Absorption coefficient regression scheme for splitting radiative heat sources across phases in gas–particulate mixtures

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ABSTRACT

In a gas–particle mixture particles of different makes and sizes may have different local temperatures and are, therefore, modeled with separate energy equations. If the important radiative heat transfer contributions are determined with sophisticated spectral models such as k-distributions, spectral information is lost during the reordering process, making it difficult to separate the resulting radiative heat source across the various energy equations. It is shown here how radiative sources can be determined accurately with the full-spectrum k-distribution assembled from a narrowband database and combined with particle properties on a narrowband level. Proper distribution of the radiative source across the various phases is achieved using regression analysis. Numerical examples demonstrate the accuracy of the model.

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1. Introduction

Thermal radiation is one of the major heat transfer modes in fluidized bed and pulverized coal combustors, due to strong particle radiation at high temperature [1,2]. A high-fidelity radiation model is necessary to improve numerical predictions of the overall heat transfer.

In gas–particle flows, polydisperse particles are grouped into phases by their size and material because of distinguishing characteristics of momentum transfer [3]. Particles of each phase also have individual dynamical responses to heat transfer, which requires a dedicated energy equation and each energy equation requires an individual radiative heat source. On the other hand, the radiation field is described by a single radiative transfer equation (RTE), which determines the total radiative heat source. Therefore, an accurate scheme is needed to split the total heat source across phases in gas–particle mixtures.

Solving the RTE requires spectral models for radiatively participating gases commonly occurring in coal combustion, such as CO_2, CO and H_2O. Their absorption coefficients have strong spectral dependency. Common particles in coal combustion include soot, coal, char, ash and limestone [4]. Their radiative properties are not gray even for gray complex refractive indices due to dependency on the size parameter [5].

While the line-by-line (LBL) spectral model [6] provides the most accurate results of radiative heat transfer, its large computational demands prevent its use in practical engineering applications. Recently, k-distribution methods have been developed for gases [7–9]. A k-distribution is a spectrally reordered absorption coefficient over a narrow-band or the full spectrum. Using k-distributions, radiative heat

transfer can be solved with excellent accuracy, but at a small fraction of the effort compared to LBL calculations [9].

Although the total heat source can be accurately predicted using k-distribution methods, the reordering process makes splitting the total heat source across phases challenging because of the loss of spectral information. For example as shown in Fig. 2, for a nongray solid gas–particle mixture, multiple solid absorption coefficient values may correspond to one total absorption coefficient value. After reordering, due to the loss of spectral information, the individual solid phase absorption of radiation is indeterminate.

In this paper a regression scheme is introduced to extend the validity of the k-distribution scheme to multi-phase gas–particulate mixtures with multiple emission temperatures, and to accurately distribute the resulting radiative source across the phases. The new method is tested with several examples, demonstrating its validity and accuracy.

2. Theoretical analysis

Consider a gas–particle mixture with particles grouped into M different phases according to their material and/or sizes with $m = 1, 2, …, M$ and in particular let $m = 0$ be the gas phase. Particles of different sizes possess different radiative properties and may have different temperatures due to different reaction rates and responses to heat transfer. The spectral radiative transfer equation (RTE) of radiation intensity I_η at wavenumber η including absorption, scattering and multiple temperature emission for a gas–particle mixture may be stated as [5]

$$\frac{dI_\eta}{ds} = \sum_{m=0}^{M} \kappa_{m\eta} I_{b\eta}(T_m) - \sum_{m=0}^{M} \kappa_{m\eta} I_\eta - \sum_{m=0}^{M} \sigma_{sm\eta} I_\eta + \sum_{m=0}^{M} \left[\sigma_{sm\eta} \frac{1}{4\pi} \int_{4\pi} I_\eta(\hat{s}') \Phi_{m\eta}(\hat{s}, \hat{s}', \eta) d\Omega \right]$$

(1)

where $\kappa_{m\eta}$ are the absorption coefficient, $I_{b\eta}$ the Planck function, $\sigma_{sm\eta}$ the scattering coefficient and $\Phi_{m\eta}$ the scattering phase function of

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phase m. Both absorption and scattering coefficients are functions of state variable arrays $\underline{\phi}$ and $\underline{\phi}_s$, i.e., ϕ contains the gas properties, such as temperature, pressure and species concentration, and ϕ_s contains information of local particle properties such as particle number density, radius and species.

