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Spectral Photon Monte Carlo With Energy Splitting Across Phases for Gas–Particle Mixtures

In multiphase modeling of fluidized beds, pulverized coal combustors, spray combustors, etc., where different temperatures for gas and solid phases are considered, the governing equations result in separate energy equations for each phase. For high-temperature applications, where radiation is a significant mode of heat transfer, accurately predicting the radiative source terms across each individual phase is an essential task. A spectral photon Monte Carlo (PMC) method is presented here with detailed description of the implementation features, including the spectral treatment of solid particles, random number correlations, and a scheme to split emission and absorption across phases. Numerical results from the PMC method are verified against direct numerical integration of the radiative transfer equation (RTE), for example, problems including a cylindrically enclosed homogeneous gas–particulate medium and a simple fluidized bed example. The PMC method is then demonstrated on a snapshot of a pulverized-coal combustion simulation. [DOI: 10.1115/1.4030959]

Keywords: heat transfer, radiation, photon Monte Carlo, multiphase media, Buckius and Hwang correlations

1 Introduction

Advanced multiscale and multiphase simulation tools play central roles in the development of clean and efficient coal combustion systems, including fluidized bed combustors, pulverized coal combustors, and oxyfuel combustors aiming at sequestration of the abundant carbon dioxide resulting from coal combustion. Radiation is a major contributor to heat transfer in all such two phase combustion systems, especially at high temperatures and low particle loading. In fluidized beds radiation (and heat transfer overall) is often dominated by particle-to-wall and particle-to-particle transfer [1], while in standard pulverized-coal combustors strong nongray gas radiation will also become important. In upcoming oxyfuel combustors, replacing nonradiating nitrogen by strongly radiating carbon dioxide, radiation becomes ever more important, and the nongray radiation from combustion gases may dominate the heat transfer in parts of the combustor. Despite the great importance of thermal radiation in such combustion systems, the quality of radiation models employed is generally inadequate, being either absent altogether or limited to trivial T^4 relationships.

Several multi-RTE approaches have been derived and applied to study heterogeneous gas–solid systems including gas-saturated particulate media [2–5]. Basically, there are two approaches: (1) a single average intensity field in a two-phase medium is assumed with appropriate terms representing different phases in the single RTE and (2) the average intensity field is decomposed into average intensities associated with individual phases, and there is one RTE per phase. Analytical and experimental studies showed that for large semitransparent particles in packed beds, approach (1) may result in considerable errors [6–8]. It has also been shown that approach (1) can be obtained by simply reducing the multiple RTEs of approach (2) to a single one in several situations, e.g., if the volume fraction of one phase (e.g., gas) is much larger than

that for the other one (e.g., particles). In the present work, approach (1) is employed, since the solid media of interest here are large number of small coal particles whose radiative properties may be represented by continuum relationships.

In models of gas–particle mixtures in fluidized bed combustors, individual gas and solid phases are treated with separate energy equations for each phase [9]. On the other hand, the RTE is a single equation for computing the radiative heat source [10]. In order to account for radiation in the separate energy equations, the radiative source must be split across gas and solid phases. Currently, there is a lack of such spectral radiation models applicable for multiphase computational fluid dynamics (CFD) simulations. One exception is a recent paper by Cai and Modest [11], which introduces an extended full-spectrum k -distribution regression scheme which splits the radiative source terms. Their full-spectrum k -distribution model was combined with the P_1 -approximation as the RTE solver and tested on a 1D fluidized bed for various gas–particle mixture parameters. This method is essentially a two-component radiation model, which uses a full-spectrum k -distribution as the spectral model and the P_1 -approximation as the RTE solver. The test cases presented in Ref. [11] were compared with a line-by-line (LBL) solution using, again, the P_1 -approximation as the RTE solver. When compared to the LBL solution, the k -distribution spectral model was shown to accurately predict the splitting of the radiation source terms. Another example of modeling the spectral radiation in a fluidized bed can be found in the work presented by Zedtwitz et al. [1,12], where a spectral Monte Carlo was developed to determine the radiative source terms within a fluidized bed, which receives concentrated thermal irradiation. This spectral model includes the splitting of absorbed radiation across gas and solid phases by statistically determining the absorbing phases [12] or scattering events. The spectral-dependence of the absorption coefficients for the gas species was based on the correlations given in Ref. [13], and for the solids the spectral dependence of scattering and absorption were based on Ref. [14].

The PMC method has been implemented in several CFD simulations of combustion, due to the continuous improvements in numerical methods and computer capabilities. Snegirev [15]

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incorporated a PMC method into a CFD code with the weighted-sum-of-gray-gases model in his study of buoyant turbulent nonpremixed flames. Tessé et al. [16,17] developed their PMC methods to model the radiative transfer in a turbulent sooty flame, in which a narrow-band correlated- k model was used for spectral integration. Wang and Modest [18,19] developed several emission and absorption schemes for discrete particle fields, which can be utilized to perform PMC simulations in such media. The PMC method has also been applied in a variety of other participating media. For example, Xia et al. [20] developed a curved Monte Carlo method for radiative heat transfer in media with variable index of refraction. Ruan et al. [21] applied the Monte Carlo method in media with nongray absorbing-emitting anisotropic scattering particles, and Mazumdar and Kersch [22] employed a Monte Carlo scheme for thermal radiation in semiconductor processing applications.

