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_2O, 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 $^\circ$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
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
  - 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
- 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
- CFD simulation
  - Radiative heat transfer in a fluidized-bed coal combustor (P-1 with CO2-char k-distribution)

RTE Solution Module

P–1 Solver:

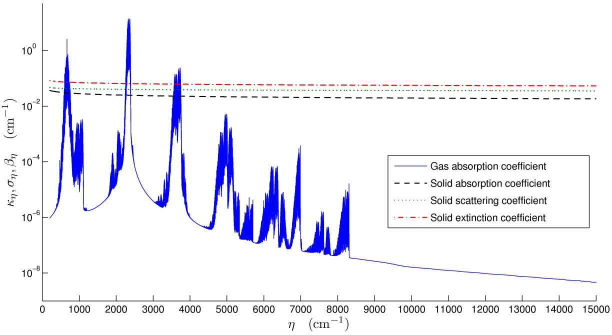
- Ideal RTE solver for expected large optical thicknesses
- Single-scale full-spectrum k-distribution, assembled from narrow-band data for particulates and gas k-distributions
- One RTE solution, but separate emission and absorption terms for individual phases

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

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



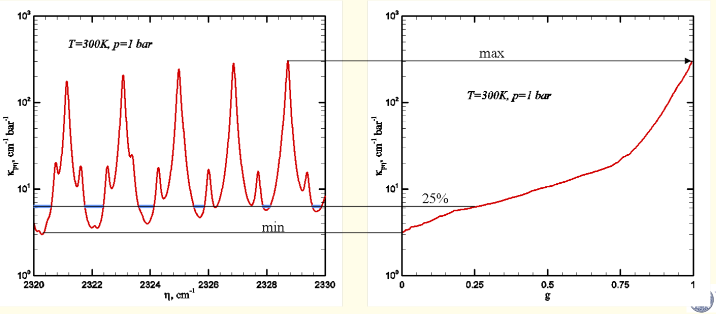
Conditions:

- Temperature 600K
- Gas: 10% CO_2
- Particle: $m = 2.2 - 1.12i$, volume fraction 0.001, diameter 400μm

Spectral Models for Combustion Gases

Narrow Band *k*-Distributions

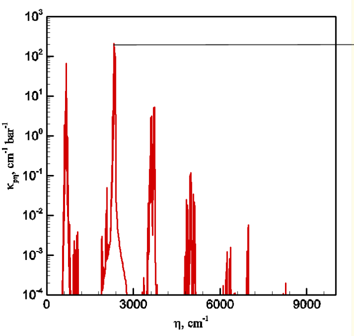
- RTE (without scattering): $\dfrac{dI_\eta}{ds} = \kappa_\eta \left(I_{b\eta} - I_\eta\right)$
- Planck function much better behaved than absorption coefficient, $\approx$ const over small part of spectrum $\Delta\eta$
- Can be reordered into a monotonically increasing function
- On right cumulative *k*-distribution of narrowband spectrum on left
- Requires "correlated" absorption coefficient

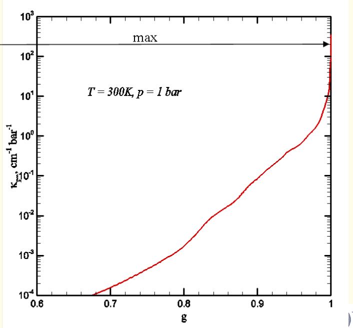


Spectral Models for Combustion Gases, cont'd

Full-Spectrum *k*-Distribution

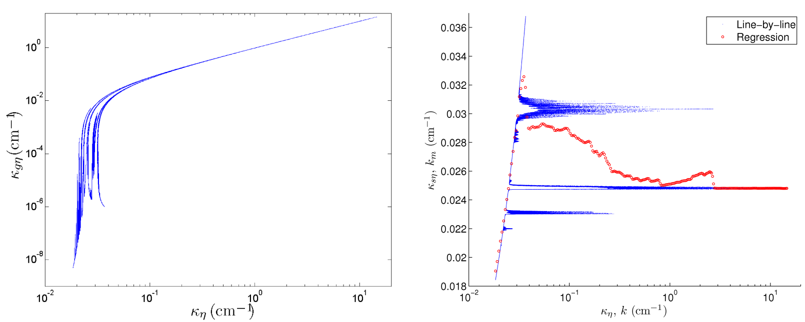
- On right cumulative full-spectrum *k*-distribution of CO_2 absorption coefficient at 300 K, 1 bar on left
  - Very steep at k_{max}
  - Covers many orders of magnitude
  - Part of spectrum has "zero" κ_η
  - 6–10 RTE evaluations as opposed to $>$1,000,000 for LBL
  - Requires "correlated" absorption coefficient





