A Hybrid Wavenumber Selection Scheme for Line-By-Line Photon Monte Carlo Simulations in High-Temperature Gases

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Recently, it has become possible to conduct line-by-line (LBL) accurate radiative heat transfer calculations in spectrally highly nongray combustion systems using the Monte Carlo method. LBL accuracy, in principle, adds little to the computational load as compared to gray calculations. However, when employing the Monte Carlo method, the original scheme for choosing appropriate emission wavenumbers for statistical photon bundles is numerically expensive. An improved wavelength selection scheme has been applied to hypersonic plasmas for Monte Carlo solvers. However, directly applying this improved scheme to combustion gases may cause significant errors. In this paper, a hybrid scheme for wavenumber selection is proposed, significantly decreasing CPU requirements compared to previous work. The accuracy of the new method is established and its time requirements are compared against the previous method. [DOI: 10.1115/1.4024385]

Keywords: radiative heat transfer, Photon Monte Carlo, wavenumber selection

1 Introduction

In many high-temperature radiative heat transfer simulations, radiation from participating media plays an important role, such as in combustion systems. Due to the rapid increase of computational power, conducting LBL calculations, the most accurate radiative heat transfer simulation, has become possible. In addition, the photon Monte Carlo (PMC) method can deal with complicated problems, such as radiation from highly nongray combustion gases, with relative ease. The combination of LBL simulations with the PMC method has first been implemented by Tang and Brewster [1], and by Wang and Modest [2] and, in the field of aerodynamics, by Ozawa et al. [3], and by Feldick and Modest [4] for nonequilibrium radiation in hypersonic plasma. For a gray analysis with the PMC method, the Planck-mean absorption coefficient is used for calculations and no spectral model is required. However, for nongray analysis the wavenumber carried by photon bundles must be determined in a statistically meaningful way. Photon bundles are emitted in random directions at random wavenumbers from random locations in each computational cell. So-called random-number relations must be developed to obtain statistically meaningful directions, wavenumbers and locations of emitting bundles [5]. Based on random-number relations, the processes of emission, scattering and absorption are simulated by tracing histories of energy bundles. When increasing the number of energy bundles, results will approach the exact solution with diminishing statistical error. Although Wang and Modest [2] developed random-number relations for LBL accurate spectral Monte Carlo models for combustion system, calculation of mixture random-number relations and computational searching make their model to be rather time-consuming. Recently, some improved wavenumber selection schemes have been proposed for hypersonic plasma radiation in Earth entry applications by Ozawa et al. [3], and by Feldick and Modest [4]. Unlike in combustion and other high-temperature systems, in Earth entry applications, 95% or more of the emitted energy comes from atomic species with very few, but strong, electronic lines. Contribution from diatomic species tend to be minor, and diatomic radiation is due to relatively few rovibrational lines. In their scheme, the rovibrational transition lines were separately databased. However, there are too many rovibrational transitions for combustion products such as CO_2, H_2O, and CO (over hundred million), making it impractical to database every individual lines. By properly applying the improved wavenumber selection scheme to high-temperature gaseous media, a hybrid scheme was developed for LBL photon Monte Carlo simulations in order to improve efficiency as well as to guarantee accuracy.

2 Wavenumber Selection for PMC Simulations

2.1 Old Scheme. The probability of the number of photons emitted in a differential wavenumber interval $d\eta$ is given by a probability density function, and the fraction of energy emitted over all wavenumbers between 0 and η can be derived as [5]

$$R_\eta = \frac{1}{E_{\text{tot}}}\int_0^\eta \kappa_\eta I_{\text{b}\eta} d\eta \tag{1}$$

where E_{tot} is the total emission per unit volume and unit solid angle over the entire spectrum. In practice, one deals with a gas mixture. For an n_s species system, total emission equals the integrated mixture absorption coefficient weighted by the Planck function over the whole spectrum

$$E_{\text{tot}} = \int_0^\infty \sum_{i=1}^{n_s} \kappa_{\eta,i} I_{\text{b}\eta} d\eta = \frac{\sigma T^4}{\pi}\sum_{i=1}^{n_s} x_i p \kappa_{P,i} \tag{2}$$