The PMC/LBL scheme developed by Wang and Modest [23], and later improved for computational efficiency by Ren and Modest [24], provides a basis for the current work. Although these PMC/LBL schemes have been applied for problems including soot radiation [25], the previous PMC/LBL models did not account for energy splitting across phases and have not been extended to include radiation with larger solid particles. This paper extends previous PMC/LBL approaches by incorporating a scheme for energy splitting across gas-particle phase, which complies with the multi-RTE approach that assumes a single averaged intensity. The current PMC implementation has several extensions to conventional PMC models employed for single gas phase media, including emission and absorption splitting across phases, an extended wavenumber selection scheme, and random number correlations for solid particles. Details of these procedures are presented in the following sections followed by numerical results. Geometrical aspects of ray tracing in axisymmetric media (as employed with examples presented here) can be found in Ref. [26].

2 Overview and Assumptions of PMC/LBL Energy Splitting Approach

The PMC method statistically simulates the process of radiative transfer using statistically emitted photon bundles. Photon bundles are absorbed throughout the domain as they are traced from one cell to the next. The strength of each photon bundle is proportional to the local emission potential of the cell it is emitted from. The directions and emission points of the rays are selected randomly within each cell. In spectral PMC, each emitted photon bundle is assigned a wavenumber so that during tracing each ray's energy is diminished according to the spectral absorption potential of the cells that the ray traverses. Once a ray's energy is depleted, another photon bundle is emitted and is traced, and so on, until all the emission of the medium has been accounted for.

The spectral PMC method can be summarized by the following set of procedures:

- (1) For each cell and each gas-particle phase, the number of photons that will be traced is determined. For each photon bundle, the direction and exact point of emission within the cell is statistically assigned.
- (2) For each emitted photon bundle, a wavenumber based on random-number relations is selected.
- (3) Each photon bundle is traced until an intersection with a cell face is reached, then the distance traversed by the ray through the cell is computed.
- (4) The absorption coefficients and optical thickness for the absorbing cells are determined.
- (5) The absorbed energies of individual phases are subtracted according to the absorption splitting scheme.
- (6) The corresponding absorbed energy is subtracted from the photon bundle and the total absorbed energy of the intersected cell is incremented.

Procedures 3–6 are continued until the photon bundle's energy is depleted, then the process is repeated from the beginning for the next photon bundle. After tracing all photon bundles, the radiative source, as it appears in the overall energy equation, is calculated as $\nabla \cdot \mathbf{q}_{\text{rad}} = Q_{\text{emi}}''' - Q_{\text{abs}}'''$, which is emission minus absorption on a per cell volume basis.

Certain assumptions are made in the current presentation: (1) all walls are gray, (2) negligible scattering, (3) constant index of refraction, and (4) absorption coefficients of particles are modeled by Buckius and Hwang correlations. Assumptions (1) and (2) are generally justified for near-black coal particles, although scattering and nongray walls are easily accommodated by PMC methods [27].

3 Emission Splitting Across Phases

3.1 Emission Energy Carried by Photon Bundles. A medium's total emission, Q_{emi} , is equal to the sum of the emission from the gas and the solid phase components. These quantities are computed on a cell basis as

$$Q_{\text{emi},i} = Q_{\text{emi},g,i} + \sum_{m=1}^{M_s} Q_{\text{emi},s,m,i}, \quad (1)$$

where

$$Q_{\text{emi},(g) \text{ or } (s,m),i} = 4\pi \bar{\kappa}_{(g) \text{ or } (s,m),i} I_b(T_{(g) \text{ or } (s,m),i}) V_i, \quad (2)$$

where $\bar{\kappa}$ denotes the Planck-mean absorption coefficients, M_s is the number of solid phases, V_i is the cell volume, and I_b is the blackbody intensity ($I_b = \sigma T^4/\pi$, also called Planck function). The gas phase Planck-mean absorption coefficient is computed as the summation of the individual gas species Planck-mean absorption coefficients $\bar{\kappa}_{g,n}$

$$\bar{\kappa}_g = \left(\sum_{n=1}^{M_g} x_n \bar{\kappa}_{g,n} \right) p_g \varepsilon_g, \quad (3)$$

where x_n is the mole fraction of the n th gas species, $\bar{\kappa}_{g,n}$ is the pressure based Planck-mean absorption coefficient of gas species n , p_g is the total gas pressure, ε_g is the gas volume fraction, and M_g is the number of gas species. Whether a gas species or a solid phase, individual Planck-mean absorption coefficients are calculated from spectral absorption coefficients by

$$\bar{\kappa} = \frac{\pi}{\sigma T^4} \int_0^\infty \kappa_\eta I_{b,\eta} d\eta \quad (4)$$

The number of photon bundles emitted from a given cell N_i is determined by

$$N_i = \frac{Q_{\text{emi},i}}{Q_{\text{emi}}} N_{\text{tot}} \quad (5)$$

where Q_{emi} is the total emission from the medium ($Q_{\text{emi}} = \sum_i Q_{\text{emi},i}$), and N_{tot} is a predetermined total number of photon bundles emitted by the internal medium. Equation (5) states that the relative proportion of photon bundles from the i th cell is proportional to the relative emission from the cell. The sum of the number of photon bundles emitted by each phase, $N_{g,i}$ and $N_{s,m,i}$, must satisfy, on a cell basis

$$N_i = N_{g,i} + \sum_{m=1}^{M_s} N_{s,m,i} \quad (6)$$

For optimal statistical sampling, every photon bundle emitted from a given cell should carry equal amounts of energy leading to

$$N_{(g) \text{ or } (s,m),i} = \frac{Q_{\text{emi},(g) \text{ or } (s,m),i}}{Q_{\text{emi},i}} N_i \quad (7)$$

which must be rounded to integers because $N_{g,i}$ and $N_{s,m,i}$ are integer-valued. The emission energy carried by photon bundle k is then adjusted to

$$Q_i^k = \frac{Q_{\text{emi},g,i}}{N_{g,i}} \text{ or } \frac{Q_{\text{emi},s,m,i}}{N_{s,m,i}} \simeq \frac{Q_{\text{emi},i}}{N_i} \quad (8)$$

