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An adaptive emission model for Monte Carlo simulations in highly inhomogeneous media represented by stochastic particle fields

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Abstract

Traditional Monte Carlo ray-tracing (MCRT) methods for continuous participating media are not applicable in media represented by point masses (or stochastic particles) frequently encountered in combustion modeling. In the authors' previous work several ray models and particle models have been proposed for radiation simulations in such media. In the present paper an efficient emission scheme is developed for MCRT in highly inhomogeneous media represented by particle fields. Ray energies are limited to a narrow range to reduce statistical error, by having particles emit numbers of photons proportional to their emissive power (including combination of weak particles). A method to evaluate the radiative heat source, required by the overall energy equation, is also developed. A particle field representing the highly inhomogeneous medium in a turbulent jet flame is employed to test the proposed methods.

Keywords: Thermal radiation; Monte Carlo method; Participating media; Combustion modeling

1. Introduction

The Monte Carlo ray-tracing (MCRT) method has been applied to all aspects of radiative heat transfer. It directly simulates the physical processes, i.e., emission, absorption, scattering and reflection, from which the radiative transfer equation (RTE) is derived. In the standard Monte Carlo method a ray carrying a fixed amount of energy is emitted and its progress is then traced until it is absorbed at a certain point in the participating medium or at the wall, or until it escapes from the enclosure. In another variation of the Monte Carlo method, referred to as the "energy-partitioning" method [1,2], the energy carried by a ray is not absorbed at a single point, but rather is attenuated gradually along its path until its depletion or until it leaves the enclosure. The locally absorbed fraction of the ray's energy contributes to the heat exchange rates of subvolumes along the ray's path. Tracing identical numbers of rays, the average CPU time for tracing a single ray is often less in the standard method than the energy-partitioning method, but the energy-partitioning method supplies more statistical samples per ray so that a smaller statistical error is achieved. Both methods

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have been widely used. However, as many researchers have pointed out [1–5], the standard Monte Carlo method is inefficient when the walls are highly reflective and/or the medium in an open configuration is optically thin, so that most photon bundles exit the enclosure without any contribution to the statistics.

In many applications involving inhomogeneous participating media, such as combustion problems, one major difficulty in MCRT methods is the evaluation of the optical thickness that a ray travels through, since the temperature and concentration fields tend to be highly inhomogeneous and turbulent. Traditionally, radiation is treated as an uncoupled process from the turbulent fluctuations of temperature and concentrations, using mean temperature and concentrations to evaluate the radiative intensities and properties [6]. However, many experimental and numerical studies have demonstrated that radiative fluxes can be underestimated by a factor of up to 3 in this way [7,8]. The treatment of turbulence–radiation interactions (TRI) is a challenging task because of the nonlinear coupling between temperature, species concentrations and radiative intensities, which can be separated into the coupling between local blackbody intensity and local absorption coefficient and the coupling of incident radiation and local absorption coefficient. The former coupling is referred to as "emission TRI" and determined by local properties only, while the latter is referred to as "absorption TRI" and determined by properties at every point in the domain. Virtually all studies on nonlinear TRI to date have employed a major simplifying assumption, the so-called "optically thin fluctuation assumption" (OTFA) [9,10], which assumes that, if the eddies are optically thin and statistically independent, the local fluctuations in the absorption coefficient will not affect the net radiation intensity passing through that eddy. By applying the OTFA, the absorption TRI can be neglected. Among the various schemes to predict the emission TRI the most promising one appears to be the joint-probability-density-function (joint-PDF) method, which was first developed by Pope [11] to treat chemical sources in turbulent reacting flows. In this method, any term can be evaluated exactly as long as it is a function of local scalars (such as temperature, species concentrations, etc.) only, by solving the joint-PDF of scalars using a particle Monte Carlo method [11], in which the flow is represented by a sufficiently large number of discrete particles (point masses) evolving with time. This method has been employed by Modest et al. [12,13], and the emission TRI was evaluated exactly. To date the only attempt to take the effects of absorption TRI into account was conducted by Tessé et al. [14], while modeling radiative transfer in a turbulent, sooty ethylene/air jet flame. A MCRT method was employed in their study to investigate the coupling of the incident intensity and the local absorption coefficient without applying the OTFA. However, their study of absorption TRI was carried out by assuming that the turbulent structures of the flame were homogeneous to simplify ray tracing and smaller scales of turbulence were neglected. All the above studies were carried out in continuous media, i.e., media with defined values for temperature and radiative properties for every point in the enclosure.

