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A Multi-Spectral Energy Bundle method for efficient Monte Carlo radiation heat transfer computations in participating media

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ABSTRACT

The Monte Carlo method is a powerful technique for simulating radiation heat transfer processes. The method can easily deal with irregular three-dimensional geometries, anisotropic scattering of radiation and other complexities, which are usually difficult to be tackled with other numerical techniques. On the other hand, Monte Carlo computations are highly time consuming. In addition, accurate radiation heat transfer solutions require that spectral properties be taken into account in a detailed manner, being the line-by-line integration the more accurate but also more computationally expensive technique. Due to these reasons, Monte Carlo computations that accurately consider the spectral properties of radiation are impracticable for several cases of interest in engineering. Therefore reducing the computer time associated to Monte Carlo simulations is highly desirable. This paper presents the Multi-Spectral Energy Bundle method, which reduces the computational time of Monte Carlo simulations in which the spectral properties are accurately taken into account. The method can be applied for line-by-line computations as well as along with spectral models. Here, the proposed method is applied with the accurate full-spectrum k-distribution method, and the obtained results are analyzed.

1. Introduction

Radiation heat transfer in participating media is important in diverse physical processes in nature and engineering. Since emission of radiation is proportional to the fourth power of the temperature, radiation is usually the dominant heat transfer mode when high temperatures does occur. It is the case in many combustion processes, as those occurring in combustion chambers. However, radiation heat transfer calculations are generally considerably difficult. The intensity field of radiation depends strongly on the spectral properties, spacial coordinates, and direction. This makes analytical solutions virtually impossible for the great majority of the cases and computationally tedious. In participating media, as emitting/absorbing gases, the radiative properties are usually strongly dependent on the wavelength, making it necessary to take into account hundreds of thousands or even millions of spectral intervals to perform accurate line-by-line computations. Thus, accurately considering the spectral dependence of the radiative properties is computationally expensive, and consequently one of the major issues in radiation heat transfer simulations concerns with efficient accounting of the spectral dependence of the radiative properties.

The simplest spectral model is the gray gas, in which the averaged value of the absorption coefficient is assumed to be independent of the wavenumber, and usually computed as the Planck mean absorption coefficient. Although the model can be accurate for uniform media, its application to more realistic non-uniform media can lead to unacceptable errors. The Weighted-Sum-of-Gray Gases (WSGG) model, first proposed by Hottel and Sarofim [1], treats the entire spectrum by a few bands having uniform absorption coefficient, each band corresponding to a gray gas. Smith et al. [2] obtained useful coefficients for the WSGG gray gases and correlations for computing their weights. The gray gas model as well as the WSGG are named global models, since they model the entire spectrum. Another class of spectral models corresponds to the band models. Instead of modeling the absorption coefficient for the entire spectrum, the absorption coefficient is modeled in the band models inside small portions of the spectrum. An extensive overview on the band models can be found in Howell et al. [3] and Modest [4].

A particular type of band model is the narrow band k-distribution. This model uses the fact that even within a small portion of the spectrum the absorption coefficient attains the same

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value several times while the blackbody spectral intensity of radiation remains essentially constant. Therefore the blackbody intensity is assumed as constant inside a band, and the absorption coefficient is reordered into a smooth monotonically increasing function to allow the computation of the intensity field only once for all spectral positions where the absorption coefficient assumes a same specific value. Modest and Zhang [5] presented a global version of the k-distribution method, the so called full-spectrum k-distribution (FSK). However, unlike in the narrow band k-distribution, the blackbody intensity cannot be assumed as constant across the entire spectrum. Thus, in order to allow variation of the blackbody intensity, it is defined a cumulative k-distribution, which gives the fraction of the blackbody energy in the portions of the spectrum where the spectral absorption coefficient is less than a prescribed value. A cumulative k-distribution defined in such a way is equivalent to the Absorption-Line-Blackbody distribution function (ALBDF), previously defined by Denison and Webb [6] for application in the Spectral Line-Based Weighted-Sum-of-Gray-Gases (SLW) model, proposed by Denison and Webb [7]. In order to apply the SLW to nonhomogeneous media, Denison and Webb [6] assumed correlated absorption coefficients (correlated-k). This assumption was also applied to the FSK by Zhang and Modest [8]. Approximations for joint ALBDFs, which provide higher efficiency, were proposed by Denison and Webb [9] and Solovjov and Webb [10]. Such approximations can be applied along with the FSK as well including media in non-local thermodynamic equilibrium, as accomplished by Maurente et al. [11].

The FSK cumulative k-distribution functions (or, alternatively, ALBDFs) are calculated from the line-by-line spectrum. Thus it is necessary to precalculate them before performing radiation heat transfer computations, otherwise the FSK would become even more computationally expensive than line-by-line calculations. The line-by-line absorption coefficients are obtained from databases, such as HITRAN and HITEMP [12,13]. Denison and Webb [6] and Denison and Webb [9] presented useful correlations computed from an old version of HITRAN presented by Rothman et al. [14], which can be used to generate ALBDFs for media composed respectively of H_2O and CO_2. Pearson et al. [15] updated the correlations for H_2O using the current version of the HITEMP database, more suited for higher temperatures.

