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Technical Notes

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Monte Carlo Simulation of Radiation in Scattering Volumes with Line Structure

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Introduction

ACCURATE consideration of line structure in scattering media remains a problem in radiant heat exchange and applied computational physics. Calculation of spectral radiation transfer requires integration of the transfer equation over thousands of spectral bands, over which the optical thickness in the spectrum may change by orders of magnitude. Including scattering and realistic geometries makes this task difficult even for modern supercomputers. Significant recent work addresses this problem.[1–4]

For radiative transfer in the infrared region ($\Delta\omega$ = 500–10,000 cm^{-1}), two other scales are important: 1) the half-width of a rotational line, $\gamma \sim 0.01$–$1\ cm^{-1}$, and 2) the width of a vibrational band, $\Delta\omega_v \sim 200$–$500\ cm^{-1}$. Various degrees of detail can be used to describe the spectral characteristics. To describe the rotational structure of a spectrum, line-by-line integration requires wave number increments smaller than the size of a rotational line. In each spectral element, averaged absorption and scattering coefficients are used. To describe the vibrational structure of a spectrum, the wave number range for averaging should contain many rotational lines but must not be so large that averaging over the vibrational structure introduces significant error. The characteristic range for averaging over the rotational structure within a vibrational band is $\Delta\omega_g$ = 50–100 cm^{-1}.

One approach is to develop approximate methods that include radiation transfer relationships, the line structure of the spectrum, and scattering with a precision sufficient for practical needs. Monte Carlo simulation has a significant advantage in this type of problem, in that if careful statistical averaging methods are applied, the accuracy of the radiative energy transfer predictions depends only on the number of samples chosen; i.e., accuracy is independent of the complexity of the spectrum. This paper compares five algorithms that are based on direct Monte Carlo simulation of photon trajectories. Comparisons are shown for radiation transfer in a one-dimensional slab with line absorption and scattering.

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Line-by-Line Integration over a Spectrum

For line-by-line calculation, the given spectral range is divided into N spectral subregions $\Delta\omega_g$. In each subregion the averaged absorption coefficient is

$$\kappa_g = \frac{1}{\Delta\omega_g}\int_{\Delta\omega_g}\left[\kappa^p(\omega) + \kappa^c(\omega) + \sum_{i}^{N_l}\kappa_i^l(\omega)\right]d\omega$$

where $\kappa_i^l(\omega)$ is the spectral absorption coefficient of the ith line, N_l is the number of lines located in the subregion $\Delta\omega_g$, and $\kappa^c(\omega)$, $\kappa^p(\omega)$ are the continuum spectral absorption coefficients of the gas and solid particles. It is assumed that all lines are of Lorentzian shape

$$\kappa_i(\omega) = \frac{S_i\gamma_{L,i}}{\pi[(\omega - \omega_{0,i})^2 + \gamma_{L,i}^2]}$$

where S_i, $\gamma_{L,i}$ are the intensity and half-width of the ith line, and $\omega_{0,i}$ is the wave number at the center of the ith line.

Within each spectral subregion $\Delta\omega_g$, a simulation of photon trajectories is carried out by the Monte Carlo method as for a gray medium.[4] For a nonuniform but gray medium, the coefficients κ_g, κ^p, κ_i^c, κ^l, $\kappa_i(\omega)$, S_i, and γ are functions of the coordinates.

Hybrid Statistical Method

In the hybrid statistical method, a Monte Carlo simulation is used to track photon groups whose energy is averaged over a spectral band. Averaged energies of photon groups for various optical paths are determined using statistical models of real-line spectra, and the Curtis–Godson method is used to account for inhomogeneity of the optical path. The spectrum is divided into a number of bands with $\Delta\omega_g$ of 50–250 cm^{-1} in the infrared region. Many spectral lines and a continuous (or quasicontinuous) absorption spectrum may exist in each band.