To take absorption TRI fully into account, detailed knowledge of instantaneous fields of temperature and species concentrations are required, which can be obtained by assuming the instantaneous particle field in joint-PDF methods to be a snapshot of the real flow. For such a particle representation of flows, traditional continuum ray-tracing methods are no longer useful. Recently, Wang and Modest [15] have developed several MCRT schemes for the evaluation of radiative heat transfer for problems, in which the participating medium is represented by discrete point masses (particles). In several 1-D radiative heat transfer problems they demonstrated that their schemes can achieve high accuracy by tracing a small number of rays. In their preliminary work each particle emits a fixed number of rays, which leads to a wide range of ray energies in highly inhomogeneous media encountered in combustion problems, since different particles emit different amounts of energy. Therefore, its statistical error will be larger than a scheme in which rays carry a relative constant amount of energy. It is the purposes of the present paper to develop an efficient emission scheme for highly inhomogeneous particle fields. Ray energies will be limited to a small range by adaptive control of number of rays per statistical particle, including the combination of cold particles to be represented by a single ray, thus reducing the statistical error. In addition, a method to evaluate the radiative heat source term in nonhomogeneous particle fields will be developed as required by the overall energy equation.

2. Emission scheme

In a small volume of a physical gas, photons are emitted into all directions from every point in the volume. Some of the photons can escape and enter into adjacent volumes but others are absorbed by the small volume

itself. In particle Monte Carlo simulations, the emitted energy comes from the inside of a gas particle and is divided into a limited number of photon bundles (rays), which are released into random directions. If the particle is optically thin, the self-absorption of emission is negligible and the total emission from particle i is calculated from [16]

$$Q_{\mathrm{emi},i} = 4\kappa_{\rho,i} m_i \sigma T_i^4, \tag{1}$$

where $\kappa_{\rho,i}$ is the density-based Planck-mean absorption coefficient at particle temperature T_i, σ the Stefan–Boltzmann constant, and m_i the mass. If self-absorption is considered, a more sophisticated expression for the total emission can be obtained from Chapter 9.9 in Ref. [16].

The number of rays emitted by a specific particle should be determined by the total emission of the particle, guided by the average value of energy that the rays carry, i.e.,

$$Q_{\mathrm{avg}} = \sum_{i=1}^{N_{\mathrm{p}}} Q_{\mathrm{emi},i}/N_{\mathrm{r}}, \tag{2}$$

where N_{p} is the total number of particles in the computational domain and N_{r} is the prescribed total number of rays to trace. The range of ray energy $[Q_{\min}, Q_{\max}]$ can be chosen around the average ray energy:

$$Q_{\min} < Q_{\mathrm{avg}} < Q_{\max}, \tag{3}$$

since the total emission from a particle cannot be expected to be an integer multiple of the average ray energy.

