The Monte Carlo Method Applied to Gases With Spectral Line Structure

Michael F. Modest
Department of Mechanical Engineering
The Pennsylvania State University

Contents

Abstract

The necessary statistical relationships have been developed for the application of the Monte Carlo method to radiative heat transfer within media including molecular gases, which have absorption coefficients that vary strongly across the spectrum due to a multitude of partially-overlapping lines. The statistical narrow band model is applied to obtain the necessary random number relationships for wavelength of emission and for absorption path length. It is observed that absorption path lengths are considerably different, depending on whether emission is from a surface or from within the medium. The Monte Carlo method approach is verified by comparison with "exact" wide band model results for a few cases, for which such "exact" results are easily obtainable.

Nomenclature

A	area, cm^2
A^*	nondimensional band absorptance
d_η	spectral line spacing, cm^{-1}
E_n	exponential integral
G	incident radiation, W/cm^2
I, I_b	intensity (of a blackbody), W/cm^2 sr
L	thickness of slab, cm
q	radiative heat flux, W/cm^2
R_η	random number for wavenumber of emission
R_κ	random number for absorption path length
s, S	geometric coordinate, distance, cm
S_η	line intensity, $\int_{\text{line}} \kappa_\eta \, d\eta$, cm^{-2}
T	temperature, K
x, y, z	Cartesian coordinates, cm
α	absorptivity, or band strength parameter $= \int_{\text{line}} \kappa_\eta \, d\eta$, cm^{-2}
β	line overlap parameter
ϵ	emissivity
η	wavenumber, cm^{-1}
κ	absorption coefficient, cm^{-1}
μ	cosine of polar angle
σ	Stefan-Boltzman constant, $= 5.670 \times 10^{-12}$ W/cm^{2}K^4
τ	optical thickness
ω	bandwidth parameter, cm^{-1}
Ω	solid angle, sr

SUBSCRIPTS

g	gas
p	particles
P	Plank-mean
η	spectral value
0	at line or band center

OVERSCRIPTS

$\overline{}$	narrow band average
$\sim$	path average for variable properties

Introduction

There are several different computational methods with which radiative heat transfer problems may be analyzed. One of the more popular ones is the Monte Carlo method, a statistical method in which the history of large numbers of photon bundles is traced. The Monte Carlo method has the advantage that almost any problem of arbitrary complexity can be addressed with relative ease, but has the disadvantages of statistical scatter in the results and its large appetite for computer time. With the advent of faster and faster computers the second disadvantage is rapidly disappearing, and the popularity of the Monte Carlo method is expected to increase. Like other radiative heat transfer models, the Monte Carlo method was first employed in the field of neutron transport. The first radiative heat transfer papers using this method are due to Howell and Perlmutter (1964,1964), and Perlmutter and Howell (1964). While the necessary statistical relationships have been well established for problems of arbitrary complexity [*cf., e.g.*, the reviews by Howell, 1968; and Haji-Sheikh, 1988], most publications in the area have been concerned with relatively simple problems (simple geometries, gray and/or constant absorption coefficients, simple scattering behavior, etc.), or they have addressed computational aspects [*e.g.*, efficiency considerations, Kobiyama, 1989; the hybrid Monte Carlo method, Edwards, 1985; etc.]. Few investigations have dealt with non-gray media, and still fewer with non-gray molecular gases. For example, Modest (1989,1990) applied the Monte Carlo method to a gas at the high-pressure limit (strongly-overlapping spectral lines). To date, no attempt appears to have been made to apply the Monte Carlo method to gases with strong line structure effects. It is the purpose of the present paper to demonstrate that the Monte Carlo method can be applied to such problems by combining it with the narrow-band model, which is commonly used to model line structure effects. Comparison with results using the exponential wide band model demonstrates the validity of the present formulation.