where x_i is the mole fraction of species i, $\kappa_{\text{P},i}$ is its pressure-based Planck-mean absorption coefficient, p is the total pressure, σ is the Stefan-Boltzmann constant, and T is the temperature. Eq. (1) can be written as

$$R_\eta = \frac{\pi}{\sigma T^4}\frac{1}{\sum_{i=1}^{n_s} x_i \kappa_{\text{P},i}}\int_0^\eta x_i \sum_{i=1}^{n_s} \kappa_{\text{p}\eta,i} I_{\text{b}\eta} d\eta = \frac{\sum_{i=1}^{n_s} x_i \kappa_{\text{P},i} R_{\eta,i}}{\sum_{i=1}^{n_s} x_i \kappa_{\text{P},i}} \tag{3}$$

where $\kappa_{\text{p}\eta,i}$ is the pressure-based spectral absorption coefficient, and $R_{\eta,i}$ is the fraction of energy from species i emitted in the spectral range $(0, \eta)$, i.e.

$$R_{\eta,i} = \frac{\pi}{\kappa_{\text{P},i}\sigma T^4}\int_0^\eta \kappa_{\text{p}\eta,i} I_{\text{b}\eta} d\eta \tag{4}$$

Since fractional $(0, \eta)$ emissions for individual species, $R_{\eta,i}$, are different, for a gas mixture the mixture fractional emission R_η corresponding to η needs to be calculated using Eq. (3) employing species fractional emission relations $R_{\eta,i} - \eta$. However, direct inversion from R_η to η of Eq. (3) is impossible and must be done by trial-and-error. In Wang and Modest's model [2] (the old scheme), first an emission wavenumber is guessed for which the mixture fractional emission R_η is calculated, and then a bisectional

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search algorithm is employed to find the correct wavenumber of for a given random number R_η.

2.2 Improved Scheme. In the scheme of Ozawa et al. [3], the independence of emission from difference species is used to allow for separation of species. Feldick and Modest [4] more extensively utilized the additive property of emission by separating all lines and all continuum transitions. In their scheme an emitting line was identified and then the emitting wavelength was selected within the line. Because of the hundreds of millions of rovibrational transitions for combustion species, it is not practical to separate transition types and particular transitions. in the improved wavenumber selection scheme, emission from different species is considered separably, i.e., Eq. (2) is rewritten as

$$E_{\text{tot}} = \sum_{i=1}^{n_s} \int_0^\infty \kappa_{\eta,i} I_{\text{b}\eta} \text{d}\eta \tag{5}$$

emphasizing that emission from individual species is independent of another, i.e., there are no overlap effects for emission. Rather than looking for the appropriate wavenumber for the mixture, one may first determine the emitting species s and then the appropriate wavenumber. Following this idea, Eq. (1) can be rewritten as

$$R_\eta = \frac{\sum_{i=1}^{s-1} E_i}{E_{\text{tot}}} + \frac{\int_0^\eta \kappa_{\eta,s} I_{\text{b}\eta} \text{d}\eta}{E_{\text{tot}}} \tag{6}$$

where s is the number index of the emitting species. E_i is the total emission by species i in the given cell, i.e.

$$E_i = \int_0^\infty \kappa_{\eta,i} I_{b\eta} \text{d}\eta \tag{7}$$

In the improved wavenumber selection scheme, first a random number for emission wavenumber, R_η, is drawn, and the emitting species s is determined according to

$$s = j \qquad \text{if} \qquad \frac{\sum_{i=1}^{j-1} E_i}{\sum_{i=1}^{n_s} E_i} < R_\eta \le \frac{\sum_{i=1}^{j} E_i}{\sum_{i=1}^{n_s} E_i} \tag{8}$$

This ensures that the fraction E_i/E_{tot} of random numbers is employed to pick emission wavenumbers for species i, in accordance with the fractional emission from the species. Once the emitting species is found, R_η is rescaled according to

$$0 \le R_{\eta,s} = \frac{R_\eta E_{\text{tot}} - \sum_{i=1}^{j-1} E_i}{E_j} < 1 \tag{9}$$