Extension to gas-particle flows

- Reordering by *total* absorption coefficient
  - Spectral information is lost
  - Difficult to track fraction of gas or particle contribution
  - Multiple solid absorption coefficient values may correspond to the same total absorption coefficient (right figure)
- Correlation assumption requires gas and particle absorption coefficient to be correlated with total absorption coefficient
  - Gas correlation is approximately valid (left figure)
  - Solid correlation is not valid (right figure)



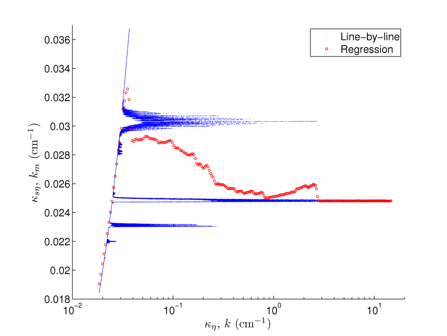
Regression

- 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

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



k-distribution for gas-particle mixtures

Challenge	Solution
Nongray absorption coefficients	k-distribution, reordering by total absorption coefficient at reference state
Gas emission, absorption	Gas absorption correlation with total absorption coefficient
Solid emission, absorption	“Effective” absorption coefficient from regression
Total emission, absorption	Conserved through summation over phases
Multiple temperature emission	Exact (assuming gas is correlated)
Scattering	Gray

Sample calculation–inhomogeneous medium

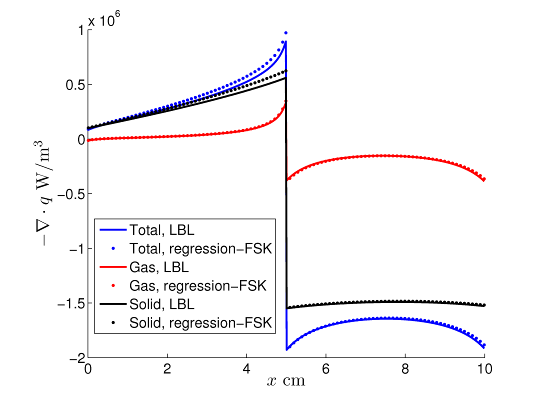
- One dimensional slab with two layers

	Left	Right
Width	5cm	5cm
Gas		
Temperature	600K	1200K
Composition	5%CO_2, 95%(N_2+O_2)	10%CO_2,90%(N_2+O_2)
Paticles		
Temperature	500K	1300K
Diameter	200μm	100μm
Volume fraction	10^{-3}	2.5×10^{-4}
Refractive index	$2.2 - 1.12i$	

- RTE solver P_1
- 64 quadrature points

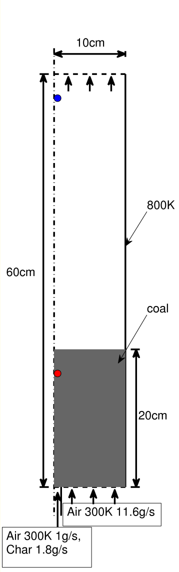
Sample calculation–inhomogeneous medium, cont'd

- 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%



Test Configuration

- 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 particle, 1000K

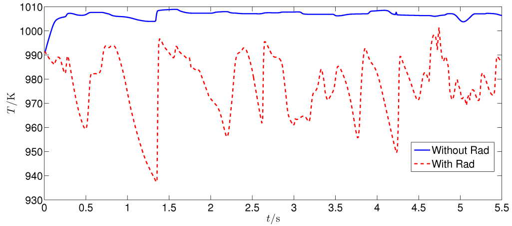


Test Configuration cont’

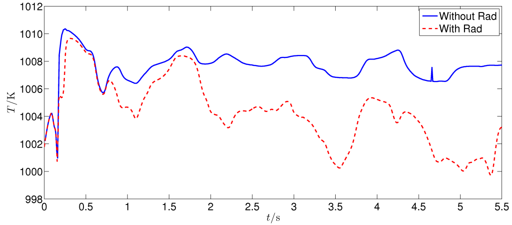
- Reactions
  - $C + \frac{1}{2} O_2 \longrightarrow CO$
  - $C + CO_2 \longrightarrow 2CO$
  - $CO + \frac{1}{2} O_2 \longrightarrow CO_2$
  - Cold-char $\longrightarrow$ Hot-char (pseudo reaction to model char heating)
- Radiation
  - Nongray CO_2, CO and char
  - P–1 RTE solver
  - Split radiative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