Random Number Relations

In the Monte Carlo method a large statistical sample of photon energy bundles are traced from their point of emission to their point of absorption (or their leaving the geometry under investigation). To obtain statistically meaningful results relations need to be developed between random numbers and points of emission (from a surface, or from within the medium), direction of emission, wavenumber of emission, distance traveled before absorption (within the medium), distance traveled before

scattering, scattering direction, probability of reflection from a surface, and reflection direction. Of these various random number relations, two depend on the spectral absorption coefficient of the medium [Siegel and Howell, 1981; Modest, 1992]:

Wavenumber for emission from within the medium:

$$R_\eta = \frac{\pi}{\kappa_P \sigma T^4} \int_0^\eta \kappa_\eta \, I_{b\eta} \, d\eta, \tag{1}$$

Distance traveled before absorption within the medium:

$$R_\kappa = \exp\left[- \int_0^S \kappa_\eta \, ds \right]. \tag{2}$$

Here R_η and R_κ are random numbers which determine wavenumber of emission, η, and distance traveled between emission ($s = 0$) and absorption points ($s = S$), $I_{b\eta}$ is the Planck function or blackbody intensity, T is local temperature, κ_η is the local, spectral absorption coefficient, and κ_P is the Planck-mean absorption coefficient.

If the participating medium contains an absorbing/emitting molecular gas, the gas will have a number of vibration-rotation bands which—in turn—consist of hundreds of overlapping spectral lines. If line overlap is not very strong (small line overlap parameter β), the absorption coefficient becomes a strongly gyrating function of wavenumber making the use of equation (1) (emission wavenumber) and equation (2) (absorption location) impractical: (i) many digits of accuracy would be required in the evaluation of η, to ascertain whether emission occurs near a line center (with large κ_η) or between lines (small κ_η), (ii) accurate knowledge of the spectral gyration of κ_η is rarely known. To simplify the analysis one may employ the narrow band model described by, *e.g.*, Tien (1968). First, the absorption coefficient is split into two components,

$$\kappa_\eta = \kappa_{p\eta} + \kappa_{g\eta}, \tag{3}$$

where $\kappa_{p\eta}$ is the (spectrally-smooth) absorption-coefficient of other participating material (such as particles or ions), and $\kappa_{g\eta}$ is the rapidly-varying gas absorption coefficient. Taking a narrow band average over the Planck function-weighted absorption coefficient leads to

$$\int_0^\eta \kappa_{g\eta} \, I_{b\eta} \, d\eta = \int_0^\eta \left(\frac{1}{\delta\eta} \int_{\delta\eta} \kappa_{g\eta} \, I_{b\eta} \, d\eta' \right) d\eta \simeq \int_0^\eta \overline{\kappa}_{g\eta} \, I_{b\eta} \, d\eta,$$

where $\overline{\kappa}_{g\eta} = (S/d)_\eta$ is the narrow band average of the gas absorption coefficient, $S_\eta = \int_{\text{line}} \kappa_\eta \, d\eta$ is the line strength parameter, and d_η is the average line spacing.[1] The wavenumber of emission is determined with equation (1) from

$$R_\eta = \frac{\pi}{(\kappa_{pP} + \kappa_{gP}) \sigma T^4} \int_0^\eta \left(\kappa_{p\eta} + \overline{\kappa}_{g\eta} \right) I_{b\eta} \, d\eta, \tag{4}$$

or, after inversion,

$$\eta = \eta(R_\eta, \, x, \, y, \, z). \tag{5}$$

[1] Care must be taken to distinguish the line strength parameter $S_\eta = \int_{\text{line}} \kappa_\eta d\eta$ in the the locally averaged absorption coefficient from geometric distance S.

Application of the narrow band model to find the location of absorption within the participating medium is somewhat more complicated. The random number relations are different for photon bundles emitted from a surface (with spectrally-smooth emissivity ϵ_η), as opposed to bundles emitted from within the medium (with strongly varying absorption coefficient κ_η): bundles emitted from a wall are equally likely to have wavelengths close to the center of a line or the gap between two lines, causing them to travel a certain distance before absorption. Bundles emitted from within the medium are likely to have wavenumbers for which κ_η is large, making them much more likely to be absorbed near the point of emission.