The Monte Carlo method was first applied to consider the spectral properties of participating media by Modest [16]. However, the application of the method for accurate line-by-line computations is relatively recent [17], since both Monte Carlo and line-by-line are associated to high computational cost. The Monte Carlo method was applied with accurate spectral models by Wang et al. [18] and Maurente et al. [19], who combined the Monte Carlo respectively with the FSK and ALBDF. The method proposed by Maurente et al. [19], was next applied by Maurente et al. [20] to generate results for a cylindrical enclosure whose temperature field and mole fractions of H_2O and CO_2 were similar to those encountered in combustion chambers. The obtained results were used to evaluate the WSGG method, whose absorption coefficients and respective weights were computed using the correlations proposed by Smith et al. [2]. The evaluation indicated that the inaccuracy associated to the WSGG was due to the mentioned correlations, which had been fitted from the databases available in early 1980's. Recently, Dorigon et al. [21] presented updated correlations for the WSGG obtained from the current version of the HITEMP database and demonstrated that the WSGG can be in fact considerably accurate.

Although the methods proposed by Wang et al. [18] and Maurente et al. [19] combine the Monte Carlo with the spectral models, the computations are still highly expensive. In this study, it is presented and analyzed a method aimed at reducing the computational cost associated to Monte Carlo spectral radiation heat transfer computations, namely, the Multi-Spectral Energy Bundle (MSB). This method can be applied in line-by-line computations or along with spectral models, as the FSK and ALBDF. Results in which the Monte Carlo is applied along with the FSK are presented, and compared to a conventional approach in order to evaluate the efficiency of the MSB method.

2. The Multi-Spectral Energy Bundle method

In traditional applications of the Monte Carlo method to media with spectrally dependent properties, the energy bundles are modeled as monochromatic. The main idea behind the Multi-Spectral Energy Bundle (MSB) method is to treat the energy bundles as multi-spectral and composed of a set of sub-bundles to make the method more efficient in the treatment of the spectral integration. Thus, the next subsections present some fundamental ideas regarding the Monte Carlo method, and the MSB formulation.

2.1. The Monte Carlo method

The Monte Carlo is a stochastic numerical method with application in diverse areas, including radiation heat transfer. Accordingly, the radiative energy exchange is modeled as emission and absorption of energy bundles, which are associated to probabilities of occurrence. As an example, consider an uniform gas volume, V, emitting radiation. The energy emitted from this volume per unity of time, independently of escaping or being reabsorbed in the volume itself, is given by:

$$Q_e = \int_V \int_{4\pi} \int_0^\infty \kappa_\eta I_{b,\eta} d\eta d\Omega dV = 4\pi V \int_0^\infty \kappa_\eta I_{b,\eta} d\eta \tag{1}$$

where $I_{b,\eta}$ is the blackbody spectral intensity given by the Planck distribution, κ_η is the spectrally dependent absorption coefficient, η is the wavenumber and Ω is the solid angle. In the above relation, it is assumed that the blackbody intensity is uniform in the volume. Thus, the fraction of energy emitted in the wavenumber η around $d\eta$ is

$$P(\eta)d\eta = \frac{4\pi V \kappa_\eta I_{b,\eta} d\eta}{4\pi V \int_0^\infty \kappa_\eta I_{b,\eta} d\eta} = \frac{\kappa_\eta I_{b,\eta} d\eta}{\int_0^\infty \kappa_\eta I_{b,\eta} d\eta} \tag{2}$$

where the numerator is the amount of energy emitted in the wavenumber η, per unity of time and the denominator is the rate of emission of energy, that is, the total energy emitted per unit of time.

Assuming that the energy is emitted in N energy bundles per unity of time, all carrying the same amount of energy (Q_e/N), the fraction $P(\eta)d\eta$ may be thought as the probability of emission of an energy bundle of wavenumber η. Therefore, from the probability and statistical theory, $P(\eta)$ is the *probability density function*. Consequently, the *cumulative distribution function* of probabilities is

$$R(\eta) = \int_{-\infty}^{\eta} P(\eta^*) d\eta^* = \frac{\int_0^\eta \kappa_\eta I_{b,\eta} d\eta^*}{\int_0^\infty \kappa_\eta I_{b,\eta} d\eta} \tag{3}$$

where the asterisk denotes a dummy variable of integration.

The cumulative distribution function given by Eq. (3) is equivalent to the probability that a given energy bundle has a wavenumber between $-\infty$ and η. However, since a negative wavenumber has no physical meaning, Eq. (3) is equivalent to the probability that the bundle has a wavenumber between 0and η. Thereafter, the probability that a bundle has a wavenumber between 0 and $+\infty$ (when $\eta \to \infty$) is equal to 1.

According to the demonstration presented by Howell et al. [3], the cumulative distribution function can be used for Monte Carlo simulations of radiation heat transfer. In the case of the example,