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Relationship between the spectral line based weighted-sum-of-gray-gases model and the full spectrum *k*-distribution model

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ABSTRACT

The relationship between the spectral line based weighted-sum-of-gray-gases (SLW) model and the full-spectrum *k*-distribution (FSK) model in isothermal and homogeneous media is investigated in this paper. The SLW transfer equation can be derived from the FSK transfer equation expressed in the *k*-distribution function without approximation. It confirms that the SLW model is equivalent to the FSK model in the *k*-distribution function form. The numerical implementation of the SLW relies on a somewhat arbitrary discretization of the absorption cross section whereas the FSK model finds the spectrally integrated intensity by integration over the smoothly varying cumulative-*k* distribution function using a Gaussian quadrature scheme. The latter is therefore in general more efficient as a fewer number of gray gases is required to achieve a prescribed accuracy. Sample numerical calculations were conducted to demonstrate the different efficiency of these two methods. The FSK model is found more accurate than the SLW model in radiation transfer in H_2O; however, the SLW model is more accurate in media containing CO_2 as the only radiating gas due to its explicit treatment of 'clear gas.'

1. Introduction

Thermal radiation plays an important role in heat transfer in various practical high-temperature systems, such as furnaces, engines, and combustors, as well as in fire spread. The main challenges of modeling thermal radiation in gaseous media containing high temperature combustion products are twofold: (1) accurate and efficient solution to the spectral radiative transfer equation (RTE) and (2) accurate and efficient modeling of the spectral radiative properties of the combustion products. Significant research efforts have been devoted to real-gas radiative properties since the 1950s.

Remarkable progress in the development of accurate and efficient global non-gray gas radiation methods has been achieved in the last two decades or so. These developments were largely based on the *k*-distribution methodology first applied to atmospheric sciences by Arking and Grossman [1]. Several global non-gray gas models have been developed in recent years, which include the spectral line-based weight-sum-of-gray-gases (SLW) [2,3], the full-spectrum *k*-distribution (FSK) [4,5] model, the absorption distribution function (ADF) model [6,7], and the spectral-line moment-based (SLMB) model [8]. Among these models SLW and FSK are by far the two most popular models for the reasons that they have been extensively developed for gas radiation calculations in non-isothermal and inhomogeneous gas mixtures [3,9,5,10] and their model parameters for CO_2 and H_2O have been determined by line-by-line calculations. Both models are

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considered as modern development of the classical weight-sum-of-gray-gases (WSGG) model proposed by Hottel and Sarofim within the framework of the zone method [11]. The connection of the SLW and FSK models to the classical WSGG model has been discussed by Denison and Webb [2] and Modest and Zhang [4].

Although the starting points of derivation, the resultant transfer equations, and the numerical implementations of the SLW and FSK models differ, they are actually closely related to each other as first discussed by Modest [5] and recently by Solovjov and Webb [12]. Modest showed that the SLW RTE can be derived from the FSK RTE by approximating the integration over the cumulative k-distribution function by a trapezoidal scheme [5]. Consequently, Modest concluded that the SLW is the crudest possible implementation of the FSK method [5]. In a recent paper, Solovjov and Webb [12] showed that in isothermal and homogeneous media the FSK model can be derived from the SLW model in the limit of small absorption cross section increment and the two models are just different forms of the very same equation. Although these studies provided some useful insights into the relationships between the two models, the findings are still incomplete and the relationships between the key quantities in the two models have not been thoroughly explored.

The objective of this study is to offer new insights into the relationship and main differences between the SLW and FSK models by conducting a further analysis of the two models in isothermal and homogeneous media.

2. SLW and FSK models in isothermal and homogeneous media

2.1. The SLW model

Although detailed derivations of the SLW model have been given originally by Denison and Webb [2] two decades ago and more recently by Solovjov and Webb [12], it is useful to present the key steps in arriving at the RTE and the key variables of the SLW model to facilitate the present discussion. The spectral RTE in an absorbing and emitting medium can be written as

$$\frac{dI_\eta(s)}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta} \tag{1}$$