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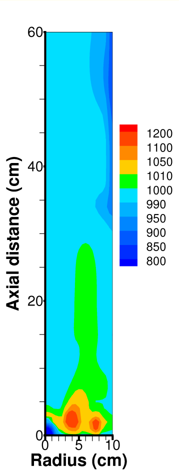
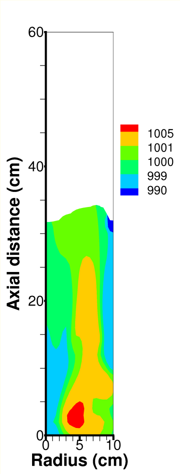
Instantaneous Flow Fields

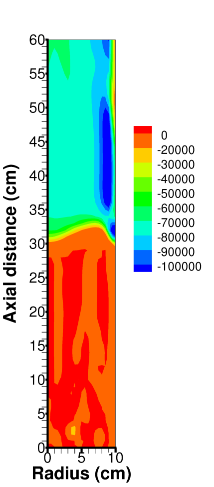
Gas temperature (K)



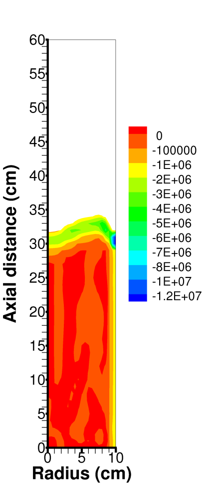
Solid temperature (K)



Gas radiative heat source (W/m^3)



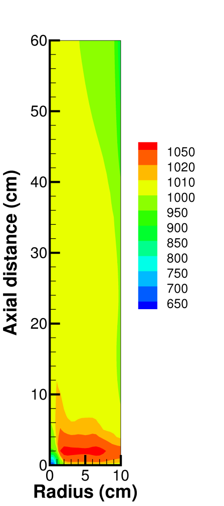
Solid radiative heat source (W/m^3)



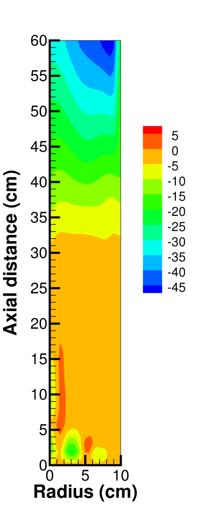
Time Averaged Temperature

Time averaged gas temperature (K)

Without radiation



ΔT with radiation



Time averaged solid temperature

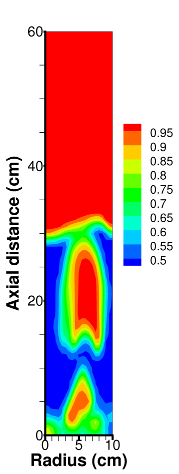
- Relatively unaffected
- ΔT from +5 to -15K

Effort for Next Year

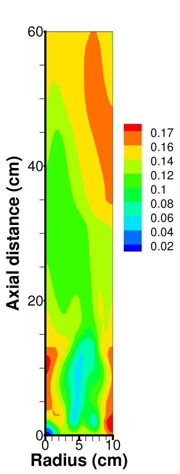
- Implement turbulent mixing and combustion model
- Implement higher-level char combustion kinetics
- Set up simulation of radiative heat transfer in a pulverized coal combustor
- Comparisons between P-1 and Monte Carlo RTE solver
- Comparisons between various spectral models

Instantaneous Flow Fields

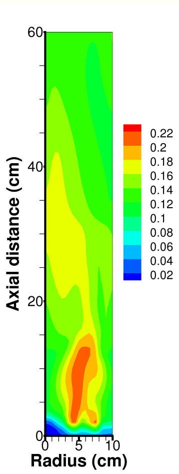
Void Fraction



CO Mass Fraction



CO_2 Mass Fraction



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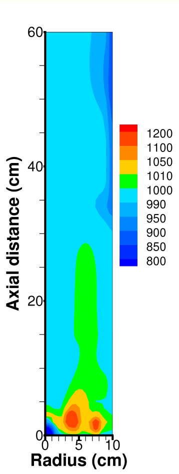
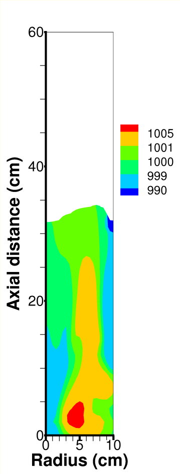
Instantaneous Flow Fields

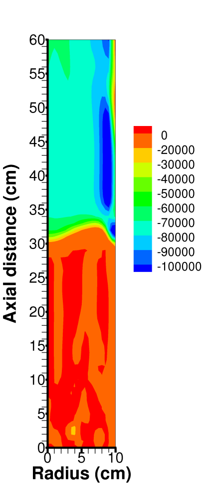
Gas temperature (K)