The amount of energy emitted by a surface element dA over a wavenumber range $d\eta$ into a pencil of rays $d\Omega$ is

$$\epsilon_\eta \, I_{b\eta} \, dA_p \, d\eta \, d\Omega,$$

where dA_p is projected area normal to the pencil of ray. Of this, the amount

$$\epsilon_\eta \, I_{b\eta} \, dA_p \, d\eta \, d\Omega \, \exp\left[- \int_0^S \kappa_\eta \, ds \right]$$

penetrates a distance of S into the medium. Taking a narrow band average of both expressions leaves the first one unchanged while the second becomes

$$\epsilon_\eta \, I_{b\eta} \, dA_p \, d\eta \, d\Omega \frac{1}{\delta\eta} \int_{\delta\eta} \exp\left[- \int_0^S \kappa_\eta \, ds \right] d\eta \\ = \epsilon_\eta \, I_{b\eta} \, dA_p \, d\eta \, d\Omega \, (1 - \overline{\alpha}_\eta) \, ,$$

where $\overline{\alpha}_\eta$ is the narrow band average of the spectral absorptivity. The ratio of the two expressions gives the *fraction of energy* traveling a distance of S. For an isothermal path with spatially invariant κ_η the narrow band average for the absorptivity, using the statistical model, has been summarized, *e.g.*, by Tien (1968) and Edwards (1976), leading to

$$R_\kappa = 1 - \overline{\alpha}_\eta \simeq \exp\left[- \kappa_{p\eta} S - \frac{\tau_\eta}{\sqrt{1 + \tau_\eta / \beta}} \right] , \tag{6}$$

where $\tau_\eta = \overline{\kappa}_{g\eta} S$ and β is the line overlap parameter. In the high pressure limit (strong line overlap with $\beta \to \infty$) equation (6) reduces to

$$R_\kappa = \exp\left[- \left(\kappa_{p\eta} + \overline{\kappa}_{g\eta} \right) S \right] \quad \text{or} \quad S = \frac{1}{\kappa_{p\eta} + \overline{\kappa}_{g\eta}} \ln \frac{1}{R_\kappa}, \tag{7}$$

which is the expression regularly employed in Monte Carlo simulations (without line structure effects).

If the path through the absorbing/emitting medium is not isothermal (or if the absorption coefficient varies due to concentration changes), the narrow-band absorptivity may be approximated as outlined, *e.g.*, by Edwards (1976), using path averages for τ_η and β, or

$$\widetilde{\tau}_\eta = \int_0^S \overline{\kappa}_{g\eta} \, ds, \tag{8a}$$

$$\widetilde{\beta} = \frac{1}{\widetilde{\tau}_\eta} \int_0^S \overline{\kappa}_{g\eta} \beta \, ds, \tag{8b}$$

Therefore, for a non-isothermal gas equation (6) is replaced by

$$R_\kappa = 1 - \overline{\alpha}_\eta = \exp\left[-\int_0^S \kappa_{p\eta} ds - \frac{\widetilde{\tau}_\eta}{\sqrt{1+\widetilde{\tau}_\eta/\widetilde{\beta}}}\right]. \tag{9}$$

Explicit inversion of equations (6) and (9) is not possible (unless $\kappa_{p\eta} = 0$ and $\overline{\kappa}_{g\eta}$ =const).

If emission is from a volume element, we have for a volume dV, a wavenumber range $d\eta$ and a pencil of rays $d\Omega$ the total emitted energy [Siegel and Howell, 1981; Modest, 1992]:

$$\kappa_\eta \, I_{b\eta} \, dV \, d\eta \, d\Omega,$$

of which the amount of

$$\kappa_\eta \, I_{b\eta} \, dV \, d\eta \, d\Omega \, \exp\left[-\int_0^S \kappa_\eta \, ds\right]$$

is transmitted over a distance of S. Taking the narrow band average of both expressions, and dividing the second by the first gives the transmitted fraction as

$$\begin{aligned} R_\kappa &= \frac{\dfrac{1}{\delta\eta}\displaystyle\int_{\delta\eta} \kappa_\eta \, \exp\left[-\int_0^S \kappa_\eta \, ds'\right] d\eta}{\dfrac{1}{\delta\eta}\displaystyle\int_{\delta\eta} \kappa_\eta \, d\eta} \\ &= -\frac{1}{\kappa_{p\eta}+\overline{\kappa}_{g\eta}} \frac{d}{dS}\left[\frac{1}{\delta\eta}\int_{\delta\eta} \exp\left(-\int_0^S \kappa_\eta \, ds'\right) d\eta\right], \end{aligned} \tag{10}$$

where $s' = S - s$ is measured from the point of absorption back to the point of emission (this ensures, upon differentiation with respect to S, that the absorption coefficient at the point of emission appears in front of the exponent). For a gas medium with constant absorption coefficient the differentiation is readily carried out to yield