If the total emission of a particle is in the range defined in Eq. (3), its total energy will be lumped into one ray. However, particles in hot zones of the medium tend to emit more energy, and if the total emission of particle i exceeds the maximum ray energy, it needs to emit more than one ray in order for each ray to obey Eq. (3). The number of rays emitted by particle i can be determined by

$$N_{\mathrm{r},i} = \lfloor Q_{\mathrm{emi},i}/Q_{\mathrm{avg}} + 0.5 \rfloor. \tag{4}$$

Because the energy of each ray after splitting should also satisfy Eq. (3), a requirement of choosing the ray energy range is obtained as

$$Q_{\max} \geqslant 2Q_{\min}. \tag{5}$$

One convenient choice is

$$Q_{\min} = \tfrac{2}{3}Q_{\mathrm{avg}} \quad \text{and} \quad Q_{\max} = \tfrac{4}{3}Q_{\mathrm{avg}}. \tag{6}$$

In cold zones particles emit little energy and, for increased efficiency, it is advantageous to combine the emission of several particles into one ray. To be meaningful, a low-emission particle should be combined with particles in its close proximity. In the PDF modeling of combustion flows a finite-volume mesh is often used to control the particle number density and resolve different levels of gradients. The particle size and other properties tend to be relatively uniform in a single finite-volume cell, which means that a low-emission particle tends to be surrounded by other low-emission particles. Therefore, the finite-volume mesh can be utilized to search low-emission particles and combine their emission. The emission point of the resultant ray is then determined as

$$\mathbf{x} = \sum_c Q_{\mathrm{emi},c}\mathbf{x}_c \Big/ \sum_c Q_{\mathrm{emi},c}, \tag{7}$$

where the subscript c denotes those particles combined together. Eq. (5) also guarantees that the resultant ray energy falls into the prescribed ray energy range during the particle emission combination process.

3. Radiative heat source evaluation

The local radiative heat source of a particle is determined by the energy it emits and the radiation it absorbs. The emission can be simply evaluated from Eq. (1). However, the absorption (interaction between

rays and particles) necessitates ray models and particle models so that the optical thickness a ray travels through by interacting with a specific particle can be evaluated. Wang and Modest [15] developed three absorption models, in which either a ray or a particle or both are assigned a volume so that the ray can interact with particles. In their first absorption model, the cone-PPM model, the ray is assigned a small solid angle and treated as a cone. The ray energy propagates axisymmetrically along the cone, with its strength decaying in the radial direction normal to the cone axis. Particles are treated as point masses without a prescribed shape. The contribution of particle i to the optical thickness ray j travels through is evaluated as

$$\Delta\tau_{ij} = \frac{\kappa_{\rho,i} W_{ij} m_i}{\pi R_{\mathrm{c},ij}^2}, \tag{8}$$

where $\kappa_{\rho,i}$ is the density-based absorption coefficient of particle i, m_i the mass of particle i, $R_{\mathrm{c},ij}$ the local cross-sectional radius of ray j where particle i is located, and W_{ij} the weight of particle i in ray j and is computed from a normalized two-dimensional center-symmetric weight function, which models the decaying strength of ray energy in the radial direction. In Wang and Modest's [15] second absorption model, the cone-CDS model, rays are also modeled as a cone. However, particles are assumed to be constant-density spheres, and the contribution of a particle i to the optical thickness a ray j travels through is evaluated as

$$\Delta\tau_{ij} = \kappa_i R_{\mathrm{c},ij} f\left(\frac{r_{ij}}{R_{\mathrm{c},ij}}, \frac{R_i}{R_{\mathrm{c},ij}}\right), \tag{9}$$

where $\kappa_i = \rho_i \kappa_{\rho,i}$ is the linear absorption coefficient of particle i, r_{ij} the distance from the center of particle i to the ray axis, R_i the radius of particle i, and f a nondimensional function, which can be tabulated beforehand. In their third absorption model, the line-CDS model, a ray is simply treated as a volumeless line and energy propagates one dimensionally along a line, which is the standard model for ray tracing in continuous media. Particles are treated as constant-density spheres as in the cone-CDS model. The optical thickness contribution of particle i to a ray j that it interacts with is simply

$$\Delta\tau_{ij} = \kappa_i \sqrt{R_i^2 - r_{ij}^2}. \tag{10}$$

The total optical thickness of ray j is accumulated as

$$\tau_j = \sum_{i \in I_j} \Delta\tau_{ij}, \tag{11}$$

where I_j denotes the particles ray j interacts with along its path. In the standard Monte Carlo method, before ray j is traced, a random number is drawn to determine the optical thickness the ray can travel through:

$$\tau_{o,j} = -\ln \eta, \tag{12}$$

where η is a random number uniformly distributed in $[0, 1)$. As ray j travels on, as soon as the total optical thickness τ_j exceeds its predetermined value $\tau_{o,j}$, all the energy ray j carries is dumped into the last particle it interacts with. If τ_j never exceeds $\tau_{o,j}$ before ray j leaves the domain, its energy contributes to the heat loss from the domain. Therefore, after all the rays have been traced, the energy absorbed by a particle i is the sum of the ray energies carried by rays, which end at particle i:

$$Q_{\mathrm{abs},i} = \sum_{j \in J_i} Q_j, \tag{13}$$

where J_i denotes all the rays absorbed by particle i and Q_j is the energy carried by ray j.

In the energy-partitioning Monte Carlo method the energy carried by ray j is dropped bit by bit into all the particles it has interacted with, until depleted or escaping from the domain. When a ray escapes, its remaining energy contributes to the heat loss from the domain. The energy contributed by ray j to particle i is evaluated from the optical thickness contribution from the particle to the ray as

$$\Delta Q_{ij} = Q_j^{(i)}[1 - \exp(-\Delta\tau_{ij})], \tag{14}$$

where $Q_j^{(i)}$ is the energy currently carried by ray j before interaction with particle i. Therefore, after the entire MCRT process is completed, the total energy absorbed by particle i is computed as

$$Q_{\mathrm{abs},i} = \sum_{j \in J_i'} \Delta Q_{ij}, \tag{15}$$

where J_i' denotes all the rays that interacted with particle i.

Required by the overall energy equation in the combustion model, the cell-averaged radiative heat source term needs to be evaluated from the underlying particle field. By its definition, the average radiative source term in a small volume V can be expressed as

$$\bar{S}_{\mathrm{rad}} = -\frac{1}{V}\int_V (\nabla \cdot \mathbf{q}_{\mathrm{rad}})\,\mathrm{d}V = -\frac{1}{V}\int_{\partial V} \mathbf{q}_{\mathrm{rad}} \cdot \mathrm{d}\mathbf{A} = \frac{1}{V}(Q_{\mathrm{rad,in}} - Q_{\mathrm{rad,out}}), \tag{16}$$

where $\mathbf{q}_{\mathrm{rad}}$ is the radiative heat flux, $\mathbf{A}$ the surface vector of the volume, $Q_{\mathrm{rad,in}}$ is the radiative energy entering the volume across its surface and $Q_{\mathrm{rad,out}}$ is the radiative energy leaving the volume. According to the energy balance in a finite-volume cell, the amounts of radiative energy entering and leaving the cell must be balanced by the energy emitted and absorbed by particles in the cell. Thus,

$$\bar{S}_{\mathrm{rad}} = \frac{1}{V}(Q_{\mathrm{rad,in}} - Q_{\mathrm{rad,out}}) = \frac{1}{V}\sum_{i \in I_c}(Q_{\mathrm{abs},i} - Q_{\mathrm{emi},i}), \tag{17}$$

where I_c denotes particles in the cell.