3.2 Emission From Walls. Emission from a wall is treated by increasing the overall total number of photon bundles. Assuming the walls are gray, the emission from the i th wall face is calculated as

$$Q_{\text{emi},w,i} = \epsilon_{w,i} \sigma A_{w,i} T_{w,i}^4 \quad (9)$$

where $\epsilon_{w,i}$, $A_{w,i}$, and $T_{w,i}$ are, respectively, the wall face emittance, surface area, and temperature. To keep strengths of photon bundles from the wall faces at the same level, their number $N_{w,i}$ is proportional to the wall emission of the face

$$N_{w,i} = \frac{Q_{\text{emi},w,i}}{Q_{\text{emi}}} N_{\text{tot}} \quad (10)$$

where Q_{emi} and N_{tot} are the total internal emission and number of photon bundles, respectively. By including wall emission, the overall number of photon bundles emitted in the PMC method becomes $N_{\text{tot}} + \sum_i N_{w,i}$. The energy of a photon bundle emitted from a wall is then adjusted to

$$Q_i^k = \frac{Q_{\text{emi},w,i}}{N_{w,i}} \quad (11)$$

After determining the emission strengths and locations of photon bundles emitted from the wall faces, they are traced and absorbed in the same manner as photon bundles emitted by interior cells.

3.3 Wavenumber Selection. Wavenumber selection requires inverting the random-number relations

$$R_\eta = \frac{\int_0^\eta \kappa_\eta I_{b\eta} d\eta'}{\int_0^\infty \kappa_\eta I_{b\eta} d\eta'} \quad (12)$$

to obtain η as function of R_η , where R_η is a uniformly distributed random number. The current implementation of the PMC utilizes the LBL spectral scheme developed by Ren and Modest [24] for combustion gas mixtures. This spectral model, referred to here as the hybrid selection scheme (HSS), involves first selecting an emitting gas species, then determining wavenumbers based on the specific random-number relations of the selected gas species. Following this approach of independence of emission for all gas species and solid phases, emission wavelengths for solid phases are also determined independently.

3.3.1 Wavenumber Selection for Gas Mixtures Using the HSS Scheme. The procedure of the HSS consists of the following steps:

- (1) A uniformly distributed random number, $0 < R_{\eta,g} < 1$ is selected.
- (2) From that random number, the emitting species is selected, denoted by subscript n^* , that satisfies the condition

$$\frac{\sum_{n=1}^{n^*-1} E_n}{E_{\text{tot}}} < R_{\eta,g} \leq \frac{\sum_{n=1}^{n^*} E_n}{E_{\text{tot}}} \quad (13)$$

where

$$E_n = \int_0^\infty \kappa_{\eta,g,n} I_{b\eta} d\eta = \bar{\kappa}_{g,n} \sigma T_g^4 \quad (14)$$

is the emission of gas species n , and

$$E_{\text{tot}} = \sum_{n=1}^{M_g} E_n \quad (15)$$

- (3) The wavenumber η is determined from the random number relations of the selected gas species, with a random number rescaled from $R_{\eta,g}$ [24].

The selection criterion of Eq. (13) effectively splits the emission of photon bundles among gas species by comparing random numbers to the relative emissions of each gas species. In contrast, Eq. (7) splits the emission of photon bundles among phases prior to emitting any photon bundles, thereby avoiding steps for random number generation and phase selection. Either approach is valid since the photon bundle distributions are based on preserving relative gas species and gas-particle phase emissions.

A database for each gas species' random numbers versus temperature and emission wavenumbers built from spectroscopy data sets of fractional emission, such as HITEMP [28], must be available for the HSS scheme. Wavenumbers are determined from the database by using linear interpolation for T_g and using a bisectional search for η [24].

3.3.2 Wavenumber Selection for Solid Phases Derived From Buckius and Hwang Correlations. In this PMC implementation, we consider previously derived correlations of spectral absorption coefficients for solid particles $\kappa_{\eta,s}$, which can be found in [10,29]. With these empirically derived correlations as a starting point, we derive correlations of random numbers versus wavenumbers and other physical properties of particles. The convenience of producing these random-number relations is that it avoids the need for databasing and inverting Eq. (12) is trivial, thereby saving on computational effort.

The particle absorption coefficient correlations of Buckius and Hwang [29] define a normalized absorption coefficient

$$\kappa_{\eta,s}^* = \kappa_{\eta,s} / f_A \quad (16)$$

where f_A is the total cross-sectional area per unit volume defined as

$$f_A = \int_0^\infty \pi r^2 n(r) dr \quad (17)$$

where r is the radius of the particles and $n(r)$ is the per volume number density. The mean particle radius $\bar{r}$ is related to f_A by

$$\bar{r} = \frac{3\epsilon_s}{4f_A} \quad (18)$$

where ϵ_s is the solid volume fraction. The correlations for the normalized absorption coefficients utilize the small particle limit value

$$\kappa_{\eta,s,0}^* = C_0 \frac{\epsilon_s}{f_A} \eta \quad (19)$$

where C_0 is a property constant that depends on the particle's complex index of refraction

$$C_0 = \frac{36\pi n k}{(n^2 - k^2 + 2)^2 + 4n^2 k^2} \quad (20)$$

where the n and k are the real and imaginary components of the complex index of refraction of the solid particles. For reference, complex indices of refraction of selected solids are provided in Table 1.