In the old scheme, databases tabulating both $R_{\eta,i} - \eta$ and $\kappa_{\eta,i} - \eta$ relations for each species were established. When a random number is chosen, the appropriate wavenumber can be found by searching through the mixture random-number relations. In the improved wavenumber selection scheme, first the emitting species is determined, and then the rescaled random number $R_{\eta,s}$ selects photons of equal strength from species s, with wavenumber found from the probability density function Eq. (4).

Instead of tabulating fractions $R_{\eta,i}$ versus η through Eq. (4), in the improved scheme an inverted relation $\eta - R_{\eta,i}$ is tabulated. Once the emitting species s is determined from Eq. (8), the emission wavenumber can be found directly (or by linear interpolation) from the $\eta - R_{\eta,s}$ database. By eliminating expensive computational searching, the improved scheme with the new database should be more efficient. The new database has the form of

$$\eta = f_{\eta,i}(R_{\eta,i}, T, x_i), \quad \kappa_{\eta,i} = f_{\kappa,i}(\eta, T, x_i), \quad i = 1, 2, \ldots, n_s \tag{10}$$

The $\eta - R_{\eta,i}$ database again includes 28 temperatures, which are equally spaced between 300 K and 3000 K, a single mole fraction, say, 0.0, for CO_2 and CO (due to weak self-broadening effects) and two mole fractions, 0.0 and 0.25, for H_2O. One million random-number entries are tabulated for each temperature and mole fraction to build the $\eta - R_{\eta,i}$ databases.

2.3 Verification and Sample Calculations. When carrying out a Monte Carlo simulation, the many emitted and traced photon bundles must accurately reflect spectral emission of each species, as well as that of the mixture. This is readily verified by collecting all photon bundles emitted over a narrow spectral interval $\Delta\eta$, say, n bundles chosen out of a total of N. Then, the probability of energy emitted from this range is

$$P(\eta) \approx \frac{n}{N} \tag{11}$$

and the fraction of energy emitted at this interval must also equal

$$P(\eta) \approx \frac{\kappa_\eta I_{\text{b}\eta} \Delta\eta}{\int_0^\infty \kappa_\eta I_{\text{b}\eta} \text{d}\eta} \tag{12}$$

which is valid for any individual species or a mixture. Using $\Delta E = E_{\text{tot}}/N$ (each photon carries equal energy), the absorption coefficient is evaluated as

$$\kappa_\eta \approx n \frac{\Delta E}{I_{\text{b}\eta} \Delta\eta} \tag{13}$$

Figure 1 presents a comparison of the reconstructed pressure-based absorption coefficient distribution of CO_2 at 300 K in several small spectral intervals using the newly built $\eta - R_{\eta,i}$ database, with the original absorption coefficients obtained by Wang and Modest [6] but updated to HITEMP2010 [7].

Different sample sizes of random numbers were drawn to reconstruct the absorption coefficients, as shown in the figure. The reconstructed absorption coefficients perfectly match with the original data at strong values, even if only 1×10^6 random numbers are drawn, although the reconstructed absorption coefficients fluctuate somewhat around the original data at weak values (Fig. 1(*a*)). If 10×10^6 wavenumbers are picked randomly, even small values of the absorption coefficients can be reconstructed accurately as shown in Fig. 1(*b*).

A gas mixture of 10%CO_2-25%H_2O-10%CO-55%N_2 at 600 K was chosen for an example calculation. In the old scheme, the wavenumber is found via the mixture random-number relation, as shown in Fig. 2. In the improved scheme, when a random number is picked, a species is selected first and then the appropriate wavenumber is found from the $\eta - R_{\eta,s}$ database for that specific species. As shown in Fig. 2, for the improved scheme, the data for each species are squeezed into a fraction of the random-number range, which depends on the contribution of the species to the total emission from the cell. When the random number is below the fraction of energy emitted by CO_2, CO_2 is selected as the emitting species, otherwise H_2O or CO become the emitting species.

