THE MULTI-SPECTRAL BUNDLE MODEL FOR MONTE CARLO RADIATION HEAT TRANSFER COMPUTATION

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Abstract. *The Monte Carlo method is powerful in radiation heat transfer computations, since it is able to deal with complex geometries and scattering phenomena without highly increase the difficulties associated to the model implementation. On the other hand, the Monte Carlo is highly computer time consuming, specially when necessary accounting for the detailed spectral behavior. The Monte Carlo, as other numerical techniques, can be applied with spectral models. Here we propose the Multi-Spectral Bundle model, which improves the computational efficiency of the Monte Carlo and can be applied in line-by-line computations as well as when spectral models are employed.*

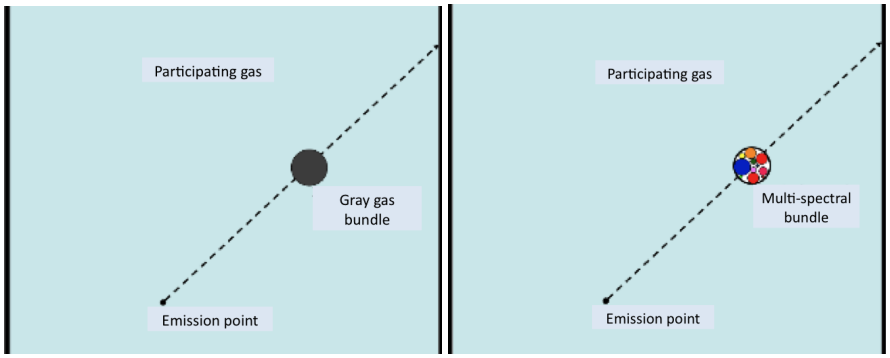
Keywords: *Radiation heat transfer, non-uniform absorbing-emitting gases, Monte Carlo method, spectral model.*

1. INTRODUCTION

Radiation heat transfer occurs in several processes in physics and engineering. In combustion chambers, thermal radiation is often the dominant heat transfer mode due to the formation of gases at high temperatures. However, computing radiation exchange in participating gases is in general a complex task, a reason for this being the highly irregular dependence of the radiative properties with the wavelength.

Gas emission and absorption results from transitions between energy states, for which a number of models have been proposed for the structure of the bands. The simplest model is the gray gas, which considers the absorption coefficient to be wavelength independent. The weighted-sum-of-gray gases (WSGG) model, first proposed by Hottel and Sarofim (1967), models the entire spectrum by a few bands having uniform absorption coefficient, each band corresponding to a gray gas. Band models are based on the fact that the absorption coefficient varies much more rapidly across the spectrum than the blackbody intensity and then actual spectral absorption can be replaced by a value averaged over a spectral region. A number of band models have been proposed. An extensive overview of those models can be found in Howell et al. (2011) and Modest (2003). A particular type of band models are the band k-distributions. These models use the fact that even within a small portion of the spectrum the absorption coefficient attains the same value several times. Therefore the absorption coefficient can be reordered into a smooth, monotonically increasing function inside a band, assuming that each intensity field calculation is carried out only once.

Contemporary full spectrum k-distribution (FSK) methods have led to helpful simplifications. In these methods the absorption coefficient is reordered into a monotonically increasing function. However, unlike the band k-distribution, the blackbody intensity is allowed to vary across the spectrum. It is attained by defining a cumulative k-distribution, which is the fraction of the blackbody energy in the portions of the spectrum where the spectral absorption coefficient is less than a prescribed value. The cumulative k-distribution for gas species encountered in atmospheric and combustion problems are generated from fundamental data for the spectral line absorption behavior, such as the HITRAN and HITEMP database. The cumulative k-distribution is equivalent to the absorption-line-blackbody distribution function (ALBDF), first defined by Denison and Webb (1993a) for application in the spectral line-based weighted-sum-of-gray-gases model proposed by Denison and Webb (1993b). Modest and Zhang (2002) have demonstrated the equivalence between the ALBDF and the cumulative k-distribution and applied it to formulate the FSK method. In order to apply the FSK to nonhomogeneous



(a) (b)

Figure 1: Representation of bundles traveling in the gas: (a) a gray gas bundle and (b) a multi-spectral bundle.

media, the absorption coefficient is assumed to be correlated, Denison and Webb (1995a) and Zhang and Modest (2003).