We now apply reordering according to the total absorption coefficient at reference state (κ_η^0) over the full spectral range [5,10]:

$$\int_\eta [\bullet]\delta\left(k-\kappa_\eta^0\right)d\eta. \tag{2}$$

The superscript ^{0} indicates a reference state, i.e., $\kappa_\eta^0 = \kappa_\eta(\underline{\phi}^0, \underline{\phi}_s^0)$ indicates the absorption coefficient at a reference state specified by state variable arrays $\underline{\phi}^0$ and $\underline{\phi}_s^0$. Similar to the full spectrum k-distribution method [5], after performing the integration indicated by Eq. (2), each term in Eq. (1) is transformed (reordered) as follows:

The path derivative (term on the left) becomes

$$\int_\eta \frac{dI_\eta}{ds}\delta\left(k-\kappa_\eta^0\right)d\eta = \frac{d}{ds}\int_\eta I_\eta\delta\left(k-\kappa_\eta^0\right)d\eta = \frac{d}{ds}I_k \tag{3}$$

where

$$I_k = \int_\eta I_\eta\delta\left(k-\kappa_\eta^0\right)d\eta. \tag{4}$$

The emission term (first on the right) becomes

$$\begin{aligned}
&\int_\eta \sum_{m=0}^M \kappa_{m\eta}I_{b\eta}(T_m)\delta\left(k-\kappa_\eta^0\right)d\eta \\
&= \sum_{m=0}^M \int_\eta \kappa_{m\eta}I_{b\eta}(T_m)\delta\left(k-\kappa_\eta^0\right)d\eta \\
&= k_0^*(k) + \int_\eta I_{b\eta}(T_0)\delta\left(k-\kappa_\eta^0\right)d\eta \sum_{m=1}^M \hat{k}_m(k;T_m)\int I_{b\eta}(T_m)\delta\left(k-\kappa_\eta^0\right)d\eta \\
&= k_0^* I_b(T_0)f_{FS}\left(T_0, \underline{\phi}^0, \underline{\phi}_s^0, k\right)\sum_{m=1}^M \left[\hat{k}_m(k;T_m)I_b(T_m)f_{FS}\left(T_m, \underline{\phi}^0, \underline{\phi}_s^0, k\right)\right]
\end{aligned} \tag{5}$$

where the gas absorption coefficients are assumed to be correlated with total absorption coefficients, i.e., there exists a map K_0 [10]

$$\kappa_{0\eta}\left(\underline{\phi}, \underline{\phi}_s, \eta\right) = K_0\left(\underline{\phi}, \underline{\phi}_s, \kappa_\eta\left(\underline{\phi}^0, \underline{\phi}_s^0, \eta\right)\right) = K_0\left(\underline{\phi}, \underline{\phi}_s, \kappa_\eta^0\right) \tag{6}$$

which gives

$$k_0^* = K_0\left(\underline{\phi}, \underline{\phi}_s, k; \underline{\phi}^0, \underline{\phi}_s^0\right). \tag{7}$$