4. Case study

To demonstrate the proposed emission scheme and the radiative heat source evaluation method, a particle field containing roughly 85,000 particles was extracted from the particle Monte Carlo solution of a composition-PDF study of a methane/air axisymmetric jet flame, obtained from the Sandia D flame by doubling its geometric size and halving its velocities [17]. The central jet is pure methane at 293 K flowing into the domain at 24.8 m/s and the outer coflow of air is at 291 K and 0.45 m/s. Around the fuel jet an annular pilot flow of burnt gas enters at 1880 K and 5.7 m/s and the pilot's composition is the equilibrium composition for burning of methane with an equivalence ratio of 0.77. The diameter of the fuel jet is $D = 14.4$ mm and the outer diameter of the pilot flow annulus is $2.62D$. Fig. 1 shows the contours of cell-mean fields of temperature and the Planck-mean absorption coefficient, computed from the particle field for this snapshot in time. Temperature is one of the scalar properties carried by particles, while the Planck-mean absorption coefficient is calculated based on the particle temperature and species concentrations using a high-accuracy narrow-band k-distribution database developed by the authors [18]. From Fig. 1 it is clear that the particle field represents a highly inhomogeneous medium. The contours in Fig. 1 are not smooth because the particle field studied in the present paper represents just one single snapshot in time of the turbulent flame. Although it is well known that

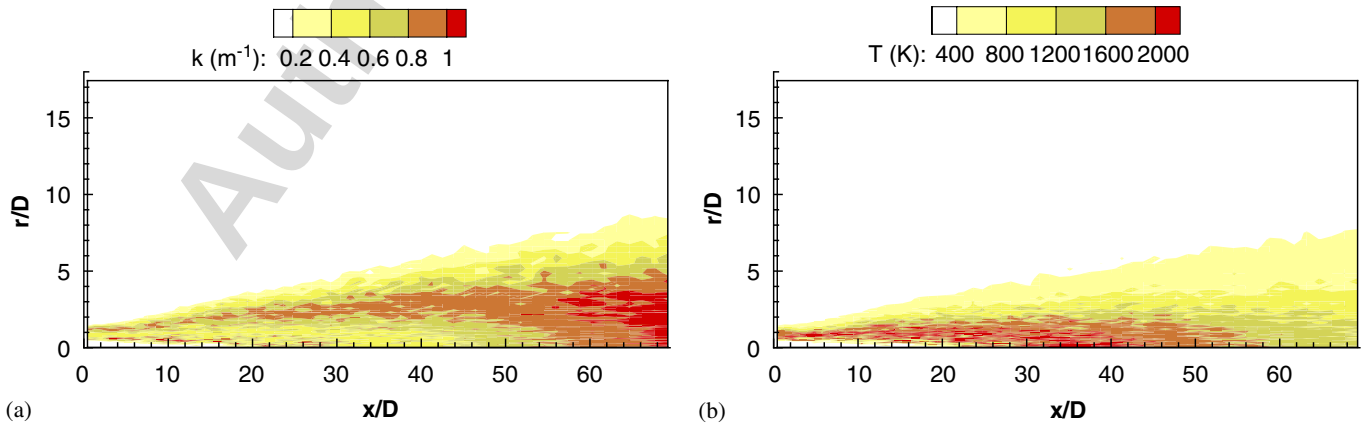

Fig. 1. Contours of cell-mean values of a particle field: (a) Planck-mean absorption coefficient; (b) temperature.

it is problematic to use Planck-mean absorption coefficients to model strongly nongray combustion gases, it is not the purpose of the present paper to study spectral models. Techniques from the present paper can be readily implemented using more advanced spectral models.

In the inhomogeneous medium shown in Fig. 1 the emissive energy of different particles varies by several orders of magnitude. If all particles emit the same number of rays, ray energies will vary over a wide range, as shown in Fig. 2(a) depicting the PDF and the cumulative-density function (CDF) of ray energies when each particle emits only a single ray. The peak of the PDF at very low ray energies is due to the fact that a large part of the domain is dominated by cold particles, which emit little energy. Using roughly the same number of rays, the proposed emission scheme results in a very small range of ray energy as shown in Fig. 2(b). For convenience we call the emission scheme, in which each particle emits a fixed number of rays, the "fixed scheme" and the proposed scheme, in which particles emit variable numbers of rays, as the "adaptive scheme."