The Buckius and Hwang correlation equation for particle absorption coefficients is [10,29]

$$\kappa_{\eta,s}^* = \left[\frac{1}{\left(\kappa_{\eta,s0}^* (1 + 2.30 \kappa_{\eta,s0}^{*2}) \right)^{1.6}} + \frac{\kappa_{\eta,s0}^{*0.256}}{1.66^{1.6}} \right]^{-1/1.6} \quad (21)$$

According to Eq. (12), the fraction $R_{\eta,s}$ of energy emitted by particles at wavenumbers below η , depends on three variables: $\kappa_{\eta,s0}^*$, η , T_s . The following combination of variables helps to simplify development of subsequent correlations by reducing the number of dependent variables from 3 to 2: letting

$$\xi = \frac{\eta}{T_s} \quad (22)$$

and

$$\gamma = C_0 \frac{\varepsilon_s}{f_A} T_s \quad (23)$$

The dependent variable of Eq. (21) becomes

$$\kappa_{\eta,s0}^* = \gamma \xi \quad (24)$$

and the random number relation, Eq. (12), can be re-expressed in terms of the new grouped variables γ and ξ as

$$R_{\eta,s} = \frac{\int_0^\xi \kappa_{\eta,s}^*(\gamma \xi') I_{b\xi}(\xi') d\xi'}{\int_0^\infty \kappa_{\eta,s}^*(\gamma \xi') I_{b\xi}(\xi') d\xi'} \quad (25)$$

where $\kappa_{\eta,s}^*$ becomes a function of the product $\gamma \xi$ and $I_{b\xi}$ is a modified Planck function defined as

$$I_{b\xi} = \frac{I_{b\eta}}{T_s^3} = \frac{C_1 \xi^3}{\pi (\exp C_2 \xi - 1)}$$

where $C_1 = 3.7418 \times 10^{-16} \text{ W m}^2$ and $C_2 = 1.4388 \text{ cm K}$. Focusing on $\kappa_{\eta,s}^*$, separate regimes for small, intermediate, and large particles can be readily observed. In the limiting case of very small particles, where $\kappa_{\eta,s0}^* \ll 1$, Eq. (21) yields

$$\kappa_{\eta,s}^* \approx \gamma \xi \quad (26)$$

At the other extreme of very large particles, where $\kappa_{\eta,s0}^* \gg 1$, Eq. (21) simplifies to

$$\kappa_{\eta,s}^* \approx 1.66 (\gamma \xi)^{-0.16} \quad (27)$$

Since γ can be factored out of the integrals in Eq. (25) for the extreme situations, $R_{\eta,s}$ can be expected to be sensitive to γ only

Table 1 Representative values of complex index of refractions for selected solids [10]

	$m = n - ik$	C_0
Anthracite coal	$m = 2.05 - 0.54i$	3.143
Char (fixed carbon)	$m = 2.20 - 1.12i$	5.023
Ash	$m = 1.50 - 0.02i$	0.189

for intermediately sized particles as confirmed with numerical calculations of $R_{\eta,s}$ shown in Fig. 1(a). Profiles of $R_{\eta,s}$ versus η overlap each other and, thus, no longer change when γ exceeds certain lower ($\gamma < 10^{-4}$) and upper limiting values ($\gamma > 0.1$).

Since the profiles of $R_{\eta,s}$ appear sigmoidal (S-shaped) with respect to ξ and asymptotically approach values of 0 and 1, the hyperbolic tangent function becomes an excellent candidate curve fitting function. Employing the hyperbolic tangent function, the following was found to well approximate $R_{\eta,s}$ for various values of γ

$$R_{\eta,s}(\gamma, \xi) = \frac{1}{2} + \frac{1}{2} \tanh(a_1(\gamma) \xi^{0.4} - a_2(\gamma)) \quad (28)$$

This expression is easily inverted to obtain η (or ξ) as a function of R_{η} and solid particle properties through the dependence on the fitting coefficients, a_1 and a_2 , which are in turn functions of γ . The fitting coefficients were successively determined by incrementally stepping through $\lg \gamma$ for $-6 < \lg \gamma < 1$, where $\lg$ is the base 10 logarithm function, holding γ constant each time and applying least-square minimization to Eq. (28). A plot for the values of a_1 and a_2 in the range mentioned is shown in Fig. 1(b). When γ is too

(a)

(b)

Fig. 1 Random-number relations and regression coefficients for particles as functions of grouped variables γ and ξ . The regression coefficients a_1 and a_2 were computed *directly* using least squares regression from the random-number relations, then *approximated* through a second regression function. (a) Random-number relations for solids and (b) regression coefficients.

small ($\gamma < 10^{-4}$) or larger ($\gamma > 10^{-1}$), the coefficients a_1 and a_2 go to values expected from the limiting case analysis of Eq. (21).

Using simple power functions with correct asymptotic behavior for $\gamma \rightarrow 0$ and $\gamma \rightarrow \infty$, the coefficients a_1 and a_2 as functions of γ are fitted according to

$$a_1(\gamma) = \frac{b_{11}}{c_{11}\gamma^{c_{12}} + 1} + \frac{b_{12}}{c_{13}\gamma^{-c_{14}} + 1} \quad (29)$$

$$a_2(\gamma) = \frac{b_{21}}{c_{21}\gamma^{c_{22}} + 1} + \frac{b_{22}}{c_{23}\gamma^{-c_{24}} + 1} \quad (30)$$

Values of the coefficients b_{ij} and c_{ij} , for $i = 1, 2$, and $j = 1, \dots, 4$, determined through least squares minimization, are given in Table 2.