Accuracy and efficiency of the two schemes incorporated into the PMC model are compared for a one-dimensional example (in the z-direction). The example deals with an isothermal gas at 600 K and 1 bar contained between two parallel cold black walls. A mixture of 10%CO_2-25%H_2O-10%CO (by mole fraction) and 55% N_2 is investigated, and the resulting divergence of the radiative flux is shown in Fig. 3, comparing results from exact LBL calculations and the old as well as the improved emission wavenumber selection schemes. The absorption coefficient data are taken from the HITEMP2010 database in all three cases. It is

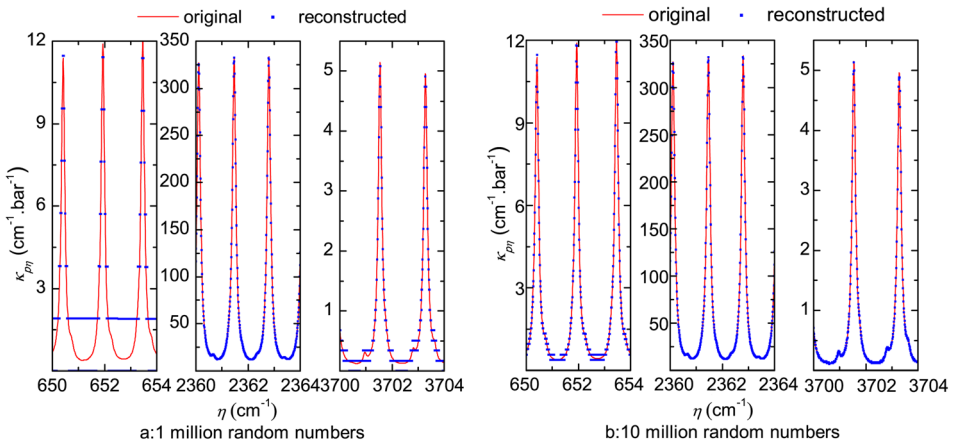

Fig. 1 Recovery of pressure-based absorption coefficients by Monte Carlo method

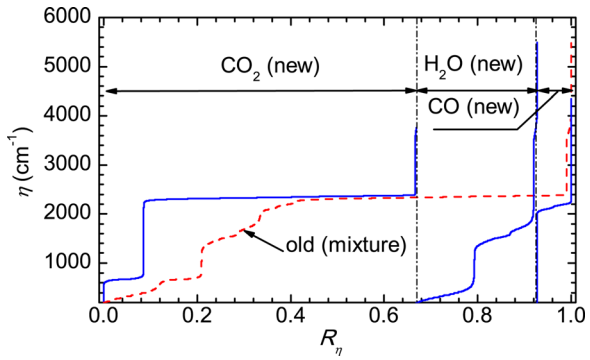

Fig. 2 Random-number relations of 10% CO_2-25%H_2O-10%CO mixture at 600 K for the improved scheme using the $\eta - R_\eta$ database as compared with the old scheme

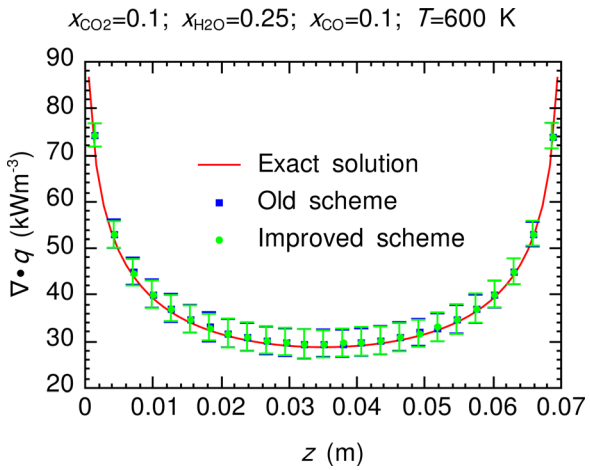

Fig. 3 Divergence of radiative flux for 10% CO_2-25%H_2O-10%CO mixture at 600 K using the old scheme and the improved scheme

observed that both Monte Carlo schemes perform equally well, correctly following the LBL solution.