$$\begin{aligned} R_\kappa &= \frac{1}{\kappa_{p\eta}+\overline{\kappa}_{g\eta}} \frac{d\overline{\alpha}_\eta}{dS} \\ &= \frac{\kappa_{p\eta} + \dfrac{\overline{\kappa}_{g\eta}(2+\tau_\eta/\beta)}{2(1+\tau_\eta/\beta)^{3/2}}}{\kappa_{p\eta}+\overline{\kappa}_{g\eta}} \exp\left[-\kappa_{p\eta} S - \frac{\tau_\eta}{\sqrt{1+\tau_\eta/\beta}}\right]. \end{aligned} \tag{11}$$

Again, equation (11) reduces to equation (7) for $\beta \to \infty$.

For a medium with spatially varying properties equation (9) must be differentiated (from the point of absorption toward the point of emission), leading to

$$R_\kappa = \frac{\kappa_{p\eta} + \dfrac{\overline{\kappa}_{g\eta}(2+\widetilde{\tau}_\eta\beta/\widetilde{\beta}^2)}{2(1+\widetilde{\tau}_\eta/\widetilde{\beta})^{3/2}}}{\kappa_{p\eta}+\overline{\kappa}_{g\eta}} \exp\left[-\int_0^S \kappa_{p\eta} ds - \frac{\widetilde{\tau}_\eta}{\sqrt{1+\widetilde{\tau}_\eta/\widetilde{\beta}}}\right]. \tag{12}$$

Note that in this equation $\kappa_{p\eta}$, $\overline{\kappa}_{g\eta}$ and β are local values at the point of emission.

To demonstrate the difference between surface emission and medium emission for the distance traveled by a photon bundle before absorption, consider the following simple example: A photon bundle is traveling through a molecular gas. The wavelength of the bundle is such that $\overline{\kappa}_{g\eta} = 1\,\mathrm{cm}^{-1}$ and $\beta = 0.1$. Drawing a randum number of $R_\kappa = 0.200$, how far will the bundle travel before absorption, if it was emitted by a gray wall, or from within the gas? If the bundle originates from a wall, we have from equation (6)

$$R_\kappa = 0.200 = \exp\left[-\frac{\tau_\eta}{\sqrt{1+10\tau_\eta}}\right].$$

By trial and error (or solution of a quadratic equation), it follows that $\tau_\eta = 25.9$ and $S = \tau_\eta/\overline{\kappa}_{g\eta} = 25.9\,\mathrm{cm}$. For medium emission equation (11) is applicable, and

$$R_\kappa = 0.200 = \frac{1+5\tau_\eta}{(1+10\tau_\eta)^{3/2}} e^{-\tau_\eta/\sqrt{1+10\tau_\eta}},$$

or $\tau_\eta \simeq 0.48$ and $S = 0.48\,\mathrm{cm}$. Therefore, as expected, the bundle travels *much* farther if emitted from a wall. For comparison, in a gray medium the bundle would have traveled

$$S = \frac{1}{\kappa}\ln\frac{1}{R_\kappa} = \frac{1}{1\,\mathrm{cm}^{-1}}\ln\frac{1}{0.200} = 1.61\,\mathrm{cm}$$

for both cases.

Numerical Examples

To validate the present Monte Carlo relations, results have been obtained for two relatively simple cases, for which "exact", *i.e.*, wide band results can be found with relative ease. First the case of a one-dimensional, isothermal slab with cold boudaries is considered, testing the validity of equation (11). Secondly, the problem of radiative equilibrium in a plane-parallel medium is investigated. In both cases, the gas is idealized to have a single exponential vibration-rotation band, such that the narrow-band averaged absorption coefficient may be written as

$$\overline{\kappa}_\eta = \kappa_{p\eta} + \left(\frac{S}{d}\right)_\eta = \kappa_{p\eta} + \frac{\alpha}{\omega} e^{-2|\eta-\eta_0|/\omega}, \tag{13}$$

where $\alpha = \int_{\text{band}} \kappa_{g\eta}\, d\eta$ is the band strength parameter, η_0 is the wavenumber of the band center, and ω is the band width parameter. For the purposes of the validation η_0 and ω will be fixed as $\eta_0 = 3000\,\mathrm{cm}^{-1}$, $\omega = 200\mathrm{cm}^{-1}$, while α will be varied such that the effect of optical thickness of the band center, $(\alpha/\omega)L = \overline{\kappa}_{g0}L$, may be studied parametrically. In all cases, to make the problem mathematically tractable, we will assume κ_p, α, ω, and η_0 to be constant, *i.e.*, not to depend on location and/or temperature.