3.4 Planck-Mean Absorption Coefficients Derived From Buckius and Hwang Correlations. The Planck-mean absorption coefficients are directly calculated using the Buckius and Hwang [29] correlations for κ_s given by Eq. (21), and using the grouped variables defined by Eqs. (22) and (23)

$$\bar{\kappa}_s^*(\gamma) = \bar{\kappa}_s/f_A = \frac{\pi}{\sigma} \int_0^\infty \kappa_s^*(\gamma\xi) I_{b\xi}(\xi) d\xi \quad (31)$$

Here $\bar{\kappa}_s^*$ is a normalized Planck-mean absorption coefficient, which depends only on γ . Data obtained from direct numerical evaluations of Eq. (31) for $-6 < \lg \gamma < 1$ are plotted in Fig. 2(a) as a function of $\lg \gamma$. For the purpose of producing fitting correlations, it is more convenient to consider the variation of $\lg(\bar{\kappa}_s^*/\gamma)$ as a function of $\lg \gamma$ as shown in Fig. 2(b). For the limiting small particle case, the quantity $\lg(\bar{\kappa}_s^*/\gamma)$ approaches a constant value, while for the large particle limiting case, this quantity approaches a linear relation with respect to $\lg \gamma$, as indicated by the line equation in Fig. 2(b). Both of these limiting situations, as well as intermediate situations, can be modeled similar to the fits for a_1 and a_2 leading to

$$\lg\left(\frac{\bar{\kappa}_s^*}{\gamma}\right) = \frac{b_{31}}{c_{31}\gamma^{c_{32}} + 1} + \frac{b_{32} \lg \gamma + b_{33}}{c_{33}\gamma^{-c_{34}} + 1} \quad (32)$$

The fitting coefficients, c_{3j} , with $j = 1, \dots, 4$, and asymptote parameters, b_{3j} , with $j = 1, 2, 3$, are also given in Table 2, and the accuracy of the fit is demonstrated in Figs. 2(a) and 2(b).

4 Absorption Splitting Across Phases

The amount of energy absorbed by cell j from the k th photon bundle emitted from cell i is computed as

$$Q_{\text{abs},ij}^k = Q_{ij}^k (1 - \exp(-\Delta\tau_{\eta,ij}^k)) \quad (33)$$

The quantity in parentheses is the absorptivity of cell j , which depends on the local optical distance $\Delta\tau_{\eta,ij}^k$, and Q_{ij}^k is the energy

Table 2 Correlation coefficients for random number relations (Eqs. (29) and (30)), and Planck-mean absorption coefficient relations (Eq. (32)). Coefficients require units of γ to be (m K).

b_{ij}	$j=1$	$j=2$	$j=3$	
$i=1$	4.4716×10^{-1}	4.2351×10^{-1}		
$i=2$	4.4854	3.7377		
$i=3$	2.4251	-1.1598	-0.15558	
c_{ij}	$j=1$	$j=2$	$j=3$	$j=4$
$i=1$	7.7212×10^4	1.8913	1.4348×10^{-7}	2.5438
$i=2$	8.8771×10^4	1.9467	1.5863×10^{-7}	2.5156
$i=3$	1.2881×10^4	1.3492	8.9608×10^{-5}	1.3986

Fig. 2 Directly calculated and approximated Planck-mean absorption coefficients for particles as functions of γ . The linear function $b_{32} \lg \gamma + b_{33}$ represents the right asymptote of $\lg \bar{\kappa}_s^*/(f_A \gamma)$ versus $\lg \gamma$. (a) Normalized Planck-mean absorption coefficient and (b) ratio of normalized Planck-mean absorption coefficient and solids property variable γ .

of the photon bundle as it enters the absorbing cell. The optical thickness across cell j for the k th ray is computed as

$$\Delta\tau_{\eta,ij}^k = \kappa_{\eta_i^k,j} S_{ij}^k = \left(\kappa_{\eta_i^k,g,j} + \sum_{m=1}^{N_s} \kappa_{\eta_i^k,s,m,j} \right) S_{ij}^k \quad (34)$$

The distance traveled by the ray through the cell is represented by S_{ij}^k as shown in Fig. 3. The gas absorption coefficient is equal to the weighted sum of the gas species absorption coefficients

$$\kappa_{\eta,g,j} = \left(\sum_{n=1}^{N_g} x_{n,j} \kappa_{\eta,n,g,j} \right) p_{g,j} e_{g,j} \quad (35)$$

The solid phase absorption coefficients are computed from the Buckius and Hwang correlations given by Eq. (21).

The energy of a photon bundle diminishes as it traverses each cell as it is traced according to

$$Q_{ij}^k = Q_i^k - \sum_{j' \in \mathbb{J}_{i(j-1)}^k} Q_{\text{abs},ij'}^k \quad (36)$$

Fig. 3 Illustration of a single ray emitted from cell i and traversing cell j . The absorbed energy depends on the absorptivity of cell j , the distance traversed S_{ij}^k , and the energy of the photon bundle as it enters the absorbing cell $Q_{i,j}^k$.

where the set $J_{i(j-1)}^k$ denotes all cells crossed by the k th ray emitted from cell i before intersecting cell j , and Q_i^k is the initial photon bundle energy given by Eq. (8).

The formulation for absorption partitioning across gas and solid phases is based on the following criterion: If, for example, solids $m=1$ and $m=2$ are identical (same $\kappa_{\eta,s,m}$), then energy splitting should give identical results if the two solids were instead analyzed as a single solid phase. Therefore, the amount of energy absorbed by the m th solid phase must be proportional to its volume fraction, or $Q_{\text{abs},sm} \propto \varepsilon_{s,m}$. In addition, absorption by a phase or species should be proportional to its local absorption coefficient. The simplest way to satisfy the above physical criterion is to assign weights for each phase according to

$$w_{\eta_i^k,(g) \text{ or } (s,m),j} = \frac{\kappa_{\eta_i^k,(g) \text{ or } (s,m),j}}{\kappa_{\eta_i^k,g,j} + \sum_{m=1}^{N_s} \kappa_{\eta_i^k,s,m,j}} \quad (37)$$

and the gas and solid phase absorbed energies are computed as

$$Q_{\text{abs},(g) \text{ or } (s,m),j} = \sum_{i,k \in J_j} Q_{\text{abs},ij}^k w_{\eta_i^k,(g) \text{ or } (s,m),j} \quad (38)$$

In contrast to the absorption splitting scheme presented in Ref. [12], the above absorption splitting scheme Eq. (38) avoids random number generation and phase selection steps, and instead splits the absorption by using weights based on the relative strengths of the phase absorption coefficients.