where I_η is the spectral radiation intensity along a path s, η is the wavenumber, $I_{b\eta}$ is the blackbody spectral radiation intensity, κ_η is the spectral absorption coefficient of the medium and is related to the spectral absorption cross section of the absorbing molecule $C_\eta(T_g)$ through $\kappa_\eta = NYC_\eta(T_g)$ with N being the gas molar density, Y is the mole fraction, and T_g is the gas temperature. The high resolution spectral absorption cross section $C_\eta(T_g)$ can be obtained from a line-by-line (LBL) spectroscopic database. The boundary condition at a diffuse gray wall is written as

$$I_{w\eta} = \varepsilon_{w\eta} I_{wb\eta} + (1-\varepsilon_{w\eta}) \frac{1}{\pi} \int_{\hat{\mathbf{n}}} \bullet \hat{\mathbf{s}} < 0 I_{w\eta} |\hat{\mathbf{n}} \bullet \hat{\mathbf{s}}| \, d\Omega \tag{2}$$

where the subscript w stands for quantities at the wall and $\varepsilon_{w\eta}$ is the wall spectral emissivity. In what follows, the discussion will be focused on the transfer equations of the SLW and FSK models, since inclusion of the boundary condition in the discussion does not alter the findings of this study.

An important quantity in the SLW method is the absorption line blackbody distribution function (ALBDF), first introduced by Denson and Webb [2], given as

$$F(C_{abs}, T_b, T_g, Y) = \frac{1}{I_b(T_b)} \sum_i \int_{\Delta\eta_i(C_\eta(T_g) < C_{abs})} I_{b\eta}(T_b) d\eta \tag{3}$$

where T_b and T_g are, respectively, the blackbody temperature and gas temperature and I_b is the spectrally integrated blackbody intensity. Although not explicitly indicated, the spectral absorption cross section C_η and ALBDF also depend on the total pressure of the medium. In this study the total pressure is restricted to $p = 1$ atm. A detailed discussion of how the gas and blackbody temperatures affect ALBDF was given by Denison [13]. It is noticed that the gas temperature affects ALBDF through the integration regions, as shown in Fig. 1 (the shaded spectral regions represent the integration regions), which will be discussed later on. ALBDF varies between 0 (for very small values of absorption cross section C_{abs}) and 1 (for sufficiently large values of C_{abs}).

The development of the SLW model starts with representing the high-resolution spectral absorption cross section by a set of discrete values C_j ($j = 1, 2, \ldots, n$) with the help of a set of supplemental cross section $\tilde{C}_0, \tilde{C}_1, \ldots, \tilde{C}_n$ [2,12] as shown in Fig. 1. Because the absorption cross section varies rapidly with the wavenumber over many orders of magnitude, the supplemental cross sections have often been chosen logarithmically equally spaced between the minimum value $\tilde{C}_0 = C_{min}$ and the maximum value $\tilde{C}_n = C_{max}$ [12], i.e.

$$\tilde{C}_j = C_{\min}(C_{\max}/C_{\min})^{j/n}, \quad j = 0, 1, \ldots, n \tag{4}$$

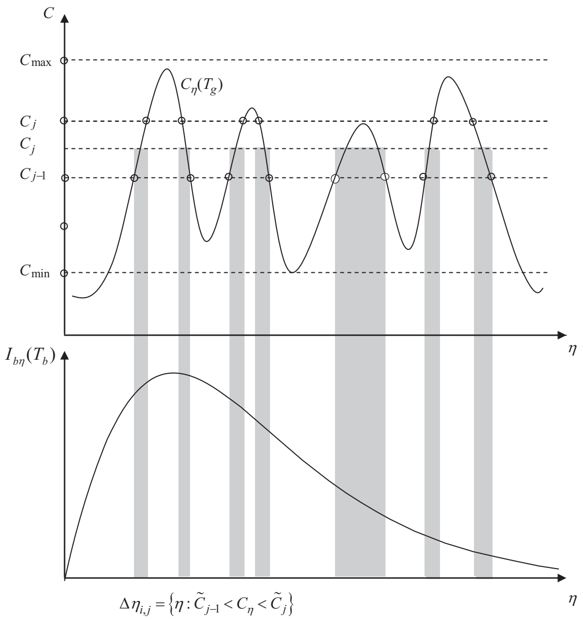

Fig. 1. Schematic showing the discretization of the absorption cross section and the corresponding wavenumber intervals of the SLW model.