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A new radiative transfer scattering phase function discretisation approach with inherent energy conservation

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ABSTRACT

In the popular Discrete Ordinates Method (DOM) formulation of the Equation of Radiative Transfer (ERT), the 4π solid angle range of directions is divided into a finite number of discrete directions or ordinates. This requires that the continuous distribution of the scattering phase function of the medium under consideration must be discretised to suit the different number, weightings and directions of the S_N ordinate set being used. This must be done such that the sum of scattered energy is conserved relative to the continuous distribution, and that the asymmetry factor g is similarly conserved. This paper introduces a discretisation technique with inherent energy conservation, suitable for any quadrature scheme. The technique was tested on two large sphere scattering phase function distributions of interest for packed bed radiative heat transfer: the analytic distribution for a diffusely reflecting sphere (a back-scattering test case) and the distribution for a transparent sphere ($n = 1.5$) obtained by ray tracing (a test case with strong forward scatter and some back-scatter). In both cases the resultant discretised phase function distributions for the S_4, S_6 and S_8 ordinate sets produced errors for the sum of scattered energy conservation of less than 0.035% and errors for g less than 1.3%. This demonstrates the inherent energy conservation of the method, as well as visible reductions in g errors. The phase function values for each case are tabulated in the paper. The major benefit of the method is the fact that computationally costly matrix calculations are avoided at run-time: the discretisation for a given scattering medium using a quadrature scheme of given order is performed only once beforehand, and the resultant distributions can be stored in an input file or look-up table for future computations with different boundary conditions, different meshes and even different geometries.

1. Introduction

1.1. Fundamentals of the discrete ordinate method

The solution of the Equation of Radiative Transfer (ERT) is required whenever a scattering, absorbing and/or emitting medium is present in a volume of radiative heat transfer interest:

$$\frac{dI}{ds} = \hat{s}\cdot\nabla I = \kappa I_b - \beta I + \frac{\sigma}{4\pi}\int_{4\pi} I(\hat{s}_j)\Phi_{(}\hat{s}_j,\hat{s})d\Omega_j \quad (1)$$

where Eq. (1) is valid for grey media (or non-grey media on a spectral basis) [1]. The final term on the right hand side of Eq. (1) is the in-scattering term. The scattering phase function $\Phi_{(}\hat{s}_j,\hat{s})$ represents the probability that a photon travelling in direction $\hat{s}_j$ will be scattered in direction $\hat{s}$ (the direction represented on the left hand side by $dI/ds = \hat{s}\cdot\nabla I$). An alternative representation of $\Phi_{(}\hat{s}_j,\hat{s})$ is $\Phi(\theta)$, where θ is the angle between the $\hat{s}$ direction of the beam being calculated in Eq. (1) and incoming direction $\hat{s}_j$ of radiation being considered in the in-scatter term. The scattering phase function distribution $\Phi(\theta)$ is continuous with angle θ, and is axisymmetric about the axis of the incoming beam.

Of the different techniques available for simulating radiative heat transfer in participating media, the S_N or Discrete Ordinates Method (DOM) is popular and widely used [2]. The development and applications of the DOM have been extensively described by many authors, so will not be repeated here. In the DOM, the continuous 4π solid angle range is divided into a finite number n of discrete directions or ordinates, so in Eq. (1), numerical quadrature (with quadrature weights w_j for each direction $\hat{s}_j$) replaces the integral over direction in the in-scattering term [3,4]:

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Nomenclature

DOM	discrete ordinates method
ERT	Equation of Radiative Transfer
$f(\cdot)$	function of $(\cdot)$
g	asymmetry factor
HG	Henyey–Greenstein
I	radiative intensity, (W m^{-2} sr^{-1})
k	current interval number
LA	linear-anisotropic
MDOM	modified discrete ordinates method
n	number of directions $\hat{s}_i$ in current S_N quadrature set
N	order of S_N quadrature set
$N_{intervals}$	number of intervals
$N_{w\ k}$	number of different weightings of ordinates in interval number k
$\hat{s}$	unit direction vector
w_i	discrete direction weight for direction $\hat{s}_i$
x, y, z	directions in Cartesian coordinate system
x_k	angle of lower boundary of kth interval

Greek symbols

β	extinction coefficient $(\kappa + \sigma)$ (m^{-1})
η	direction cosine with respect to the z-axis
θ	polar angle between i and j directions
κ	absorption coefficient (m^{-1})
μ	direction cosine with respect to the x-axis
ξ	direction cosine with respect to the y-axis
σ	scattering coefficient (m^{-1})
φ	azimuthal angle
Φ	continuous scattering phase function
Φ_{ij}	discretised scattering phase function
$\tilde{\Phi}_{ij}$	normalised scattering phase function
Φ_{step}	step-wise discontinuous axisymmetric scattering phase function
$d\Omega$	solid angle, $\sin\theta\, d\theta d\varphi$