5 Applications

The PMC method is demonstrated with a few sample problems in this section. The configuration of each of the example problems considered here are all 1D or 2D axisymmetric. Therefore, the examples given here are based on the procedures for axisymmetric PMC tracing, as described in Ref. [30]. All calculations were carried out on a single Intel (R) Xeon (R) CPU X7460 running at 2.66 GHz.

5.1 Homogeneous Medium Example. This example consists of a homogeneous medium with a gas phase (10% CO₂, 90% N₂ by mole fraction) and one solid phase where both phases have a temperature of 650 K. The medium is enclosed within a cylinder composed of cold, black side walls ($T_w = 0$ and $\varepsilon_w = 1$) and perfectly specular reflecting lower- and upper-walls, with a cylinder radius of $R = 0.1$ m, and length $L = 1$ m. The volume fraction of the solid phase is set to $\varepsilon_s = 10^{-4}$ and is composed of solid char particles with $\bar{r}_s = 10 \mu\text{m}$ and $C_0 = 5.02$. Under these conditions, $\bar{k}_g = 3.37 \text{ m}^{-1}$ and $\bar{k}_s = 8.65 \text{ m}^{-1}$, and the Planck-mean based

radial optical thickness is $\tau_r = \tau_{r,g} + \tau_{r,s} = 0.337 + 0.865 = 1.202$ (intermediate optical thickness).

The domain was meshed into 50×10 grid (50 cells in the radial direction and 10 cells in the axial direction), N_{tot} was set to 8×10^6 . The models used were the full spectral PMC using LBL spectral data (PMC/LBL), and PMC with gray properties for both gas and particles (PMC/gray). A direct numerical integration of the RTE [27], referred to as *exact*, serves as a target reference for the PMC/LBL. The cross-sectional profile of $Q_{\text{abs}}''' = Q_{\text{abs}}/V$ for each phase as a function of r taken at $z = 0.5$ m is plotted in Fig. 4. Overall, the PMC/LBL yields results very close to the exact solution. This close agreement is to be expected since the PMC/LBL is itself an exact method to within statistical uncertainty.

This example shows that the difference between PMC/LBL and PMC/gray can be quite substantial. Using gray properties, Q_{abs}''' is underestimated for the gas phase, while overestimated for the solid phase. In the nongray analysis, however, the gas emits over a few wavenumbers, where $\kappa_{g,\eta} \gg \kappa_{s,\eta}$, resulting in little gas emission absorbed by the solids. On the other hand, particles emit at all η , but CO₂ absorbs only over a few η , so only a small amount of particle emission is absorbed by the gas phase. Therefore, gray analysis can be particularly poor for gas-particle mixtures.

The sensitivity of the PMC/LBL method to N_{tot} and the meshing is illustrated in Table 3. A coarse mesh case includes 30 cells in the radial direction and 10 cells in the axial direction, or a 30×10 grid. Also included are 40×10 , 50×10 , and 50×20 grids. The number of photon bundles include $N_{\text{tot}} = 10^5$, 10^6 , and 10^7 . For these combinations of grids and N_{tot} , the time elapsed to compute the PMC results on a 2.66 GHz processor, and the relative standard deviations of Q_{abs}''' for the gas and the solid phase were computed. The standard deviation of Q_{abs}''' at the centerline is used to quantify the uncertainty in the PMC calculations. The relative standard deviation is defined as

$$\sigma = \frac{1}{\langle Q_{\text{abs}}''' \rangle} \left[\frac{1}{N} \sum_{i=1}^N (Q_{\text{abs},i}''' - \langle Q_{\text{abs}}''' \rangle)^2 \right]^{1/2} \quad (39)$$

where

$$\langle Q_{\text{abs}}''' \rangle = \frac{1}{N} \sum_{i=1}^N Q_{\text{abs},i}''' \quad (40)$$

Fig. 4 Comparison of PMC/LBL, PMC/gray, PMC/LBL applied separately to the gas and solid phases, and an exact solution for Q_{abs}''' for first example problem. Profiles taken at $z = 0.5$ m.

Table 3 Effects of meshing and number of emitted photon bundles for the homogeneous cylinder problem

Mesh ($N_r \times N_z$)	N_{tot}	t_{elapsed} (s)	σ_{gas} (%)	σ_{solids} (%)
$10 \times 30 = 300$	10^5	1.06	5.01	1.29
	10^6	10.59	2.15	1.19
	10^7	104.95	0.37	0.36
$10 \times 40 = 400$	10^5	1.34	7.99	1.98
	10^6	13.30	2.24	0.70
	10^7	132.32	0.88	0.22
$10 \times 50 = 500$	10^5	1.63	8.96	2.84
	10^6	16.053	3.37	0.84
	10^7	160.72	0.60	0.26
$20 \times 50 = 1000$	10^5	1.68	13.98	5.94
	10^6	16.60	3.25	1.56
	10^7	166.50	1.64	0.33

The two-dimensional mesh is represented as $(N_r \times N_z)$, where N_r and N_z are the number of radial and axial cells, respectively. N_{tot} is the total number of photon bundles, t_{elapsed} is the amount of time elapsed in seconds to fully compute the PMC results, and σ is the relative standard deviation of Q_{abs} calculations, Eq. (39).

and $Q_{\text{abs},i}'''$ is the value of the PMC calculations taken at distinct centerline positions, where $r = 0$ and $z = 0.1, 0.2, \dots, 0.9$ m ($N = 9$). Any variation among $Q_{\text{abs},i}'''$ at the different coordinates along the axis line is a direct result of the inherent random variability in the PMC simulation as, physically, all $Q_{\text{abs},i}'''$ values should vary only radially for this homogeneous problem. The sensitivity of the PMC/LBL accuracy and the time of computations on N_{tot} is much more significant than for the mesh refinements. Further meshing in the axial direction is not as significant because this problem one-dimensional.