Calculation starts from the formulation of the position vector of a linear homogeneous section in the direction of motion of photons in the inhomogeneous environment (l_j, j = 1, 2, . . . , N, where $l_1 = 0$, and l_N is the coordinate of the point of intersection between the ray and the boundary surface). The node values l_j correspond to the points of intersection between the ray under consideration and the boundary surfaces of each homogeneous volume element. Each element has associated coordinates l_j, gas temperature, particle temperature, molar concentrations of optically active components of the gas mixture, concentrations of optically active solid (liquid) mixture components, and the total pressure of the gas mixture. The dimensionality of the vectors is $N - 1$, because the properties inside each element are assumed to be constant. The optical constants are the coefficients of absorption κ_j^p and scattering σ_j^p of the condensed phase; the scattering phase-function or average-scattering cosine $\bar{\mu}_j$ (considered to be independent of wave number within the spectral band $\Delta\omega_g$); absorption coefficients κ_j^c in the continuous spectrum; the average absorption coefficient in the spectral lines $(S/d)_{k,b,j}$; the line-broadening parameter $\beta_{k,b,j}$; and the effective pressure $(P_e)_{k,b,j}$. The average absorption coefficient in the spectral lines, the spectral line broadening parameter, and the effective pressure are calculated

using the wideband model[5,6] for each molecular band b for each component k that contributes to radiation absorption in band $\Delta\omega_g$.

The photon mean free path is found as usual. The point of collision between the photons and particles requires additional calculations because of the inequality of total transmission over the entire spectral interval to the sum of the individual transmissions of its components. Thus, it is necessary to use the following formulas for a random model of the optical thickness of each bth band:

$$\tau_j^a = \sum_k \sum_b \tau_{k,b,j} + \sum_k \tau_{k,j}^c + \sum_k \tau_j^p, \quad \tau_{k,j}^c = \sum_{m=2}^{j} \kappa_m^c (l_m - l_{m-1})$$

$$\tau_j^p = \sum_{m=2}^{j} \kappa_m^p (l_m - l_{m-1}), \quad \tau_{k,b,j} = \frac{\chi_{k,b,j}}{\sqrt{1 + \dfrac{\chi_{k,b,j}}{4a_{k,b,j}^L}}}$$

$$\chi_{k,b,j} = \int_{l_1}^{l_j} \rho_k \left(\frac{S}{d}\right)_{k,b} \mathrm{d}l, \quad a_{k,b,j}^L = \frac{\displaystyle\int_{l_1}^{l_j} \left(\frac{S}{d}\right)_{k,b} \left(\frac{\gamma_L}{d}\right)_{k,b} \rho_k \, \mathrm{d}l}{\displaystyle\int_{l_1}^{l_j} \left(\frac{S}{d}\right)_{k,b} \rho_k \, \mathrm{d}l}$$

where ρ_k is the density of the kth component of the mixture.

The rest of the Monte Carlo procedure is the same as for monochromatic radiation. The uniform energy for each simulated photon group is calculated by finding the integrated emissive power E of the entire volume V and its separate parts E_n on the finite difference grid; finding the energy of each photon group e_f by dividing the complete energy E by the number of simulated groups N_f; and determining the relative probability of photon emission for each volume element p_n by the relation of the emissive power of the given zone to the integrated emissive power $p_n = E_n/E$. This method of estimating the emissive power is reasonable when the volume V_n is optically thin.

Method of Smoothing Coefficients

This method is equivalent to the hybrid Monte Carlo method, but with an additional simplification: $\tau_{k,b,j} = \chi_{k,b,j}$, which is correct if $(\chi_{k,b,j}/4a_{k,b,j}^L) << 1$. Obviously, the error of this method increases with optical thickness. However, as will be shown, at large optical thicknesses this method gives more physically reasonable results than the hybrid Monte Carlo method.

Two-Group Method

Consider radiation transfer in spectral range $\Delta\omega_g$, in which N_l lines are located. It is assumed that the integrated emission in this spectral range is independent of line location. The average intensity and average half-width for all lines in the $\Delta\omega_g$ range in each spatial zone is

$$\langle S_n \rangle = \frac{1}{N_l} \sum_i^{N_l} S_{i,n}, \qquad \langle \gamma_n \rangle = \frac{1}{N_l} \sum_i^{N_l} \gamma_{i,n}$$

The average half-width for all spatial zones is

$$\langle \gamma \rangle = \frac{1}{N_n} \sum_{n=1}^{N_n} \langle \gamma_n \rangle$$

Consider two spectral ranges inside $\Delta\omega_g$

$$\Delta\omega_1 = \min \{2N_l\langle\gamma\rangle, \Delta\omega_g\}, \qquad \Delta\omega_2 = \Delta\omega_g - \Delta\omega_1$$