Approximations for treating mixtures were proposed by Denison and Webb (1995b) and Solovjov and Webb (2000). These approximations allow formulation of a joint cumulative k-distribution from cumulative k-distributions for each individual emitting-absorbing species present in the mixture and so provide a considerable reduction on the size of the k-distribution database required for performing radiative heat transfer computations.

In spite of the progresses on the spectral models, there is still a strong need to develop methods that permit their application to the solution of processes that also involve complex geometry configuration and non-diffuse walls, among other effects, for which the Monte Carlo method can be the most attractive solution technique. The Monte Carlo was first applied to deal with spectrally dependent properties by Modest (1992), considering a uniform gas. In order to consider inhomogeneous media, the Monte Carlo has been applied in conjunction with spectral models: WSGG by Snegirev (2004), narrow-band k-correlated model by Tesse et al. (2002) and Tesse et al. (2004), and FSK by Wang et al (2007). Maurente et al. (2007) have proposed the application of the Monte Carlo to the ALBDF. All these methods combine the advantages of the Monte Carlo with the efficiency of the spectral models. Nevertheless, Monte Carlo computations are still expensive. Here a method to make Monte Carlo spectral radiation heat transfer computations cheaper is proposed. This method can be applied for line-by-line computations or along with spectral models.

2. MULTI-SPECTRAL BUNDLES (MSB) FORMULATION

If not accounting for the spectral behavior, there is no uncertainty associated to the wavelength. All emitted bundles are associated to a single gray absorption coefficient, whose probability of occurrence is always equal to 1. On the other hand, accounting for the spectral behavior highly increases the amount of energy bundles required for a converged solution. In this case, spectral intervals of the radiative energy are randomly computed. Thus, there is statistical uncertainty associated to the wavelength, in addition to the uncertainties associated to the location and direction of emission. The uncertainty associated to the geometric characterization is multiplied to the uncertainty associated to the spectral characterization, thus the uncertainty in the results when modeling the spectral behavior is in fact equal to the uncertainty in the results when using the gray gas model multiplied by the uncertainty associated to the spectral interval.

The Multi-Spectral bundles model aim at reducing the effect of the multiplication of uncertainties associated to geometric and spectral characterization. The idea consists of assembling a multi-spectral bundle (MSB) composed of sub-bundles (SB), each one associated to a single wavelength. If the MSB would be composed of infinite SB, it would hold all necessary information for characterizing the spectrum. All bundles would be identical and would be associated to a probability of occurrence equal to 1. For an uniform medium, the probabilities of emission and absorption of a bundle constituted for infinite SB is the same as for a gray gas with the absorption coefficient equal to the averaged spectral absorption coefficient. Therefore, the uncertainty associated to the spectral results would be the same as for the gray gas results. Figure 1 (a) represents a gray gas bundle and Fig. 1 (b) represents a MSB composed of some SB.

In the MSB model, the uncertainty associated to the results decreases as the number of SB used to compose the MSB increases. Nevertheless, comparable decrease is not verified in the computer time. The computer time necessary for characterizing a MSB is directly proportional to its number of SB's. Therefore, an optimum number of SB's for the minimum computer time does exist.

In section 2.1 a procedure for emission of MSB's is presented. The next two sections present how to simulate the MSB absorption by two different processes: a deterministic continuous, as presented by Wang et al. (2003), and a randomly discrete processe. The MSB model is not limited to applications with line-by-line spectral integration, but can also be applied along with spectral models. Section 2.4 shows how to apply the MSB model along with the Monte Carlo applied to the Absorption-Line-Blackbody distribution function (MC-ALBDF), presented by Maurente et al. (2006).

2.1 Multi-spectral bundles (MSB) emission

For the numerical solution, in this work the medium is discretized into uniform zones of volume and surface with uniform properties and the Monte Carlo is applied for computing the radiative energy exchange between the zones. According Modest (1992) the random number from which the wavelength, λ, can be computed in the Monte Carlo simulations is

$$R_\lambda = \frac{\pi}{\kappa_M \sigma T_b^4} \int_\lambda \kappa_\lambda I_{b,\lambda} d\lambda \tag{1}$$

where κ_λ is the spectral absorption coefficient in the medium at the emission location, $I_{b,\lambda}$ is the Planck distribution for the blackbody radiative intensity and κ_M is the mean Planck absorption coefficient. Follows that the energy associated to each energy bundle emitted from the volume element, dV, is

$$dE_{P,dV} = \frac{1}{N_P} 4\kappa_M \sigma T_b^4 dV \tag{2}$$

For a finite uniform zone of volume, the energy of the bundle is given by

$$E_P = \frac{1}{N_P} \int_V 4\kappa_M \sigma T_b^4 dV = \frac{4\kappa_M \sigma T_b^4 V}{N_P} \tag{3}$$

being each bundle associated to a specific wavelength depending on the random number R_λ, which can assume values from 0 to 1. N_p is the total number of emitted bundles from the volume, V.