Using 10×10^6 photon bundles in the PMC simulation required a CPU time 30.81 s for the old wavenumber selection scheme, while for the improved scheme with the new database, the required CPU time is 1.32 s, i.e., the improved scheme is about 20 times faster than the old scheme for wavenumber selection. An investigation of database queries in the old scheme indicates that the average number of data comparisons per query is around 20.

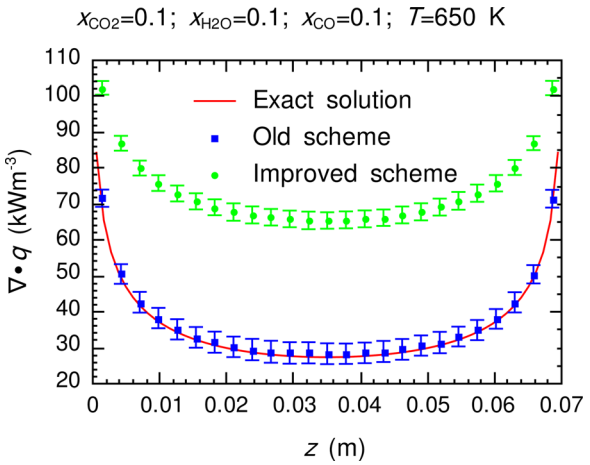

Fig. 4 Divergence of radiative flux for 10% CO_2-10%H_2O-10%CO mixture at 650 K using the old scheme and the improved scheme

This process is eliminated in the improved scheme, improving the computational efficiency by a factor of 20 for emitting wavenumber selection.

However, in this case, all data for the PMC simulation were directly taken from the $\eta - R_\eta$ database without interpolation. Because of limited data points for temperature and mole fractions in the database, interpolation is inevitable for real gas radiation simulations. Figure 4 shows the divergence of radiative flux for the same one-dimensional case, but for a gas mixture containing 10%CO_2-10%H_2O-10%CO (by mole fraction) and 70% N_2 at 650 K. Linear interpolation is employed for temperature and mole fractions. As shown in Fig. 4, when interpolation is applied, very large errors are observed for the improved scheme.

2.4 Hybrid Scheme. Careful investigation of the random-number relations indicates that interpolation from the $\eta - R_\eta$ (i.e., interpolation for temperature or concentration at fixed R_η) database can yield vastly incorrect results. An example is given in Fig. 5, showing the $\eta - R_\eta$ relationship for 25% H_2O at 600 K and 700 K, the sharp increases indicating stepping from the rotational band to the 6.3 μm band and then to the 2.7 μm band. Performing an interpolation between temperatures at fixed wavenumber, as done with the old scheme, essentially returns the correct 650 K line. On the other hand, interpolation at fixed random number generally will return an incorrect spectral line and, in the case of temperature interpolation, may even return the incorrect vibration-rotation band as shown in Fig. 5.

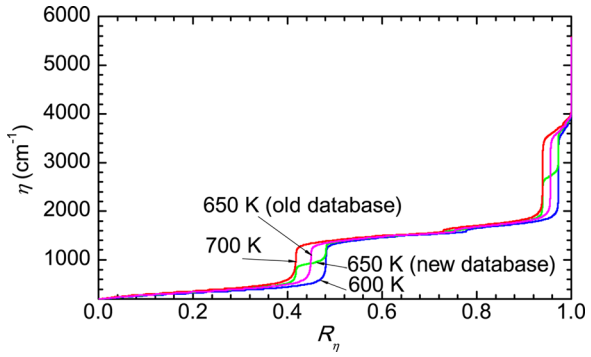

Fig. 5 Random-number relations for 25%H_2O at 600 K, 700 K, and linear interpolation values for 650 K using the $R_\eta - \eta$ and the $\eta - R_\eta$ database