Subscripts

b	blackbody
cells	pertaining to grid cells
HG	Henyey–Greenstein
i	direction of current beam being calculated
j	direction of incoming beam being considered in in-scattering term
wall	boundary surfaces of the computational volume
x, y, z	x, y or z directions

$$\frac{1}{4\pi}\int_{4\pi} f(\hat{s})d\Omega = \frac{1}{4\pi}\sum_{j=1}^{n} w_j f(\hat{s}_j) \tag{2}$$

In the standard DOM, this leads to a system of n equations described (in Cartesian coordinates) by:

$$s.\nabla I_i = \xi_i\frac{\partial I_i}{\partial x} + \eta_i\frac{\partial I_i}{\partial y} + \mu_i\frac{\partial I_i}{\partial z} = \kappa I_b - \beta I_i + \frac{\sigma}{4\pi}\sum_{j=1}^{n} w_j\Phi_{ij}I_j, \quad i = 1, 2, \ldots, n \tag{3}$$

The modified DOM or MDOM is an augmented version of the standard DOM described above. It was developed to address the known "ray effect" limitation of the conventional DOM, by splitting the intensity I in Eq. (3) into two components [5,6]:

$$I(x, y, z, \hat{s}) = I^d(x, y, z, \hat{s}) + I^s(x, y, z, \hat{s}) \tag{4}$$

The direct (or "ballistic" [5]) intensity component I^d originates from sources on the boundary surfaces of the computational volume, which may be either collimated or diffuse [7]. It is assumed in the transport equation that there is no in-scattering or emission contribution to the direct intensity component, so Eq. (3) for the direct component is simplified:

$$\xi\frac{\partial I^d}{\partial x} + \eta\frac{\partial I^d}{\partial y} + \mu\frac{\partial I^d}{\partial z} + \beta I^d = 0 \tag{5}$$

which therefore allows an analytical solution [6]:

$$I^d(x, y, z, \hat{s}) = I_{wall}(x_{wall}, y_{wall}, z_{wall}, \hat{s})e^{-\beta s(x,y,z,\hat{s})} \tag{6}$$

where $I_{wall}(x_{wall},\ y_{wall},\ z_{wall},\ \hat{s})$ is the value of intensity at the wall (collimated or diffuse) in the direction of interest $(\hat{s})$. The remaining term on the right hand side of Eq. (4) is the diffuse component I^s, which originates by scattering and emission from the participating medium within the computational volume, and (as in the conventional DOM) is solved numerically:

$$\xi_i\frac{\partial I_i^s}{\partial x} + \eta_i\frac{\partial I_i^s}{\partial y} + \mu_i\frac{\partial I_i^s}{\partial z} = -(\kappa + \sigma_{mi})I_i^s + S_i, \quad i = 1, 2, \ldots, n \tag{7a}$$

$$S_i = \kappa I_b + \frac{\sigma}{4\pi}\left(\sum_{\substack{j=1 \\ j\neq i}}^{n} w_j\Phi_{ij}I_j^s + \sum_{wall} I^d\Phi_{i\,wall}\right) \tag{7b}$$

$$\sigma_{mi} = \sigma\left(1 - \frac{1}{4\pi}w_i\Phi_{ii}\right) \tag{7c}$$

In the above formulation [5], a mechanism is included to remove the forward-scattering peak from the in-scattering term so that it is treated as transmission, to reduce the number of iterations before convergence due to scattering.

1.2. Scattering phase function discretisation

In order to be used in a DOM or MDOM analysis, the phase function $\Phi(\theta)$ must be discretised into discrete scattering values Φ_{ij} (where i represents the current ordinate direction being calculated and j represents the incoming beam).

One concern with the discretisation of the continuous phase function $\Phi(\theta)$ into discrete scattering values Φ_{ij} is that the total scattered energy fraction $(1/4\pi\int_{4\pi}\Phi(\hat{s}_j, \hat{s})d\Omega_j)$ and asymmetry factor $(g = 1/4\pi\int_{4\pi}\Phi(\theta)\cos\theta\, d\Omega)$ might not be conserved after numerical quadrature replaces the integrals, i.e.:

$$\frac{1}{4\pi}\int_{4\pi}\Phi(\hat{s}_j, \hat{s})d\Omega_j = 1 \neq \frac{1}{4\pi}\sum_{j=1}^{n} w_j\Phi_{ij}, \quad i = 1, 2, \ldots, n \tag{8}$$

$$\frac{1}{4\pi}\int_{4\pi}\Phi(\theta)\cos\theta d\Omega_j = g \neq \frac{1}{4\pi}\sum_{j=1}^{n} w_j\Phi_{ij}\cos\theta_{ij}, \quad i = 1, 2, \ldots, n \tag{9}$$

For isotropic scattering $(\Phi = 1)$, this is not a problem, as the directions $\hat{s}_i$ and weights w_i in the S_N approximation are chosen to satisfy conservation for the "zeroeth" moment:

$$\frac{1}{4\pi}\int_{4\pi} d\Omega = 1 = \frac{1}{4\pi}\sum_{j=1}^{n} w_j \tag{10}$$