To demonstrate the advantages of the adaptive emission scheme the standard deviation of net heat loss from the entire flame, calculated after 10 runs, has been investigated for both emission schemes. Results in Table 1 show that, tracing roughly the same number of rays, the adaptive emission scheme greatly reduces the standard deviation of the simulation. Table 1 displays the standard deviations for both emission schemes using different ray-particle interaction (absorption) schemes and different Monte Carlo methods.

For all three absorption schemes, the adaptive emission scheme reduces the standard deviation by a factor of 5–6 if the energy-partitioning Monte Carlo method is employed, and by a factor of more than 2 if the standard Monte Carlo method is employed. However, the average CPU time to trace a single ray, which is computed by dividing the total CPU time for the entire ray-tracing process by the number of rays traced, is

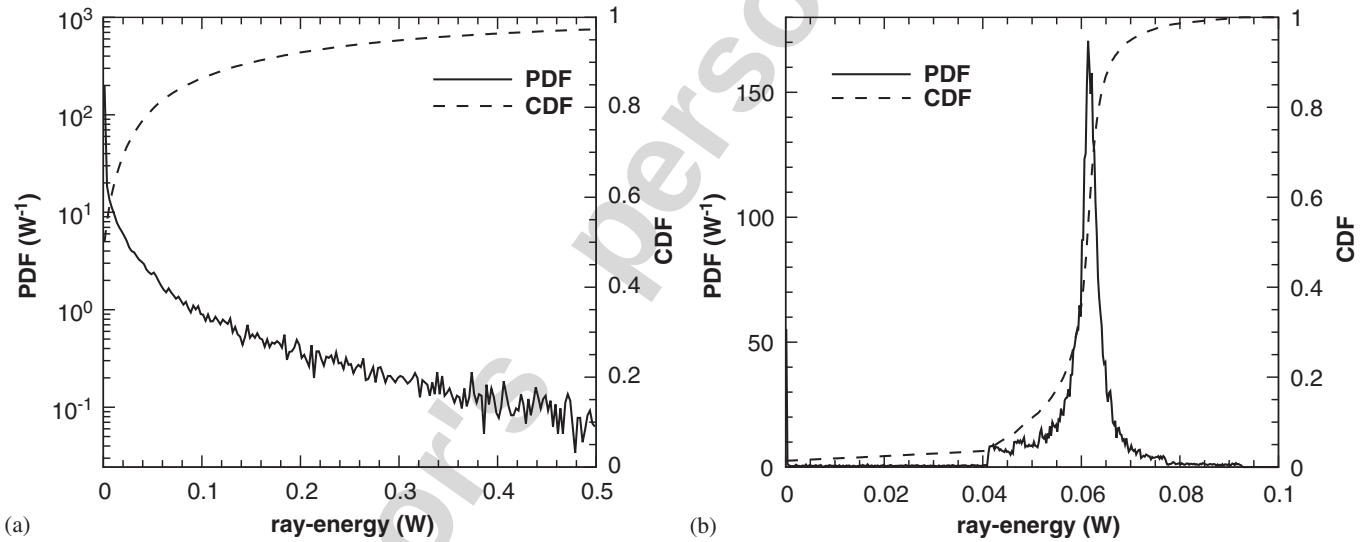

Fig. 2. PDF and CDF of ray-energy: (a) fixed scheme, 1 ray per particle; (b) adaptive scheme, 82,615 rays in total.

Table 1
Standard deviation of net heat loss from the flame (number of runs: 10; in W)

	Cone-PPM		Cone-CDS		Line-CDS	
	Fixed[a]	Adaptive[b]	Fixed	Adaptive	Fixed	Adaptive
Standard MC	16.82	6.62	15.55	7.39	18.12	8.38
Energy-partitioning MC	15.38	2.67	14.43	2.21	10.00	1.78

[a]Fixed scheme, 1 ray per particle.
[b]Adaptive scheme, 82,615 rays in total.

increased only about 10% using the adaptive scheme, as shown in Table 2. For simplicity, only results of the cone-PPM absorption scheme are listed in Table 2. Similar results have been observed for other absorption schemes. From Tables 1 and 2, it is also clear that the standard Monte Carlo method results in slightly less CPU time but considerably larger standard deviations, compared to the energy-partitioning Monte Carlo method.