The MSB is composed of $N_{P,S}$ SB's, each one associated to a specific wavelength and carrying the energy $E_{P,S}$. Thus, the energy of the MSB is

$$E_P = \sum_{j=1}^{N_{P,S}} E_{P,S,j} \tag{4}$$

where $E_{P,S,j}$ is the energy of the j-th SB. For the energy of the MSB be the same as computed by Eq. (3), the energy of the SB's must be given by

$$E_{P,S,j} = \frac{4\kappa_M \sigma T_b^4 V}{N_P N_{P,S}} \tag{5}$$

The radiation wavelength associated to each SB can be computed by Eq. (1). Observing Eq. (5), one can notice that

the number of emitted SB's is invariable.

2.2 Multi-Spectral Bundle (MSB) Absorption

Bundles absorption can be computed by two different processes: random discrete or using a partitioning scheme proposed by Modest (2003). In the second case, the energy is continuously absorbed without using random procedures. The continuous absorption procedure improves the efficiency of the Monte Carlo method for the solution of spectral radiation heat transfer. The absorption of MSB's can be better described for the procedure where the radiation is continuously absorbed. Thus, the equations for continuously energy absorption of the MSB's are first presented. Further, the equations are extended for the case of random discrete absorption.

2.3 Continuos absorption formulation

As a MSB travels through a uniform path length, l, in a zone of volume, the energy of each SB is continuously absorbed according to

$$F_{A,S,j} = \big(1 - exp\big(-\kappa_{S,j} l\big)\big) \tag{6}$$

where $\kappa_{S,j}$ is the absorption coefficient associated to the wavelength of the j-th SB. Follows that the remaining energy in the j-th SB is

$$E_{P,S,j} = E_{P,S,j} - F_{A,S,j} E_{P,S,j} \tag{7}$$

Thus, after the MSB to travel a uniform path length l, the transported energy must be updated using Eq. (7). The energy of the MSB is recalculated by Eq. (4) using the updated values of the SB energy. The total energy subtracted from the MSB is accounted as absorbed by the volume zone. The MSB remains traveling and enter the next volume zone or reach a surface. If the bundle reaches a surface, part of its energy can be absorbed and part can be reflected back to the gas. The procedure is repeated until the energy of the MSB be completely absorbed.

2.4 Random discrete absorption formulation

The random discrete energy absorption of MSB is computed by using a stratagem. The probability of a bundle to be absorbed as it travels in a uniform path length, l, is equivalent to the fraction of the energy which would be absorbed in a continuous deterministic process. To determine if a bundle is absorbed during crossing a uniform volume zone through a path l, a random number is generated and compared with the absorption probability, if the random number is lower than the absorption probability, the bundle is simulated as have been absorbed.

Equation (6) gives the fraction of energy of the j-th SB which is absorbed as the bundle travels an uniform path length l. Thus, the fraction of the absorbed energy of the whole MSB is

$$P_A = F_A = \sum_{j=1}^{N_{P,S}} F_{A,S,j} \tag{8}$$

In the random discrete absorption formulation, the MSB are either totally absorbed in a specific location or its amount of energy remain unchanged. Eq. (8) gives the probability of a MSB be absorbed during traveling a path length l. Accounting for several MSB's absorbed in a volume zone, the total energy absorbed in this zone is obtained. The bundles which are not absorbed goes to the next volume zone or reach a surface zone.

Although Eq. (8) gives the correct fractions of the energy absorbed in a finite volume, this equation provides no information about the spectral distribution of the non absorbed MSB's which escape the volume. The distribution of the non absorbed energy among the SB's can be given by Eq. (9):

$$F_{A,S,j} = \frac{E_{P,S,j}}{E_{P,S}} \tag{9}$$

where $E_{P,S,j}$ and $E_{P,S}$ are respectively the updated value of the energy of the j-th SB and by the whole MSB, which are given by Eq. (7) and Eq. (4).

Thus, if the MSB is not absorbed, equation (9) can be used to redistribute the energy among the SB's. However, the energy of the MSB remain unchanged. Therefore the energy of each SB can be computed by Eq. (9) and the following relation:

$$E_{P,S,j} = E_P F_{A,S,j} \tag{10}$$

where E_p is the energy of the MSB, as computed in the emission process by Eq. (3).