Isothermal Slab. Consider an isothermal, absorbing and emitting (but not scattering) slab of temperature $T = 1000\,\mathrm{K}$ and width L, bounded by two cold, black plates. For such a slab the spectral heat flux leaving either face of the slab is [Siegel and Howell, 1981; Modest, 1992]

$$q_\eta = 2\pi \int_0^1 \left(1 - e^{-\kappa_\eta L/\mu}\right) I_{b\eta}(T)\, \mu\, d\mu. \tag{14}$$

Assuming gray particles to be present, $\kappa_{p\eta} = \kappa_p = \text{const}$, this may be rewritten as

$$q_\eta = 2\pi \int_0^1 \left(1 - e^{-\kappa_p L/\mu}\right) I_{b\eta}\, \mu\, d\mu + 2\pi \int_0^1 e^{-\kappa_p L/\mu} \left(1 - e^{-\kappa_{g\eta} L/\mu}\right) I_{b\eta}\, \mu\, d\mu. \tag{15}$$

Using the definitions for exponential integrals and for total band absorptance, integrating over all wavenumbers and making the "narrow band" assumption (*i.e.*, $I_{b\eta} \simeq I_{b\eta_0} \simeq$ const. across the band), the heat flux becomes

$$q = [1 - 2E_3(\kappa_p L)]\, \pi I_b + 2\pi\omega I_{b\eta_0} \int_0^1 e^{-\kappa_p L/\mu} A^* \left(\frac{\overline{\kappa}_{g0} L}{\mu}\right) \mu\, d\mu, \tag{16}$$

where

$$A^*(\overline{\kappa}_{g0} S) = \frac{1}{\omega} \int_{\text{band}} \left(1 - e^{-\kappa_{g\eta} S}\right) d\eta \tag{17}$$

is the nondimensional band absorptance. Nondimensionalizing, the heat flux may be stated as

$$\Psi = \frac{q}{\sigma T^4} = 1 - 2E_3(\kappa_p L) + 2\left(\frac{\omega I_{b\eta_0}}{I_b}\right) \int_0^1 e^{-\kappa_p L/\mu} A^* \left(\frac{\overline{\kappa}_{g0} L}{\mu}\right) \mu\, d\mu. \tag{18}$$

The integral in equation (18) must be solved numerically employing one of the various available wide-band correlations [Tien, 1968; Edwards, 1976; Modest, 1992]. Some results for various values of $\overline{\kappa}_{g0} L$ are shown in Fig. 1 (pure gas, $\kappa_p L = 0$) and Fig. 2 (gas with particles, $\kappa_p L = 0.1$) for two band models: (i) the original exponential wide band model by Edwards and Menard (1964), and (ii) the Tien and Lowder model (1966). Comparison with Monte Carlo results shows near perfect agreement, *i.e.*, agreement within the accuracy of the wide band models. Note that, according to Edwards (1976), the ω in wide band models should be $\simeq 20\%$ smaller than for narrow band calculations (*i.e.*, for the Monte Carlo method). Therefore, the calculations of equation (18) were carried out with $\omega_{wb} = 200\,\text{cm}^{-1}/1.2 = 167\,\text{cm}^{-1}$. Differences between wide band model and Monte Carlo results are due to two sources: (i) the Monte Carlo method is subject to small statistical scatter (estimated to $\approx \pm 0.03$ for the value of Ψ); (ii) the major differences are expected to be due to inaccuracies in the wide band model. Edwards and Menard's model is an approximate integration of the narrow band structure and neglects changes for $1 \leq \beta < \infty$, which quite apparently do exist. The Tien and Lowder formula is nothing but a continuous curve fit of Edwards and Menard's model. It is also observed that, for otherwise identical conditions, the heat flux decreases with decreasing line overlap parameter β: for small β there is considerable room between lines (small κ_η and, therefore, little emission), and most emission takes place near line centers with large κ_η (and the radiation cannot escape from the medium since it will be reabsorbed near the point of emission).