The average absorption coefficients in these two spectral ranges are

$$\bar{\kappa}_{1,n} = \kappa_n^p + \kappa_n^c + \frac{\langle S_n \rangle}{\pi \langle \gamma \rangle}$$
$$\bar{\kappa}_{2,n} = \kappa_n^p + \kappa_n^c + \left(\langle S_n \rangle N_l - \frac{\langle S_n \rangle}{\pi \langle \gamma \rangle} \Delta\omega_1 \right) \frac{1}{\Delta\omega_2} \tag{1}$$

The problem is reduced to the modeling of photon groups in two spectral regions with the absorption coefficients from Eq. (1). The emissive powers of the separate spatial regions are $E_n = 4\pi V_n \bar{J}_{b,n} \bar{\kappa}_{1,n} \Delta\omega_1$, $E_n = 4\pi V_n \bar{J}_{b,n} \bar{\kappa}_{2,n} \Delta\omega_2$. All results using this method were obtained for $\Delta\omega_1 < \Delta\omega_g$.

Line-by-Line Integration with Few Trajectories

Experience in solving gray problems indicates that about $N_f = 10^4$ to 5×10^4 photon group trajectories provide satisfactory accuracy. For the case of low albedo ($\omega < 0.9$) and moderate optical thickness ($\tau < 1$), this number can be reduced by one order, but for a multiscattering medium with large optical thickness, the number must be increased. When the averaged (or integrated) radiating characteristics are required for a spectral range $\Delta\omega_g$ containing tens to hundreds of rotational lines, the spectral absorption coefficient within the range can vary by orders of magnitude. Therefore, spectral subregions almost always contain both small and large optical thickness. For obtaining average radiating characteristics, $N_f \sim 10^4$ is sufficient. The energy of each new photon group is estimated statistically. The spectral absorption coefficient is calculated for any spectral point inside the range $\Delta\omega_g$.

The range $\Delta\omega_g$ can be further divided into spectral subelements. The number of subelements must be sufficient for detailed description of the line structure of the spectrum. For example, for $\Delta\omega_g = 20\ \mathrm{cm}^{-1}$ and average line half-width $\gamma = 0.1\ \mathrm{cm}^{-1}$, about 1000 spectral subelements are enough. To calculate average characteristics for this $\Delta\omega_g$, apply the usual procedure of line-by-line integration, but within each spectral subelement simulate trajectories of only 10–15 photon groups. It is impossible to determine spectral characteristics in this way, but averaged energy transfer characteristics within $\Delta\omega_g$ can be obtained with good accuracy.

Comparison of the Algorithms

Two problems serve to compare the algorithms: 1) determination of the reflectivity and transmissivity of a cold isotropically scattering and selective absorbing plane layer, and 2) determination of the emissivity of a plane isotropically scattering and selectively absorbing layer. There is a basic difference between the first and second cases. The hemispherical emissivity of a medium is a selective function, because it is determined as a product of the Planck spectral function at the layer temperature and the spectral absorption coefficient, which is a strong function of wave number. In contrast, the intensity of radiation falling on the boundary of the plane layer for determining reflectivity and transmissivity is assumed independent of wave number. In both cases, it is assumed that there are five identical equally spaced Lorentzian lines in the spectral range being considered, $\Delta\omega_g = 3600$–$3620\ \mathrm{cm}^{-1}$.

The line centers are located at $\omega_i = \omega_{\min} + (\Delta\omega_g/N_l)\ (i - 0.5)$, $i = 1, 2, \ldots, N_l$, where $\omega_{\min}$ is the lowest boundary of the spectral region $\Delta\omega_g$. The parameters of the problems are $\tau_0 = \kappa_0 H$, the optical thickness of the layer (for absorption) at line centers; $\gamma = \gamma_{L,i}$ the half-width of a Lorentzian line; and $\tilde{\omega} = \sigma/(\kappa_0 + \sigma)$, the albedo for single scatter.

The intensity of each spectral line is $S_i = \pi\tau_0\gamma$. The layer thickness is $H = 1$ cm. The calculations were carried out for $0.1 \le \tau_0 \le 10$, $0.05 \le \gamma \le 0.5\ \mathrm{cm}^{-1}$, and 0 (nonscattering medium) $\le \tilde{\omega} \le 0.91$. In the line-by-line calculations, the spectral range was divided into 271 spectral subregions.

