattering

3. RTE solution module
   - $P-1$ (and perhaps a $P-3$) solver (for optically thick applications)
   - Photon Monte Carlo solver (for validation and for optically thinner applications)

4. Validation of Radiation Models
   - Module connected to MFIX and OpenFOAM
   - Comparison with experimental data available in the literature
   - Simulations for fluidized beds and pulverized-coal flames
Accomplishments

- Radiative spectral properties database and regression models
  - Surveyed radiative properties measurements of coal combustion particles
  - Compiled a radiative property database of particles in coal combustion

- Spectral calculation models
  - Ported previously developed gas-soot module to MFIX
  - Generated CO₂ and H₂O k-distribution correlations
  - Developed particle spectral properties calculation module
  - Developed new regression scheme for splitting radiative heat source
  - Ported spectral module to OpenFOAM

- Radiative Transfer Equation (RTE) solver
  - Implemented P-1 RTE solver for both gray and nongray participating media
  - Implemented Monte Carlo RTE solver for both gray and nongray media
  - Verification against line-by-line (LBL) solutions for 1D homogeneous slab
  - Source code submitted for review

- CFD simulation
  - Radiative heat transfer in a fluidized-bed coal combustor (P-1 with CO2-char k-distribution)
RTE Solution Module

\(P-1\) Solver:

- Ideal RTE solver for expected large optical thicknesses
- Single-scale full-spectrum \(k\)-distribution, assembled from narrow-band data for particulates and gas \(k\)-distributions
- One RTE solution, but separate emission and absorption terms for individual phases
- Extending to higher orders – \(P-3\) and \(P-5\).

Photon Monte Carlo Solver

- Ported from our gas combustion work with LBL module
- Particulate emission and absorption added including extended wavenumber selection schemes and energy splitting across phases.
- To ascertain accuracy of \(P-1\)/replace it whenever necessary
## Sample calculation–inhomogeneous medium

- **One dimensional slab with two layers**

<table>
<thead>
<tr>
<th></th>
<th>Left</th>
<th>Right</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Width</strong></td>
<td>5cm</td>
<td>5cm</td>
</tr>
<tr>
<td><strong>Gas</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>600K</td>
<td>1200K</td>
</tr>
<tr>
<td>Composition</td>
<td>5%CO₂, 95%(N₂+O₂)</td>
<td>10%CO₂,90%(N₂+O₂)</td>
</tr>
<tr>
<td><strong>Particles</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature</td>
<td>500K</td>
<td>1300K</td>
</tr>
<tr>
<td>Diameter</td>
<td>200µm</td>
<td>100µm</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>10⁻³</td>
<td>2.5 × 10⁻⁴</td>
</tr>
<tr>
<td>Refractive index</td>
<td></td>
<td>2.2 – 1.12i</td>
</tr>
</tbody>
</table>

- **RTE solver** $P_1$
- **64 quadrature points**
Sample calculation–inhomogeneous medium, cont’d

- Predicts major trends
- Gas heat source is one order less but vary accurate
- Gas radiation is from strong bands, regression scheme picks solid absorption coefficient at the corresponding wavenumbers
- Cold layer solid heat source inaccuracy due to $I_\eta \neq I_{b\eta}$
- Hot layer solid heat source within 1%
Line-by-line Photon Monte-Carlo

- Fully implemented a LBL-PMC module on MFIX for gas-particle mixtures, including energy splitting across phases.
- Validated PMC calculations with exact calculations for simple geometries.
Buckius and Hwang Correlations

\[ f_A = \int_0^\infty \pi a^2 n(a) da = \frac{3f_v}{4\bar{r}} \]

\[ \kappa_0^* = 3 \left[ \frac{m^2 - 1}{m^2 + 2} \right] \frac{6\pi f_v \eta}{f_A} = C_0 \frac{f_v}{f_A} \eta \]

\[ \frac{\kappa}{f_A} = \kappa^* = \left[ \frac{1}{(\kappa_0^*(1 + 2.30\kappa_0^{*2}))^{1.6}} + \frac{\kappa_0^{*1.76}}{1.66^{1.6}} \right]^{-1/1.6} \]

- If \( \kappa_0^* \ll 1 \), then \( \kappa^* = \kappa_0^* \).
- If \( 1 \ll \kappa^* \), then \( \kappa^* = 1.66 \times \kappa_0^{*1.1} \)

\[ a \]

Random number relations for solid phases

Random numbers vs $\eta$, $T$, $f_v$, $f_A$, $C_0$.

$$R_\eta = \frac{\int_0^\eta \kappa_\eta I_b \eta d\eta}{\int_0^\infty \kappa_\eta I_b \eta d\eta}$$

$$= \frac{\int_0^{\eta^*} \kappa_\eta^* (\xi \times \eta^*) I_{b\eta^*}(\eta^*) d\eta^*}{\int_0^\infty \kappa_\eta^*(\xi \times \eta^*) I_{b\eta^*}(\eta^*) d\eta^*}$$

(1)

Random numbers can be reduced to 2 variables.