Slab at Radiative Equilibrium. Consider an absorbing-emitting, non-scattering gas (no particles) with a single exponential band as given by equation (13). The gas is at radiative

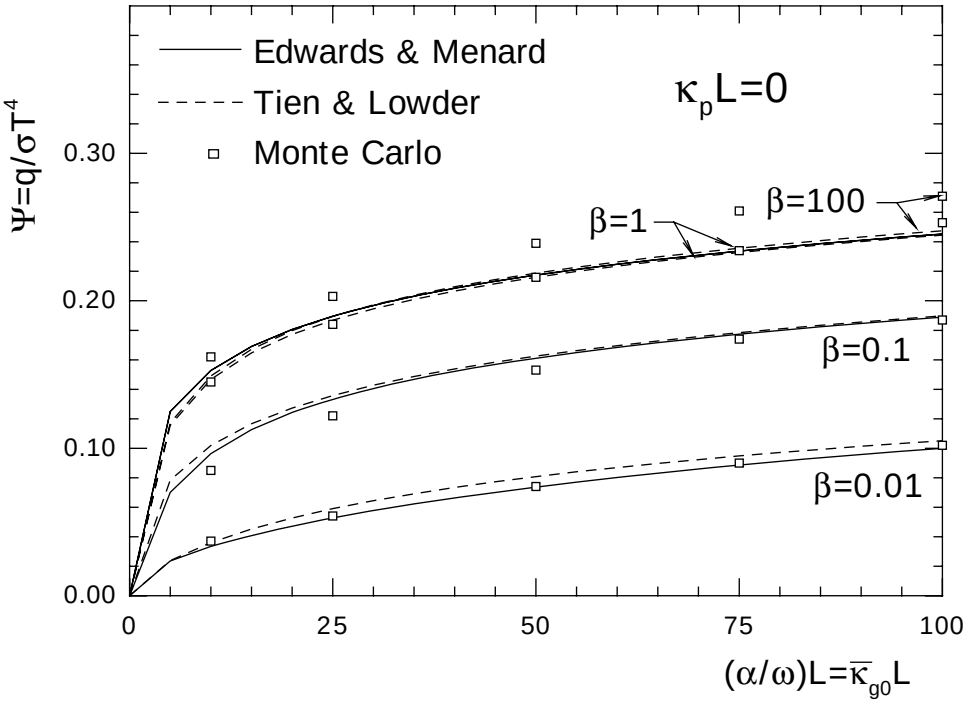

Figure 1: Total radiative heat loss from the face of an isothermal slab of non-gray molecular gas, without particles ($\kappa_p L = 0$).