5.2 Fluidized Bed Example. Next, we consider a simplistic fluidized bed problem, where the medium consists of a freeboard and bed section. Revising the cylindrical geometry described in the previous example, the lower half ($0 < z < 0.5$ m) of the cylindrical enclosure is made to be the bed section, and the upper half ($0.5 \text{ m} < z < 1$ m) is the freeboard section. In the bed section, solid volume fraction is set to $\varepsilon_s = 10^{-4}$, and in the freeboard section to $\varepsilon_s = 10^{-6}$. The particle physical properties are set to $\bar{r} = 10^{-5}$ m and $C_0 = 5.02$. In both sections the gas phase consists of 10% CO_2 by mole fraction and the rest of the gas mixture is N_2 . The gas and solid phase temperatures are set to $T_g = T_s = 650$ K uniformly in both bed and freeboard sections. The side, lower, and upper walls are all assumed to be cold and black.

This problem is set up so that there is a steep variation in ε_s at $z = 0.5$ m, which results in a commensurate variation in solid phase emission and absorption. Therefore, the mesh is partitioned more finely in the axial direction in order to model steep variations in the z -direction. The mesh is a 40×60 grid (40 cells in the r -direction and 60 cells in the z -direction). The number of photons is set to $N_{\text{tot}} = 10^7$. The computational time of the PMC method for this problem set up was 1380 s.

Profiles of Q_{abs}''' taken along the centerline of the cylindrical enclosure ($r = 0$) are shown in Fig. 5. In the bed section ($z < 0.5$ m), where the volume fraction of the solid phase is greater, most of the radiation is due to the solid phase, while in the freeboard section ($z > 0.5$ m), gas phase radiation is dominant. This example demonstrates the extent to which the PMC method can model radiation over a domain with distinct areas with properties and radiation ranging over orders of magnitude.

5.3 Pulverized Coal Flame Example. A pulverized coal ignition jet flame is utilized to study the radiative heat transfer in a pulverized coal flame, following recent simulations performed by Cai et al. [31]. This example is the same as in Ref. [31], except the geometry is rescaled by a factor of 30 and all velocities are

Fig. 5 PMC/LBL solutions of Q_{abs}''' gas and particle phases for fluidized bed example problem. Profiles are taken along the centerline axis ($r = 0$).

rescaled by a factor of 1/5. Rescaling of the problem is done to demonstrate radiation effects on an optically thicker medium.

A description of the problem is as follows. Coal particles are entrained by air through a central jet with a diameter of 6 mm. A coflow of methane through an annular slit between co-axial central jet and outer annular air coflow jets generates a flame used to ignite the central coal-air mixture. The thermophysical properties of the coal in the simulation are based on reported values [32] with some simplifications, they are listed in Table 4.

Coal feeding rate, central jet air flow rate, and methane flow rate are 2.98×10^{-5} kg/s, 3.6×10^{-5} m³/s, and 4.66×10^{-6} m³/s, respectively. The corresponding Reynolds number is 15,264. Pulverized coal particles were grouped into three solid phases in the Eulerian-Eulerian framework proposed in Ref. [31]. The nominal particle sizes of the three phases are 16.6, 24.8, and 35.9 μm , respectively. Their volume fractions relative to the total solid phases are 0.063, 0.237, and 0.70, respectively.

The computational domain is two-dimensional axisymmetric, 0.6 m in radius from the jet axis and 5 m in height from the jet exit. Radial and axial directions are uniformly discretized into 320 and 200 cells, respectively. A parabolic velocity profile is used for the central jet inlet velocity. The free slip wall boundary condition is used at the far field. The combustion model includes a turbulent combustion model, devolatilization and char reaction models. The eddy dissipation concept model [33] is employed for gaseous turbulent combustion. Turbulent flow fields are solved by the standard $k-\epsilon$ model, and the devolatilization rate is determined from Ubhayakar's two rates model [34], with model parameters identical to the original reference. The oxidation of fixed carbon in char is modeled with a single step heterogeneous reaction, i.e.,

Table 4 Thermophysical properties of coal [32]

Parameter	Value
Low heating value	28.1 MJ/kg
Proximate analysis (wt. %)	
Fixed carbon	57.9%
Ash	15.2%
Volatile matter	26.9%
Ultimate analysis (wt. %)	
Carbon	71.9%
Hydrogen	4.4%
Oxygen	8.5%

A half order reaction rate proposed by Hamor [35] is used for char mass loss rate. Conservation equations of mass, momentum, energy, and species mass fractions for gas and solid phases are solved in the open source multiphase flow solver MFIX [36].

The simulation is carried out starting at the initial conditions, using the P1/FSK spectral and radiation solver. A full description of the approach can be found in Refs. [11,31]. A snapshot of the flame at steady state serves as a basis to demonstrate the PMC method for simulating radiation of the flame. The P1/FSK method, using eight spectral quadratures, applied to the same snapshot is used for comparison. Finally, to bracket radiation potential, a

trivial optically thick (OT) model (emission only) is used to analyze the same snapshot.