2.5 The multi-spectral bundle (MSB) model along with the Monte Carlo method applied to the ALBDF

The previous sections presented a general formulation of the MSB model. Additional computer savings can be achieved by applying the MSB model along with methods for the spectral modeling, as the Absorption-Line-Blackbody distribution function (ALBDF). This section presents the equations for applying the MSB model along with the ALBDF. The main difference relative to the previous presented formulation concerns to the way as the radiative energy is distributed among the SB's. For using the ALBDF, the radiation of each SB is associated to a value of the absorption cross-section, which is associated not only to one specific, but several spectral locations. Moreover, in the formulation of the Monte Carlo applied to the ALBDF used here, the amount of energy assigned to each bundle depends on the absorption cross-section associated to the bundle radiation. The amount of energy assigned for the j-th SB can be computed by the following equation:

$$E_{P,S,j} = \frac{4 C_{S,j} \sigma T_b^4 V}{N_P N_{P,S}} \tag{11}$$

Equation (11) differs from Eq. (5). While the Planck's mean absorption coefficient is used in Eq. (5), the absorption coefficient associated to the absorption cross-section of the bundle radiation is used in Eq. (11). This absorption coefficient is computed according to the formulation presented by Maurente et. al. (2006), where instead relating a wavelength to a random number, as in Eq. (1), fractions of the blackbody energy are associated to random numbers using the ALBDF:

$$g(C_{S,j}) = \frac{\pi}{\sigma T_b^4} \sum_i \int_{\delta\lambda} I_b(T_b) d\lambda \tag{12}$$

where the $C_{S,j}$ are randomly determined by

$$g(C_{S,j}) = R_C \tag{13}$$

where R_C are random numbers which can assume values from 0 to 1.

The fraction of the energy of the j-th SB, that is absorbed as the MSB travels through a uniform path length, l, in the volume zone is given similarly as by Eq. (6) as:

$$F_{A,S,j} = \big(1 - exp\big(-C_{S,j}l\big)\big) \tag{14}$$

Equation (4) and Eq. (7) to Eq. (10) remain unchanged and can be employed along with the Eqs. (11), (12), (13) and (14) for using the MSB model along with the Monte Carlo applied to the ALBDF.

3. RESULTS

The MSB model is here analyzed. The model is employed along with the Monte Carlo applied to the ALBDF in the solution of a two-dimensional problem, which consists of a gas contained in a cylindrical enclosure. The gas is non-isothermal and non-homogeneous constituted of two emitting-absorbing species, water vapor and carbon dioxide, and a non-emitting-absorbing species, the nitrogen.

For the numerical solution, the enclosure was divided into 30 equal sized parts along the axis and 10, along the radius, totalizing 300 volume zones and 50 surface zones, being 10 surface zones in each of the flat walls in the cylinder extremities and 30 in the cylindrical wall. For statistical analysis proposes, few simulations were performed to obtain a single result, in each of them 5000 MSB's were emitted from each zone, totalizing $1{,}75{\cdot}10^6$ MSB's emitted from all zones in each simulation. Solutions were obtained considering different numbers of SB's in the MSB's.

The results were obtained with a FORTRAN 90 computer code. A very low computer power equipment was used for performing the simulations: Athlas 1.56 GHz processor with 256 MB of RAM memory. Part of the consumed processing time is for data computation and storage, it was approximately 300 s and does not change significantly with the use of the MSB model. However, the MSB model reduces the processing time to compute bundle emission and absorption. Thus, only the computer time related to emission and absorption was taken into account in this analysis.

Figure 1 shows results obtained using 3, 7, 5, 10 and 20 SB's to compose the MSB's. For all cases, the Monte Carlo statistical uncertainty level was considered satisfactory when the average of the percent standard deviation over all zones of the cylindrical wall was immediately lower than 0.3 %. For reaching this uncertainty level, was necessary 87, 66, 54, 46 and 34 simulations respectively for the cases where the number of SB's composing the MSB's were 3, 5, 7, 10 and 20. The total number of MSB's is proportional to the number of simulations for each case. Fig. 1 also shows the result obtained without the MSB model and performing 200 simulations. In this figure are also presented the computer time required for computing each result.

