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 °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 CO_2 and H_2O 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

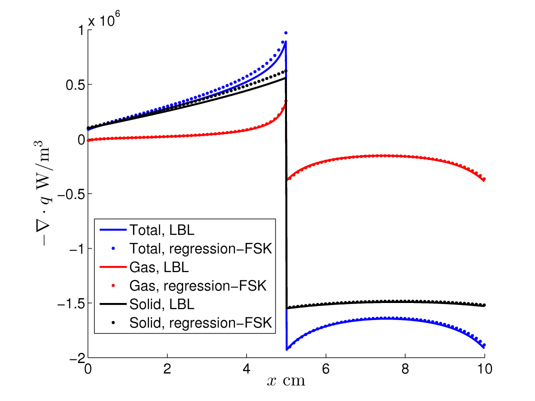
- One dimensional slab with two layers

	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	$2.2 - 1.12i$	

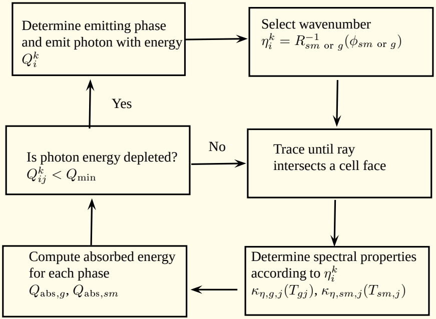
- RTE solver P_1
- 64 quadrature points

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%



Line-by-line Photon Monte-Carlo



1. Emission splitting
2. Extended wavenumber selection scheme
3. Random number relations based on Buckius and Hwang correlations
4. Absorption splitting across gas and solid-phases

- 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.

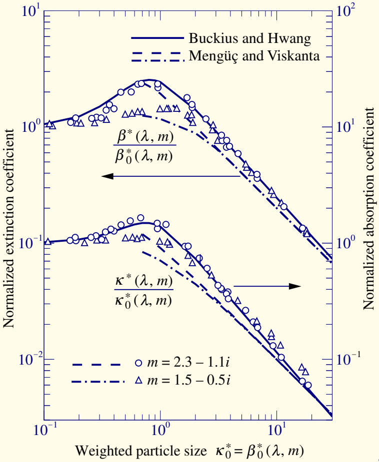
Buckius and Hwang Correlations

$$f_A = \int_0^\infty \pi a^2 n(a) \mathrm{d}a = \frac{3 f_v}{4\bar{r}}$$

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

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

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



[a]

[a] Buckius, R. O., and Hwang, D. C., 1980. "Radiation properties for polydispersions: Application to coal". ASME Journal of Heat Transfer, 102, pp. 143–159.

Random number relations for solid phases

- Random numbers vs η, T, f_v, f_A, C_0.

$$R_\eta = \frac{\int_0^\eta \kappa_\eta I_{b\eta} \mathrm{d}\eta}{\int_0^\infty \kappa_\eta I_{b\eta} \mathrm{d}\eta} = \frac{\int_0^{\eta^*} \kappa^*_\eta (\xi \times \eta^*) I_{b\eta^*}(\eta^*) \mathrm{d}\eta^*}{\int_0^\infty \kappa^*_\eta (\xi \times \eta^*) I_{b\eta^*}(\eta^*) \mathrm{d}\eta^*} \quad (1)$$

- Random numbers can be reduced to 2 variables.
- Critical value at $\xi \approx 0.001$ and $\xi \approx 0.1$

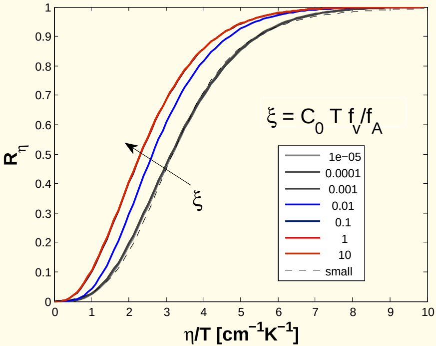
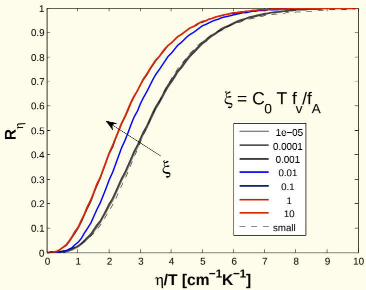
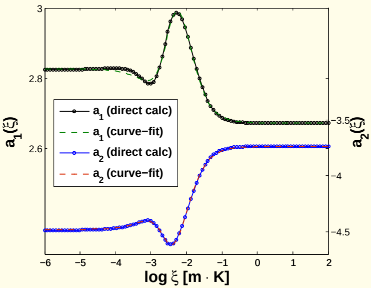


Figure : Random number vs η and T. The curve fitting is applied to the parametric function $f(\eta/T) = 1/2 + 1/2\tanh(a_1(\eta/T)^{0.4} + a_2)$.