Table 1 Hemispherical reflectivity and transmissivity of plane layer for $t_0 = 1.0$

	Line-by-line integration	Hybrid Monte Carlo method	Method of smoothing coefficients	Two-group method	Line-by-line simulation with few trajectories
N_f	1000	10,000	10,000	10,000	10
		Transmissivity (for $\sigma = 0$)			
γ, cm^{-1}					
0.05	0.950	0.953	0.933	0.950	0.954
0.1	0.902	0.907	0.857	0.899	0.902
0.5	0.583	0.642	0.578	0.582	0.587
		Transmissivity/reflectivity (for $\sigma = 10$ cm^{-1}, $\omega = 0.91$)			
0.05	0.105	0.0964	0.0912	0.1033	0.1048
	——	——	——	——	——
	0.858	0.855	0.840	0.858	0.857
0.1	0.0945	0.0834	0.0717	0.0932	0.1004
	——	——	——	——	——
	0.832	0.824	0.807	0.830	0.830
0.5	0.0330	0.0314	0.0215	0.0334	0.0384
	——	——	——	——	——
	0.671	0.689	0.648	0.673	0.663

Table 2 Hemispherical emissivity of plane layer for $t_0 = 1.0$

	Line-by-line integration	Hybrid Monte Carlo method	Method of smoothing coefficients	Two-group method	Line-by-line simulation with few trajectories
N_f	1000	10,000	10,000	10,000	10
		Emissivity for top and bottom layer surfaces (for $\sigma = 0$, $\omega = 0$)			
γ, cm^{-1}					
0.05	0.04772	0.0711	0.073	0.049	0.0437
	——	——	——	——	——
	0.04877	——	——	——	0.0536
0.1	0.09399	0.135	0.140	0.093	0.0909
	——	——	——	——	——
	0.09556	——	——	——	0.0927
0.5	0.40485	0.457	0.518	0.411	0.3720
	——	——	——	——	——
	0.40681	——	——	——	0.4267
		Emissivity for top and bottom layer surfaces (for $\sigma = 10$ cm^{-1}, $\omega = 0.91$)			
0.05	0.03819	0.0681	0.071	0.0398	0.03443
	——	——	——	——	——
	0.03733	——	——	——	0.03601
0.1	0.07433	0.121	0.128	0.0755	0.07339
	——	——	——	——	——
	0.07397	——	——	——	0.07861
0.5	0.29366	0.342	0.374	0.296	0.30121
	——	——	——	——	——
	0.29772	——	——	——	0.27747

Prediction of Hemispherical Reflectivity and Transmissivity

The results for the first problem are presented in Table 1 for a nonscattering medium (case 1) and a scattering nonradiating one with $\tilde{\omega} = 0.91$ (case 2). The number of simulated trajectories of photon groups within each spectral subregion is specified in the second line of Tables 1 and 2.

For the nonscattering medium, only transmissivity is presented (because the reflectivity of a nonscattering medium is equal to zero). For cases with scattering ($\sigma \neq 0$), the top number corresponds to the hemispherical transmissivity, and the bottom one to the reflectivity.

For a small optical thickness, $\tau_0 < 0.1$ (the results are not presented here), all of the algorithms give good accuracy compared with line-by-line results. As expected, transmissivity decreases with an increase in line half-width or scattering coefficient.

For an intermediate optical thickness, $\tau_0 \sim 1$, in the case of a nonradiating medium, the method of smoothing coefficients has poor accuracy, in particular for transmissivity. For $\gamma = 0.5$ and $\tau_0 = 10$ (not shown) the error of the smoothing coefficients calculations reaches ~35%. The error for the other algorithms does not exceed 20%. For large optical thickness, $\tau_0 > 10$ (not shown), the transmissivity becomes quite small, and large percentage errors in transmissivity are observed for all investigated algorithms, although absolute errors are small.

The growth of the errors in both absorption and scattering for the direct simulation Monte Carlo method with increasing optical thickness is expected. Statistical errors in the calculations, which are connected to the increase in the quantity of absorbed photons, inevitably grow. Also, in a number of algorithms the approximation of an optically thin layer is used (hybrid method, method of smoothing coefficients). Finally,

using integrated absorption coefficients for large line broadening ($\gamma \sim 0.5$ cm^{-1}) becomes a poor assumption, because significant absorption by the wings of the lines occurs outside the limits of the spectral range. For some of the same reasons, the results of line-by-line calculations cannot be accepted as a benchmark. Thus, the results of calculations using the direct simulation Monte Carlo method at this point must be considered as only approaching the correct results. To obtain more exact results it is necessary to either increase the number of simulated trajectories or to apply other methods.