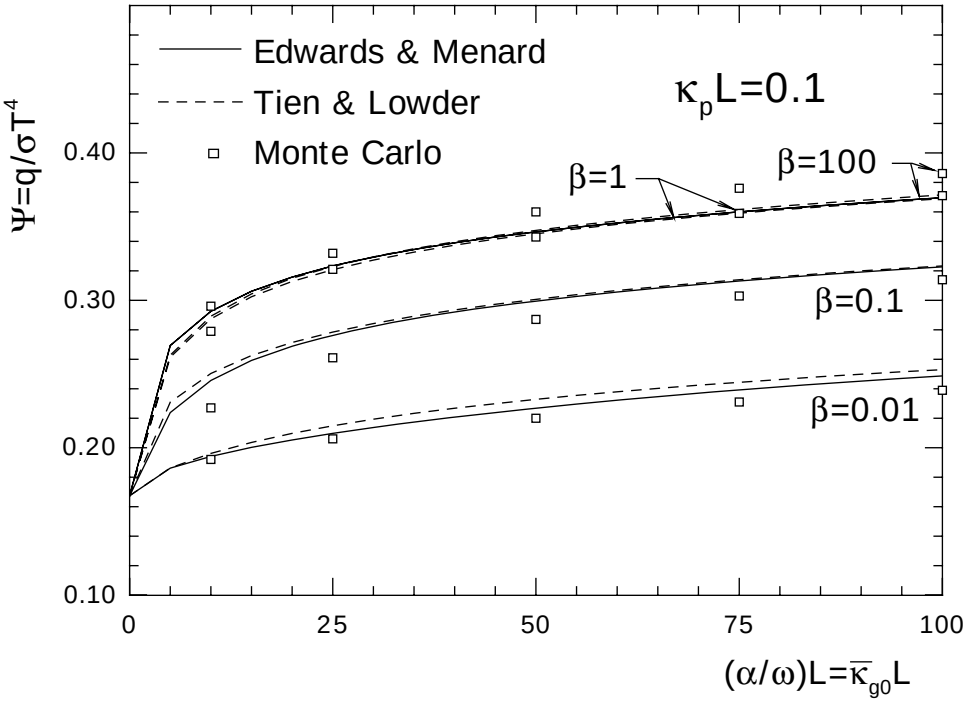

Figure 2: Total radiative heat loss from the face of an isothermal slab of a non-gray molecular gas-particulate mixture with particles ($\kappa_p L = 0.1$).

equilibrium and is bounded by two isothermal, black plates at $T_1 = 1200\,\mathrm{K}$ and $T_2 = 800\,\mathrm{K}$, respectively. For this case, spectral incident radiation and radiative heat flux follows as [Siegel and Howell, 1981; Modest, 1992]

$$\begin{aligned} G_\eta(z) &= 2\pi \int_{-1}^{1} I(\mu, z)\, d\mu \\ &= 2\pi \int_0^1 \Bigg\{ I_{b1\eta} e^{-\kappa_\eta z/\mu} + I_{b2\eta} e^{-\kappa_\eta (L-z)/\mu} \\ &\qquad + \frac{1}{\mu} \int_0^z I_{b\eta}(z')\, \kappa_\eta e^{-\kappa_\eta (z-z')/\mu} dz' \\ &\qquad + \frac{1}{\mu} \int_z^L I_{b\eta}(z')\, \kappa_\eta e^{-\kappa_\eta (z'-z)/\mu} dz' \Bigg\}\, d\mu, \end{aligned} \tag{19}$$

$$\begin{aligned} q_\eta(z) &= 2\pi \int_{-1}^{1} I(\mu, z)\, \mu\, d\mu \\ &= 2\pi \int_0^1 \Bigg\{ I_{b1\eta} e^{-\kappa_\eta z/\mu} - I_{b2\eta} e^{-\kappa_\eta (L-z)/\mu} \\ &\qquad + \frac{1}{\mu} \int_0^z I_{b\eta}(z')\, \kappa_\eta e^{-\kappa_\eta (z-z')/\mu} dz' \\ &\qquad - \frac{1}{\mu} \int_z^L I_{b\eta}(z')\, \kappa_\eta e^{-\kappa_\eta (z'-z)/\mu} dz' \Bigg\}\, \mu\, d\mu, \end{aligned} \tag{20}$$

The statement of radiative equilibrium implies

$$\nabla \cdot \mathbf{q} = \int_0^\infty \kappa_\eta (4\pi I_{b\eta} - G_\eta)\, d\eta = 0, \tag{21}$$

or

$$4\pi \kappa_P I_b = 4\pi \alpha I_{b\eta_0} = \int_0^\infty \kappa_\eta G_\eta\, d\eta \tag{22}$$

Multiplying equation (19) by κ_η and integrating over the spectrum results in (using the definition of nondimensional band absorptance)

$$\begin{aligned} 2\phi(\tau) = \phi_1 f(z) + \phi_2 f(L-z) &+ \int_0^z \phi(\tau') \frac{d}{dz'} f(z-z')\, dz' \\ &- \int_z^L \phi(z') \frac{d}{dz'} f(z'-z)\, dz' \end{aligned} \tag{23}$$

where

$$\phi(z) = \frac{\omega I_{b\eta_0}(z)}{I_{b1} - I_{b2}}, \tag{24}$$

$$f(z) = \int_0^1 A^{*\prime} \left(\frac{\overline{\kappa}_{g0} z}{\mu} \right) d\mu \tag{25}$$

and the prime attached to the A^* implies differentiation with respect to its argument.

