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

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Research Objectives

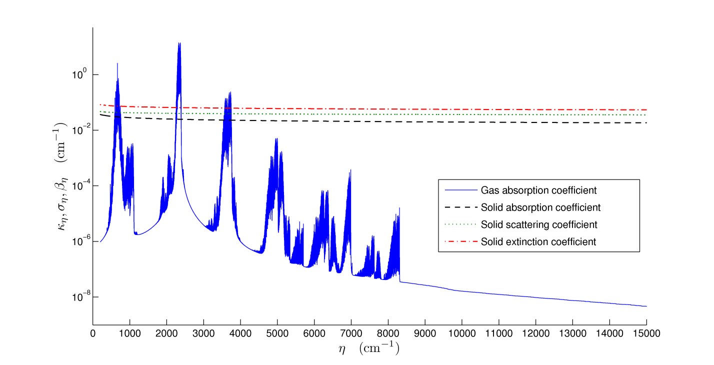
1. Spectral radiation properties of particle clouds
   - coal, ash, lime stone, etc.,
   - varying size distributions and particle loading
   - classified, pre-evaluated and stored in appropriate databases
2. Spectral radiation models for particle clouds
   - Adapt high-fidelity spectral radiation models 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_2O 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_2, H_2O 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_2
- Particle: $m = 2.2 - 1.12i$, volume fraction 0.001, diameter 400μm

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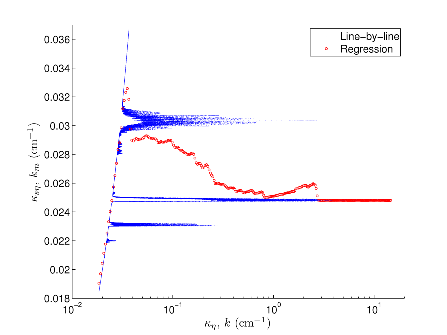
Regression

- 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

$$\hat{k}_m(k_i) = k_{m,i} = \frac{\sum_{n=1}^{N_{\text{nb}}} I_{\text{b}n} k_{m,n} \Delta g_{n,i}}{\sum_{n=1}^{N_{\text{nb}}} I_{\text{b}n} \Delta g_{n,i}}$$



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

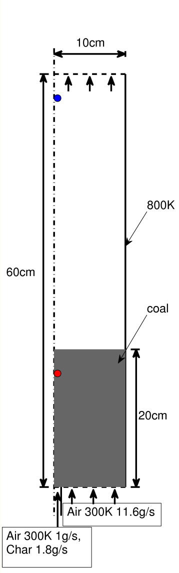
Photon Monte Carlo Solver

- Ported from our gas combustion work with LBL module
- Particulate emission and absorption added
- To ascertain accuracy of *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

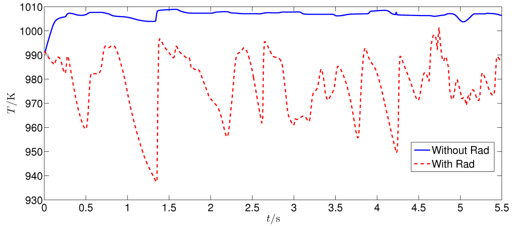


Test Configuration cont'd

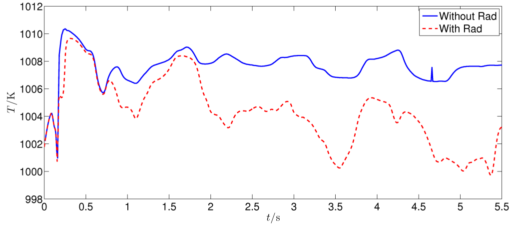
- Reactions
  - $C + \frac{1}{2} O_2 \longrightarrow CO$
  - $C + CO_2 \longrightarrow 2CO$
  - $CO + \frac{1}{2} O_2 \longrightarrow CO_2$
  - Cold-char $\longrightarrow$ Hot-char (pseudo reaction to model char heating)
- Radiation
  - Nongray CO_2, CO and char
  - P–1 RTE solver
  - Split radiative heat source across phases

Temporal behavior

Gas temperature in the free board (r=0.25cm, h=56.5cm)



Solid temperature inside bed (r=0.25cm, h=16.5cm)



Gas

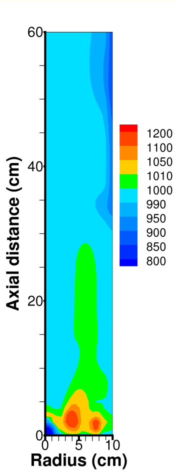
- Lower temperature due to radiation
- Larger temperature fluctuation due to radiative gas concentration variation

Solid

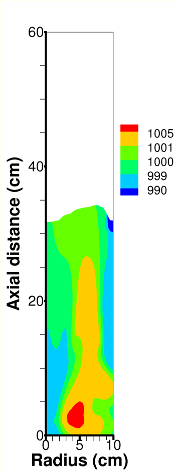
- Temperature drops due to radiation
- Larger fluctuation due to convection of cooler particle from freeboard-bed interface

Instantaneous Flow Fields

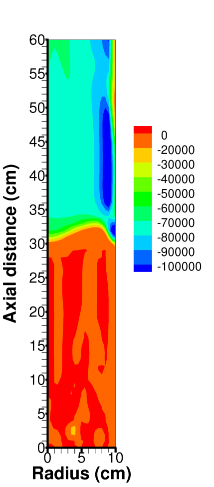
Gas temperature (K)



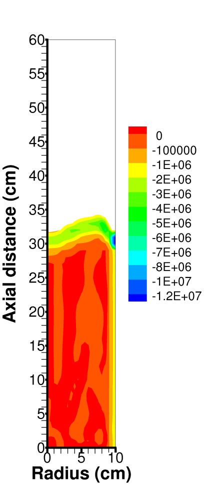
Solid temperature (K)



Gas radiative heat source (W/m^3)



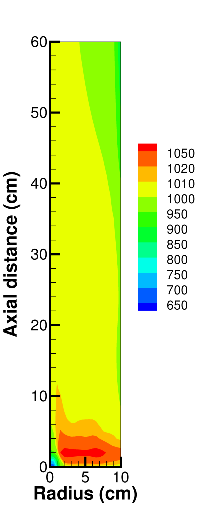
Solid radiative heat source (W/m^3)



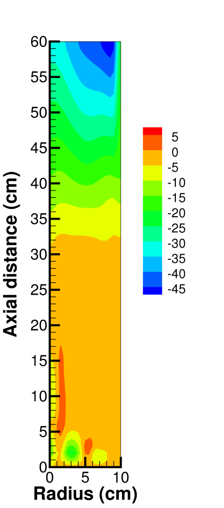
Time Averaged Temperature

Time averaged gas temperature (K)

Without radiation



ΔT with radiation



Time averaged solid temperature

- Relatively unaffected
- ΔT 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