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

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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

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 Transfer Equation (RTE) solver
  - Rewrote discretization subroutine for PDE and boundary conditions
  - 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

- Radiative spectral properties database
  - 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 CO$_2$ and H$_2$O k-distribution correlations
  - Developed particle spectral properties calculation module
  - Developed new regression scheme for splitting radiative heat source
  - Started to port module to OpenFOAM

- CFD simulation
  - Radiative heat transfer in a fluidized-bed coal combustor (P-1 with CO$_2$-char k-distribution)
Non-gray gas and particle radiative properties

- **Gases**: CO\textsubscript{2}, H\textsubscript{2}O and CO have strong spectral dependency
- **Particles**:
  - Nongray even if complex refractive index is gray
  - Much smoother than gases, can be modeled as constant over narrowbands

**Conditions**:
- Temperature 600K
- Gas: 10% CO\textsubscript{2}
- Particle: 
  - \( n = 2.2 - 1.12i \)
  - Volume fraction 0.001
  - Diameter 400\( \mu \text{m} \)
Regression

- To split heat source across phases, a regression scheme is proposed.

- Regression:

\[
\hat{k}_m(k; T_m) = \frac{\int_\eta \kappa_m \eta I_{b\eta} \delta(k - \kappa_{\eta}^0) \, d\eta}{\int_\eta I_{b\eta} \delta(k - \kappa_{\eta}^0) \, d\eta}
\]

- Gives “effective” solid phase absorption coefficient at given total absorption coefficient.

- Numerical calculation:
  - Weighted average of narrowband constant values

\[
\hat{k}_m(k_i) = k_{m,i} = \frac{\sum_{n=1}^{N_{nb}} I_{bn} k_{m,n} \Delta g_{n,i}}{\sum_{n=1}^{N_{nb}} I_{bn} \Delta g_{n,i}}
\]
RTE Solution Module

\textit{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

Photon Monte Carlo Solver

- Ported from our gas combustion work with LBL module
- Particulate emission and absorption added
- To ascertain accuracy of \textit{P–1}/replace it whenever necessary
Test Configuration

Simplistic Fluidized Bed Combustor

- **Geometry**
  - 2D cylindrical axisymmetric
  - Radius 10cm, Height 60cm
  - 20X60 cells

- **Flow**
  - Central jet
    - Air 300K, 1g/s (2.67m/s)
    - Cold char, 1.8g/s (2.67m/s)
  - Annulus coflow
    - Air 300K, 11.6g/s (0.32m/s)

- **Wall**
  - Wall temperature 800K, black

- **Initial condition**
  - Bottom 20cm filled with hot char particles, 1000K
Reactions

- $\text{C} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}$
- $\text{C} + \text{CO}_2 \rightarrow 2\text{CO}$
- $\text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2$
- Cold-char $\rightarrow$ Hot-char (pseudo reaction to model char heating)

Radiation

- Nongray CO$_2$, CO and char
- P–1 RTE solver
- Split radiative heat source across phases
**Temporal behavior**

**Gas temperature in the free board**

\((r=0.25\text{cm}, h=56.5\text{cm})\)

- Lower temperature due to radiation
- Larger temperature fluctuation due to radiative gas concentration variation

**Solid temperature inside bed**

\((r=0.25\text{cm}, h=16.5\text{cm})\)

- Temperature drops due to radiation
- Larger fluctuation due to convection of cooler particle from freeboard-bed interface
Instantaneous Flow Fields

- **Gas temperature (K)**
- **Solid temperature (K)**
- **Gas radiative heat source (W/m³)**
- **Solid radiative heat source (W/m³)**
Time Averaged Temperature

Time averaged gas temperature (K)

Without radiation

\[ \Delta T \] with radiation

Time averaged solid temperature

- Relatively unaffected
- \[ \Delta T \] from +5 to -15K
Effort for Next Year

- Implement turbulent mixing and combustion model
- Implement higher-level char combustion kinetics
- Simulation of radiative heat transfer in a realistic pulverized coal combustor
- Comparisons between P-1 and Monte Carlo RTE solver
- Comparisons between various spectral models