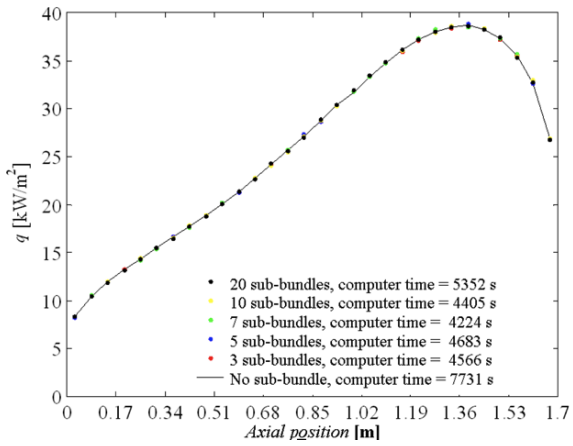
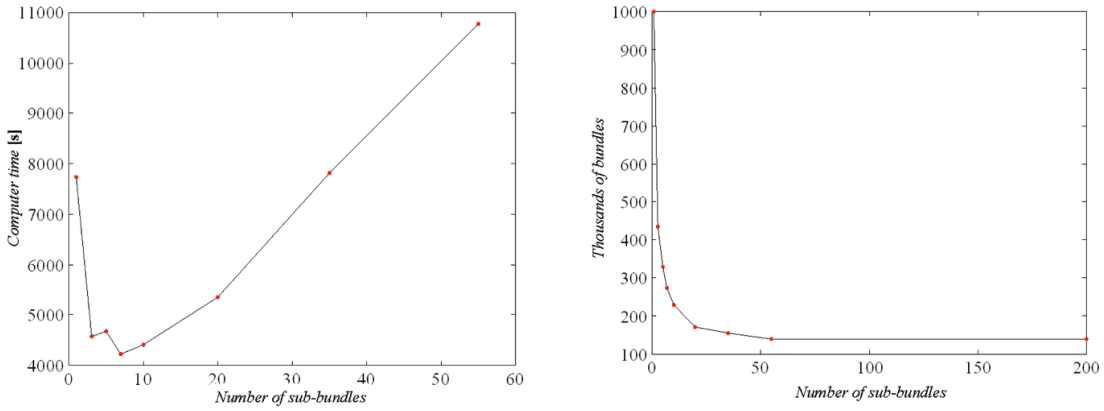


Figure 2: Heat flux in the lateral wall obtained using different numbers of SB's to compose the MSB.



(a) (b)

Figure 3: (a) Relation between processing computer time and number of SB's used. (b) Relation between number the MSB's and number of SB's.

As one can see, using 3 SB's the computer time decreases significantly compared to the case in which the MSB model is not employed. After this initial decrease in the computer time, some oscillations are verified, which can be attributed to the statistical nature of the Monte Carlo. However the general trend of computer time variation can be seen. The minimum computer time was for 7 SB's, which was of 4,224 s, which is approximately 55 % lower than for the case where the MSB model was not employed. From 7 SB's, the computer time increases nearly linearly with the number of used SB's. The computer time versus SB's number is shown Fig. 3 (a), which presents results for additional cases where 35 and 55 SB's are used.

Figure 3 (b) shows the decrease on the required MSB's in function of the increase of the SB's number. As the number of SB's increases, the number of MSB's required for an averaged standard deviation lower than 0.3 % approximates asymptotically a straight line: *Number of MSB* = 140,000.

The presented results demonstrated that the use of the MSB model can reduce the computer time. Specifically, in the approached problem, which is typical of cylindrical combustion chamber, the time savings was almost 50%.

4. conclusions

Although the advantages of the Monte Carlo, the computations efforts required restricts its application in radiation heat transfer problems. Therefore the Multi-spectral Bundles (MSB) model was here proposed to improve the Monte Carlo efficiency in the spectral modeling. In the MSB model a energy bundle is composed of sub-bundles (SB), each associated to a different wavelength.

Results were presented in order to demonstrate how the model can be better used to achieve reduction of required computer time. It was verified that there is an optimum number of SB's for the maximum time savings. Radiation heat transfer in a cylindrical enclosure was approached, which is a typical problem of combustion chambers. For this problem a reduction of almost 50% on the required computational time was achieved.

In spite of being computational expensive, the Monte Carlo method along with spectral models, as the ALBDF, has been useful for obtaining accurate solutions. The MSB model makes the Monte Carlo even more attractive to compute benchmark solutions and to provide higher efficiency if necessary its application to coupled (chemistry reaction)-(turbulent fluid flow)-(radiation heat transfer) solution.

5. ACKNOWLEDGEMENTS

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