Curve-fitting coefficients for Random Number Relations

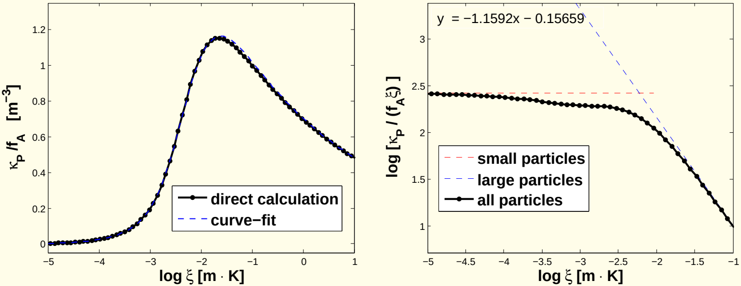




$$a_1(\xi) = \frac{2.826}{\exp(c_{12}(\log_{10}\xi + c_{11})) + 1} + \frac{2.673}{\exp(-c_{14}(\log_{10}\xi + c_{13})) + 1}$$

$$a_2(\xi) = \frac{-4.480}{\exp(c_{22}(\log_{10}\xi + c_{21})) + 1} + \frac{-3.738}{\exp(-c_{24}(\log \xi_{10} + c_{23})) + 1}$$

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

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

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

where

$$\kappa_{g,i} = \left(\sum_n \kappa_{\eta_{p,n}} x_i\right) p_{g,i}$$

$$\kappa_{s,m,i} = f_A \kappa_{\eta_{s,m}}^{*}(\xi_{m,i})$$

$$\xi_{m,i} = C_{0,m}\varepsilon_{s,m}/f_A T_{s,m,i}$$

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

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

Emission

$$Q_{\text{emi},g,i} = 4\pi\bar{\kappa}_{g,i}\sigma T_{g,i}^4 V_i$$

$$Q_{\text{emi},s,m,i} = 4\pi\bar{\kappa}_{s,m,i}\sigma T_{s,m,i}^4 V_i$$

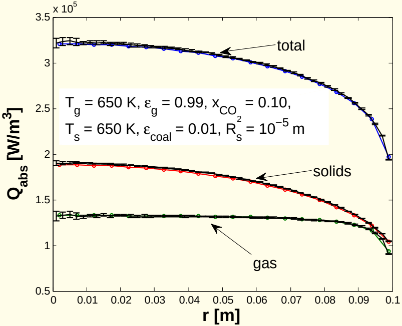
where

$$\bar{\kappa}_{g,i} = \left(\sum_n \bar{\kappa}_{p,n} x_i\right) p_{g,i}\varepsilon_{g,i}$$

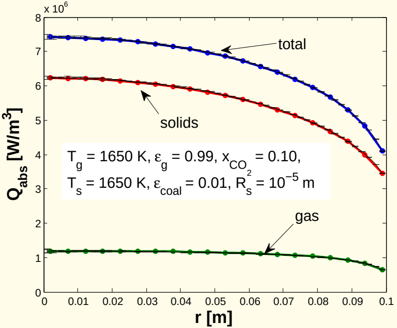
$$\bar{\kappa}_{s,m,i} = \frac{\varepsilon_{s,m,i}}{\bar{r}}\bar{\kappa}_{s,m}^{*}(\xi_{m,i})$$

$$\xi_{m,i} = C_{0,m} 4/3\bar{r} T_{s,m,i}$$

Example calculations



(a) Mixture at 650K



(b) Mixture at 1650K

Figure : line-by-line PMC and exact solutions of Q_{abs} for gas- and solid-phase mixture enclosed by a cylinder.

Fluidized bed

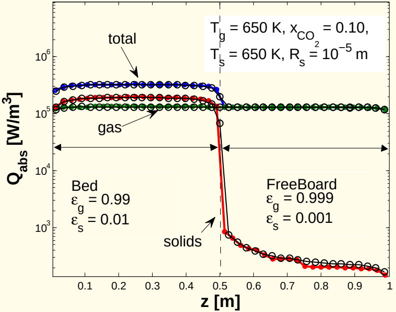


Figure : Colored lines are from exact solution. Black lines are PMC calculations.

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