Equation (23) is a relatively simple integral equation, which has been solved by a straight forward successive approximation technique. Once $\phi(z)$ is known, the heat flux may be evaluated

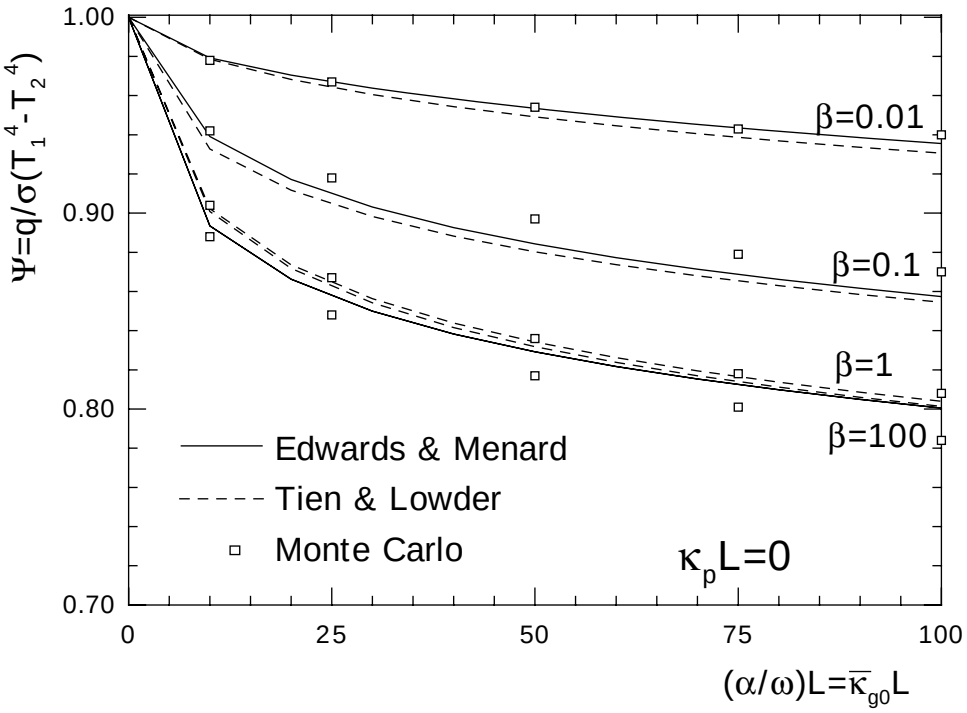

Figure 3: Radiative heat flux between black, parallel plates separated by a non-gray molecular gas at radiative equilibrium.

at any z from equation (20) as

$$
\begin{aligned}
q(z) &= \text{const} \\
&= \pi(I_{b1} - I_{b2}) + 2\pi\,(I_{b1} - I_{b2}) \Bigg\{ \phi_2 g(L - z) - \phi_1 g(z) \\
&\qquad + \overline{\kappa}_{g0} \int_0^z \phi(z') f(z - z')\, dz' \\
&\qquad - \overline{\kappa}_{g0} \int_z^L \phi(z')\, f(z' - z)\, dz' \Bigg\}, \qquad (26)
\end{aligned}
$$

$$
g(z) = \int_0^1 A^* \left(\frac{\overline{\kappa}_{g0} z}{\mu} \right) \mu\, d\mu, \qquad (27)
$$

or

$$
\begin{aligned}
\Psi &= \frac{q}{\sigma(T_1^4 - T_2^4)} = 1 - 2 \Bigg\{ \phi_1 g(z) - \phi_2 g(L - z) \\
&\qquad - \overline{\kappa}_{go} \int_0^z \phi(z') f(z - z')\, dz' \\
&\qquad + \overline{\kappa}_{g0} \int_z^L \phi(z')\, f(z' - z)\, dz' \Bigg\}. \qquad (28)
\end{aligned}
$$

Results from the Monte Carlo simulation and the wide band model are compared in Fig. 3 (again, in the wide band model calculations, the value of ω has been reduced by 20%). The agreement

between both models is excellent. Here, the heat flux increases with decreasing line overlap parameter β: for small β there are "mini-spectral windows" between the lines, through which radiation can travel unimpeded from plate to plate, increasing heat exchange.

Conclusion

The Monte Carlo method has been extended to the case of non-gray molecular gases for strongly gyrating absorption coefficient (line structure effects). It was demonstrated that the narrow band model may be applied successfully to the Monte Carlo method. In this paper verification was limited to the case of a spatially constant absorption coefficient. Verification for temperature and/or concentration dependence of the absorption coefficient needs to await extensive numerical and/or experimental study.

Acknowledgment

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