For the PMC method, this example utilizes 8×10^6 photon bundles and requires 1102 s of computer time to solve the single snapshot. On the other hand, the calculation of the radiative heat source using P1/FSK takes about 24,000 s on a single processor. Most of the time is spent on assembling the k -distributions from the narrowband k -distribution database [37]. The database offers high accuracy in return for the time cost. Because a time-marching solution method is used to advance to the steady state, the radiative heat sources are not required to be updated at each time step, when the flow fields approach steady state. In this simulation, the radiative heat sources are only updated once every

Fig. 6 $\nabla \cdot \mathbf{q}$ for gas and solid phases computed on a snapshot at steady state conditions for pulverized coal flame case. Included in the profiles are the full spectral PMC method (PMC/LBL), OT approximation, and full-spectrum k -distributions spectral model with P_1 RTE solver (P1/FSK). (a) Computed $\nabla \cdot \mathbf{q}$ using PMC/LBL and (b) profiles at $z = 1.2$ m.

2500 time steps (time step is 1 μ s). This reduces the time cost of solving radiation to about 10 s per time step, which is comparable to the cost of solving chemistry. However, the same may be said about the PMC, and/or time blending may be used (employing relatively few photon bundles at each time step [38]).

Figure 6(a) shows PMC/LBL calculations of $\nabla \cdot \mathbf{q}$ for each phase. The width of the flame is ≈ 0.1 m, which is $\approx 1/6$ of the radius of the computational domain. Significant emission occurs only within the flame region. Gas phase heat flux is 1 order of magnitude greater than for the solid phases. Minimum values of $\nabla \cdot \mathbf{q}$ (where self-absorption is greatest) for the solid phase occurs near the centerline, and away from the flame, $\nabla \cdot \mathbf{q}$ becomes negligible.

Profiles of $\nabla \cdot \mathbf{q}$ at $z = 1.2$ m plotted in Fig. 6(b) illustrate the nongray effects. For the gas phase, the PMC/LBL method and P1/FSK yield $\nabla \cdot \mathbf{q}$ values of approximately half the emission. The nongray effects for the solid phases, however, are not as significant, except near the centerline where each of the solid phases' absorption exceeds the emission ($\nabla \cdot \mathbf{q} < 0$). The FSK/P1 approach has been shown to be highly accurate in terms of approximating the spectral dependence [39,40]. Therefore, most of the FSK/P1 errors for computing $\nabla \cdot \mathbf{q}$ are believed to be a result of the RTE solver (P_1), in particular, for optically thin regions. A comparison with better RTE solvers or higher order P_N methods [39] would help explain the discrepancy between FSK/P1 and PMC/LBL.

6 Conclusions

A PMC/LBL model was developed in this paper, which can be used to accurately model the radiative heat source across phases for gas-particle mixtures. Extensions to previous PMC/LBL methods include emission and absorption energy splitting across phases, and random number relations for wavenumber selection for solid particles. The correlations that were developed are based on the Buckius and Hwang correlations for absorption coefficients, which results in a wavenumber selection scheme applicable for any size particles. The accuracy of the PMC/LBL method was validated against numerical integration of exact RTE solutions, which also accounted for energy splitting across phases.

Application of the PMC method to a pulverized coal flame, with peak temperatures above 2100 K, showed significant nongray effects for gas and solid phases. A comparison with P1/FSK as an approximate RTE solver and spectral model, showed errors of approximately 50% for the solid phases, particularly near the centerline of the flame where solid phase absorption is greater. Since the FSK model has been demonstrated to be an accurate nongray model, the P_1 RTE solver is suspected to contribute most of the error in the P1/FSK approach. The PMC method is an attractive method because of its accuracy, while approximate approaches, such as P1/FSK, can be computationally cheaper if very approximate k -distributions are employed.

Nomenclature

A = surface area (m^2)
 E_n = emission energy from the n th gas species (W)
 f_A = average particle surface area on a per volume basis (m^{-1})
 $I_{b\eta}$ = blackbody intensity/Planck function ($\text{W m}^{-2} \text{cm}^{-1}$)
 M_g = number of gas species
 M_s = number of solid phases
 N_i = number of emitted photon bundles from i th cell
 N_r = number of cells in the r -direction
 N_{tot} = total number of rays emitted from medium
 N_z = number of cells in the z -direction
 p_g = gas phase pressure (bar)
 Q_{abs} = absorption (W)
 Q_{emj} = emission (W)
 Q_i^k = photon bundle energy (W)
 r = radial coordinate, or particle radius (m)

$\bar{r}$ = average particle radius (m)
 R_η = random-number relations
 S = distance traversed by a ray (m)
 T = phase temperature (K)
 w = weights associated with absorption splitting of energy
 x = mole fraction
 z = axial coordinate (m)
 $\nabla \cdot \mathbf{q}_{\text{rad}}$ = divergence of radiative heat flux (W m^{-3})

Greek Symbols

γ = solid phase random number relation group variable, Eq. (23) (m K)
 $\Delta\tau_\eta$ = spectral optical distance
 ϵ = emittance
 ε = volume fraction
 η = wavenumber (m^{-1})
 κ_η = spectral absorption coefficient (m^{-1})
 $\bar{\kappa}$ = Planck-mean absorption coefficient (m^{-1})
 ζ = solid phase random number relation group variable, Eq. (22) ($\text{m}^{-1} \text{K}^{-1}$)

Subscripts

g = gas phase
 i = the i th emitting cell, coefficient index
 j = the j th absorbing cell, coefficient index
 m = the m th solid phase
 n = the n th gas species
 s = solid phase
 w = wall
 η = wavenumber dependent
 ζ = normalized wavenumber dependent

Superscripts

k = the k th emitted ray from a cell
 $*$ = selected value based on random number relations or normalized variable
 $'''$ = per volume basis

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