Critical value at $\xi \approx 0.001$ and $\xi \approx 0.1$

Figure: Random number vs $\eta$ and $T$. The curve fitting is applied to the parametric function $f(\eta/T) = 1/2 + 1/2 \tanh(a_1(\eta/T)^{0.4} + a_2)$. 
**Curve-fitting coefficients for Random Number Relations**

![Graph showing curve-fitting coefficients](image)

\[ a_1(\xi) = \frac{2.826}{\exp(c_{12}(\log_{10} \xi + c_{11})) + 1} + \frac{2.673}{\exp(-c_{14}(\log_{10} \xi + c_{13})) + 1} \]

\[ a_2(\xi) = \frac{-4.480}{\exp(c_{22}(\log_{10} \xi + c_{21})) + 1} + \frac{-3.738}{\exp(-c_{24}(\log_{10} \xi + c_{23})) + 1} \]
Planck-mean absorption coefficients

\[ \log \left( \frac{\kappa_P^*}{\xi} \right) = \frac{2.425}{\exp(c_{32} \log_{10}(\xi) + c_{31})} + 1 + \frac{-1.1592 \log_{10} \xi - 0.15649}{\exp(-c_{34} \log_{10}(\xi) + c_{32})} + 1. \]
LBL-PMC Energy Splitting Across Phases

**Absorption**

Absorption rates can be calculated using the following equations:

\[
Q_{\text{abs},g,j} = \sum_{i,k \in \mathbb{I}_j,\mathbb{K}_j} Q_{ij}^k \left( 1 - \exp(-\Delta \tau_{\eta,ij}^k) \right) w_g,
\]

\[
Q_{\text{abs},sm,j} = \sum_{i,k \in \mathbb{I}_j,\mathbb{K}_j} Q_{ij}^k \left( 1 - \exp(-\Delta \tau_{\eta,ij}^k) \right) w_{sm},
\]

where

\[
k_{g,i} = \left( \sum_n \kappa_{\eta,n,x_i} \right) p_{g,i}
\]

\[
k_{s,m,i} = f_A \kappa_{\eta,s,m}^* (\xi_{m,i})
\]

\[
\xi_{m,i} = C_0 \varepsilon_{s,m} / f_A T_{s,m,i}
\]

\[
w_{g,j} = \frac{\kappa_{\eta,g,j}}{\kappa_{\eta,g,j} + \sum_{m=1}^{N_s} \kappa_{\eta,s,m,j}}
\]

\[
w_{s,m,j} = \frac{\kappa_{\eta,s,m,j}}{\kappa_{\eta,g,j} + \sum_{m=1}^{N_s} \kappa_{\eta,s,m}}
\]

**Emission**

Emission rates are calculated as follows:

\[
Q_{\text{emi},g,i} = 4\pi \bar{F}_{g,i} \sigma T_{g,i}^4 V_i
\]

\[
Q_{\text{emi},s,m,i} = 4\pi \bar{F}_{s,m,i} \sigma T_{s,m,i}^4 V_i
\]

where

\[
\bar{F}_{g,i} = \left( \sum_n \bar{F}_{p,n,x_i} \right) p_{g,i} \varepsilon_{g,i}
\]

\[
\bar{F}_{s,m,i} = \frac{\varepsilon_{s,m,i}}{\bar{r}} \bar{F}_{s,m}^* (\xi_{m,i})
\]

\[
\xi_{m,i} = C_0 m^4 / 3\bar{r} T_{s,m,i}
\]
Example calculations

(a) Mixture at 650K

\[ T_g = 650 \text{ K}, \quad \varepsilon_g = 0.99, \quad x_{CO_2} = 0.10, \]
\[ T_s = 650 \text{ K}, \quad \varepsilon_{\text{coal}} = 0.01, \quad R_s = 10^{-5} \text{ m} \]

(b) Mixture at 1650K

\[ T_g = 1650 \text{ K}, \quad \varepsilon_g = 0.99, \quad x_{CO_2} = 0.10, \]
\[ T_s = 1650 \text{ K}, \quad \varepsilon_{\text{coal}} = 0.01, \quad R_s = 10^{-5} \text{ m} \]

Figure: line-by-line PMC and exact solutions of \( Q_{\text{abs}} \) for gas- and solid-phase mixture enclosed by a cylinder.
Fluidized bed

Figure: Colored lines are from exact solution. Black lines are PMC calculations.
Effort for Remaining Year

- Set up simulation of radiative heat transfer in dilute gas-solid reacting flows
- Comparisons between P-1 and Monte Carlo RTE solver
- Comparisons between various spectral models