The correlation assumption for a mixture of a gas with nongray particles may be examined by plotting line-by-line gas absorption coefficients against the total absorption coefficients as shown in Fig. 1, for a typical CO_2–N_2–char mixture with properties given in the figure caption. The gas absorption coefficients cluster around a monotonic curve, suggesting the existence of the map K_0 and the validity of correlation assumption. The correlation between gases at varying temperatures and concentrations has been found to be good in early work on nonluminous reacting flows [9]. Such correlation is not generally available for solid absorption coefficients as shown in Fig. 2 for the same mixture. For a given total absorption coefficient, several different solid absorption coefficients are possible. However, an apparent (or relevant
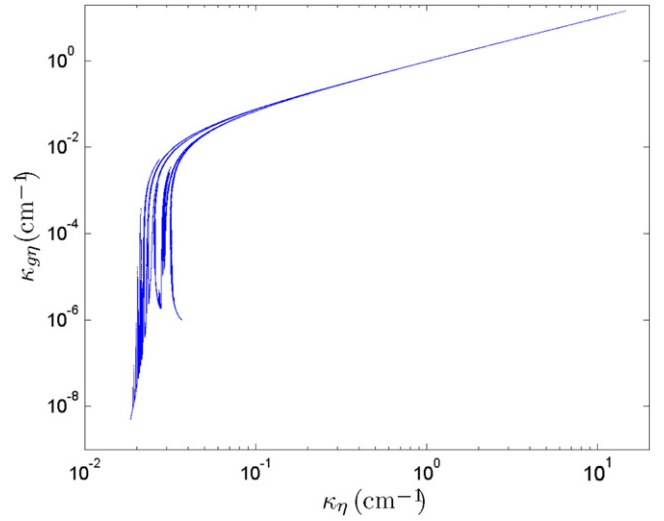

Fig. 1. Line-by-line scatter plot of gas phase absorption coefficient ($\kappa_{g\eta}$) vs total absorption coefficient (κ_η). The mixture has 10% CO_2 and 90% N_2 by volume. The particles are char with a complex refractive index $m = 2.2 - 1.12i$ and a uniform diameter of 400 μm. The volume fraction of particle is 0.001. The mixture has a temperature of 600 K.

average) solid absorption coefficient may be determined from a regression as

$$\hat{k}_m(k;T) = \frac{\int_\eta \kappa_{m\eta}I_{b\eta}(T)\delta\left(k-\kappa_\eta^0\right)d\eta}{\int_\eta I_{b\eta}(T)\delta\left(k-\kappa_\eta^0\right)d\eta}. \tag{8}$$

This allows us to find a proper average value of $\kappa_{m\eta}$ that occurs in the presence of a total absorption coefficient κ_η^0. The definition of the full spectrum k-distribution for a multi-temperature mixture remains the same as its definition for a single-temperature medium:

$$f_{FS}\left(T, \underline{\phi}^0, \underline{\phi}_s^0, k\right) = \frac{1}{I_b(T)}\int_\eta I_{b\eta}(T)\delta\left(k-\kappa_\eta^0\right)d\eta. \tag{9}$$
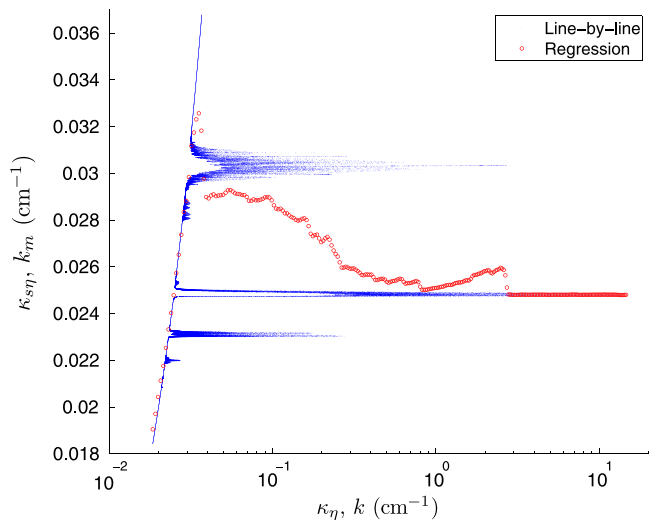

Fig. 2. Line-by-line scatter plot of solid phase absorption coefficient ($\kappa_{s\eta}$) vs total absorption coefficient (κ_η). The regression of solid absorption coefficient against the total absorption coefficient is shown by red circles. Mixture conditions are the same as in Fig. 1.