The results for transmissivity have appreciable relative errors. This occurs because of the following reasons:

1) The solution of the transmissivity of selectively absorbing scattering layers requires special consideration (it is necessary to search for the optimum number of simulated trajectories, select a special simulation algorithm or another method, etc.).

2) The chosen number of simulated trajectories N_f does not ensure acceptable accuracy for a problem of this type. However, any further increase in N_f causes the algorithms to lose their basic advantage, high computational speed.

3) Despite appreciable errors, modifications of the simple Monte Carlo method are more economical than the method of line-by-line integration applied thousands or tens of thousands of times. Therefore it is useful to continue research such as this to find the most adequate and optimum methods.

Results for Emissivity

Calculation of emissivity is complicated because it is a selective function and, therefore, incurs additional errors from the averaging procedures.

Results for the hemispherical emissivity are presented in Table 2. The hemispherical emissivity for both surfaces is shown. For an exact solution, these values should be equal; the differences in the emissivities of the two surfaces serve as an empirical estimate of the accuracy of the results.

Again, accuracy is acceptable for optically thin media ($\tau_0 < 0.1$). In spite of the rather simple analysis needed for this case, the high accuracy in average emissivity is remarkable given the range of absorption coefficient of about three orders across the spectrum. Among the algorithms investigated, the most economic is the method of smoothing coefficients. In CPU time, the hybrid Monte Carlo method took about 10% longer, the two-group method about twice as long, and the method of line-by-line integration with few trajectories took many times longer. For large optical thickness ($\tau_0 > 10$) (not presented here), the hybrid method and method of smoothing coefficients experience errors of more than 100%, and the hybrid Monte Carlo method gives nonphysical results (emissivity of the layer is predicted to be more than unity). The main reason for this error is a poor choice of average energy of the photon groups by assuming optically thin emission. The method of line-by-line integration with few trajectories has the best accuracy.

Conclusions

Four approximate fast algorithms for direct Monte Carlo simulation that take into account the line structure of an absorption spectrum have been developed and investigated. It is shown that all algorithms allow calculation of radiation transfer in scattering volumes with sufficient accuracy for practical needs, particularly at optical thickness based on line centers of order unity.

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Analysis of Transient Heat Transfer in a Cylindrical Pin Fin

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Nomenclature

A	=	dimensionless radius of fin, A^*/L
A^*	=	radius of fin
Bi_a	=	transversal Biot number, hA^*/k
Bi_T	=	tip Biot number, h_TL/k
G	=	geometry parameter for fin, L/A^*
H	=	ratio of convective heat transfer coefficients, h_T/h
h	=	convective heat transfer coefficient at lateral surface
h_T	=	convective heat transfer coefficient at tip surface
J_n	=	nth-order Bessel function
k	=	thermal conductivity of fin
L	=	fin length
$Q(t)$	=	dimensionless transient heat flow at fin base, $Q_0(t^*)/2\pi A^*k(T_0^* - T_\infty^*)$
$Q_0(t^*)$	=	transient heat flow at fin base
$T(t, x, r)$	=	dimensionless transient temperature for two-dimensional solution, $T^*(t^*, x^*, r^*) - T_\infty^*/T_0^* - T_\infty^*$
$T^*(t^*, x^*, r^*)$	=	transient temperature for two-dimensional solution
T_∞^*	=	temperature of surroundings
T_0^*	=	temperature at fin base
t	=	dimensionless time, $\alpha t^*/L^2$
t^*	=	time
x, r	=	dimensionless coordinates, x^*/L, r^*/L
x^*, r^*	=	axial and radial coordinates
α	=	thermal diffusivity
β, η	=	roots of transcendental equations

Introduction

THE use of extended surfaces or fins as heat transfer enhancement devices plays an important role in many thermal engineering applications. For one- or two-dimensional transient analysis of a fin, few papers have appeared in the literature. Chapman[1] first analyzed the transient response of an annular fin with uniform thickness subjected to a step change of base temperature. Yang,[2] Aziz,[3] and Suryanarayana[4] discussed the transient heat transfer problems with various base boundary conditions in a one-dimensional fin. Chu et al.[5] stud-

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