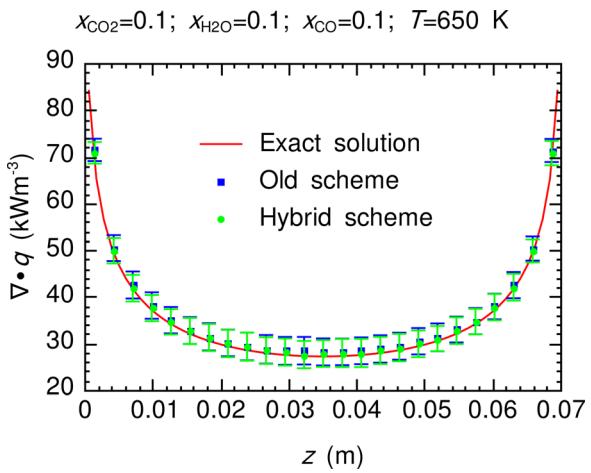

Fig. 6 Divergence of radiative flux for 10% CO_2-10%H_2O-10%CO mixture at 650 K using the old scheme and the hybrid scheme

Accordingly, while using the inverted $\eta - R_\eta$ database of the improved scheme eliminates expensive computational searching for emission wavenumber, interpolation of $\eta - R_\eta$ values can cause significant errors. On the other hand, while the old scheme is relatively inefficient, it does maintain accuracy after interpolation. A compromise between the old and the improved schemes may produce accurate results and also improve computational efficiency. One may use the old $R_\eta - \eta$ univerted database with the improved scheme, by first determining the emitting species s from Eq. (8), and then an appropriate wavenumber can be found by search through only a single species s. While still requiring computational searching to find the appropriate emission wavenumber, this search is limited to a single species. In this hybrid scheme CPU time for the calculation of mixture random-number relations is reduced, while the problem caused by interpolating the inverted $\eta - R_\eta$ database is avoided.

The previous one-dimensional case for a gas mixture of 10%CO_2-10%H_2O-10%CO and 70% N_2 at 650 K was recalculated using the hybrid scheme with the old database. The divergence of radiative flux is shown in Fig. 6. The hybrid scheme correctly follows the LBL solution, requiring 3.19 s to determine the emission wavenumbers, as opposed to the old scheme, which needed 31.08 s for the identical example; i.e., the computational efficiency for wavenumber selection is improved about by a factor of 10.

3 Conclusions

An new emission wavenumber selection scheme has been applied to line-by-line photon Monte Carlo simulations for high-temperature gases to reduce computational cost. Based on the fact that emission is not effected by overlap between species, inverted random-number databases were established for individual gas species for an improved emission scheme. Even though the new scheme with inverted random-number database can improve computational efficiency about 20 times, it can also cause significant errors when interpolation is introduced. A hybrid scheme is proposed using part of both the old and the new schemes in order to improve efficiency as well as to guarantee accuracy. In this way, an emitting species is determined first, and then the appropriate wavenumber is selected by computational searching within the chosen species using the original uninverted database. This wavenumber selection scheme produces results as accurate as the old scheme, but with a time savings factor of about 10 compared to the old scheme.

Acknowledgment

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Nomenclature

ΔE = photon bundle energy, W/m^3
E_{tot} = total specific emission from all species, W/m^3
E_i = specific emission from species i, W/m^3
$I_{b\eta}$ = black body radiative intensity, W/m^{2}cm^{-1} sr
n = numbers of radiating species
p = pressure, bar
$\nabla \cdot q$ = divergence of radiative heat flux, W/m^3
R = random number
T = temperature, K
t_{cpu} = average CPU time per run, s
x = mole fraction
z = coordinate, m

Greek Symbols

$\Delta\eta$ = wavenumber interval, cm^{-1}
η = wavenumber, cm^{-1}
κ = absorption coefficient, cm^{-1}
κ_P = pressure-based Planck-mean absorption coefficient, bar^{-1} cm^{-1}
σ = Stefan-Boltzmann constant, W/m^2 K^4

Subscripts

i, j, s = species index
η = wavenumber

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