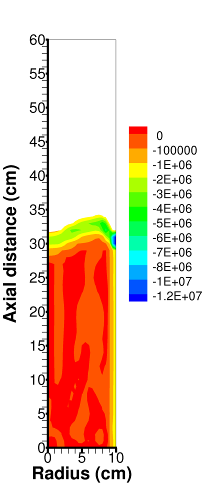
Solid temperature (K)



Gas radiative heat source (W/m^3)



Solid radiative heat source (W/m^3)



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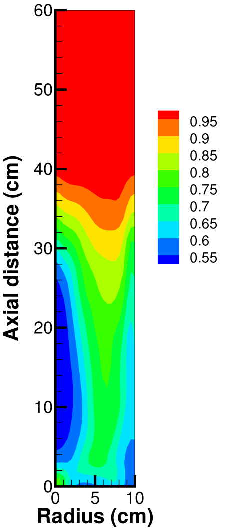
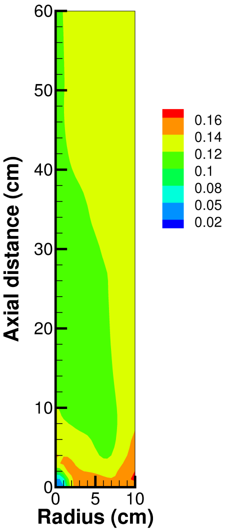
Time Averaged Flow Fields

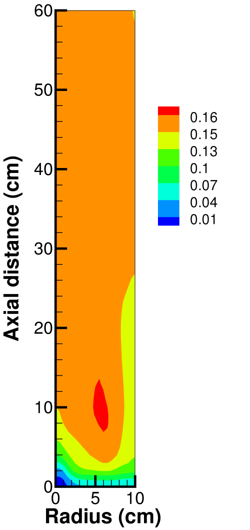
Void Fraction



CO Mass Fraction



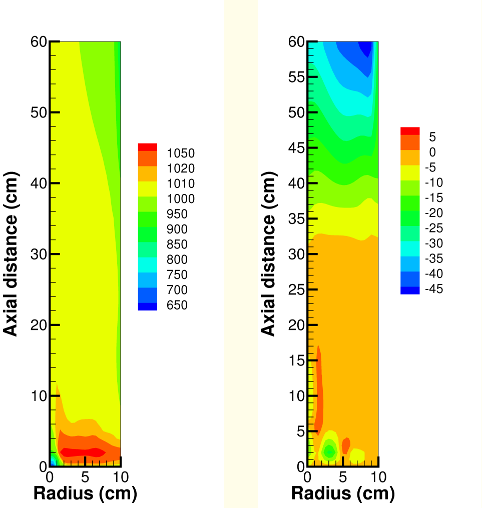
CO_2 Mass Fraction



Time Averaged Temperature

Time averaged gas temperature (K)

Without radiation ΔT with radiation



Time averaged solid temperature

- Relatively unaffected
- ΔT from +5 to -15K

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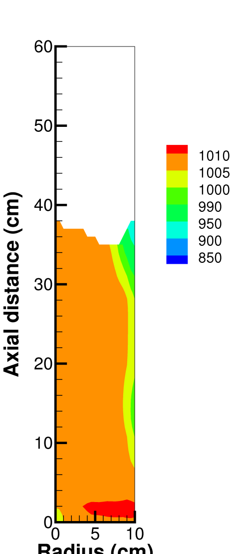
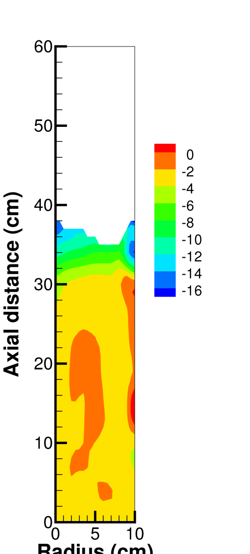
Time averaged flow field

Solid temperature without radiation (K)

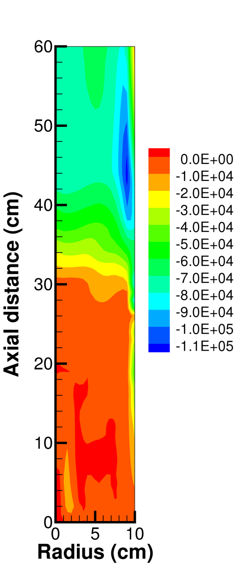


Solid temperature difference with radiation (K)



Time averaged flow field

Gas radiative heat source (W/m^3)



Solid radiative heat source (W/m^3)