The nature of TRI has been investigated as well. If the particle properties (temperature and Planck-mean absorption coefficient) are employed in both emission and absorption calculations, both emission TRI and absorption TRI can be taken into account, called "full-TRI." If the particle properties are used in emission calculations and cell-mean values are used in absorption calculations, only the emission TRI is taken into account, which is equivalent to the OTFA assumption and called here "partial-TRI." If cell-mean values are used in both emission and absorption calculations, TRI are neglected completely. It is worth noting that spectral variations also contribute to TRI effects, which are not considered here. Fig. 3 shows the contours of the cell-mean radiative heat source for the above three different TRI treatments, while Table 3 shows the total emission and the heat loss from the domain evaluated under different TRI treatments. Again, only results of the cone-PPM absorption scheme are displayed here, and similar results have been observed using other absorption schemes. The adaptive emission scheme is used with 82,615 rays traced in each run. The heat loss values in Table 3 are average values after 10 runs for all TRI treatments. It is observed that the total emission is underestimated by 16% without TRI, showing that emission TRI must be taken into account in the present turbulent jet flame. However, there is only a negligible difference between the full-TRI and the partial-TRI treatments in the heat loss estimation, which implies that the absorption TRI is negligible and the OTFA

Table 2
Average CPU time to trace a single ray (cone-PPM absorption scheme; in ms)

	Fixed	Adaptive
Standard MC	0.650	0.695
Energy partitioning MC	0.783	0.895

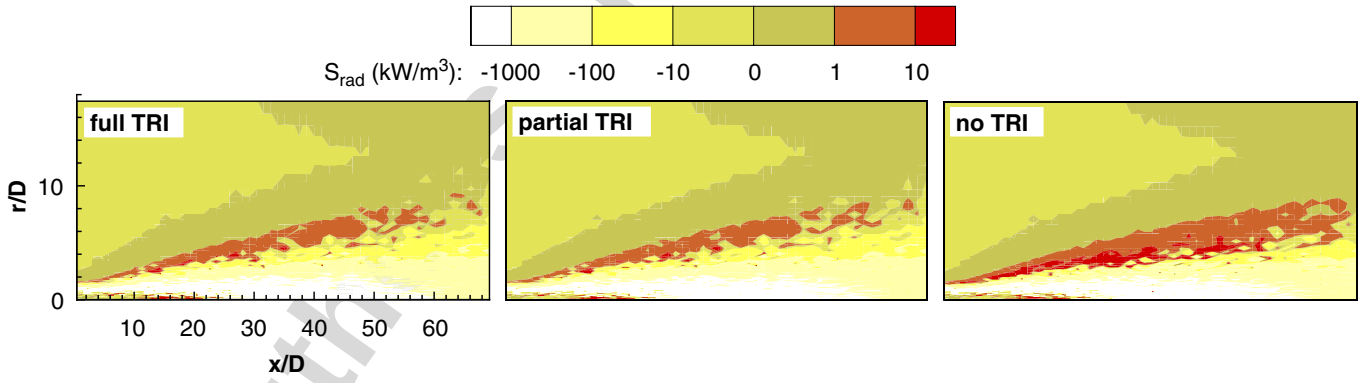

Fig. 3. Cell-mean radiative heat source (adaptive emission scheme, cone-PPM absorption scheme).

Table 3
Emission and net heat loss (adaptive scheme: 82,615 rays, cone-PPM absorption scheme, in W)

	Emission	Net heat loss
Full-TRI	4936	4149
Partial-TRI	4936	4153
No-TRI	4152	3493

assumption is valid in the present flame model. This was to be expected, since a gray analysis was used here (with a relatively low absorption coefficient across the spectrum). In a nongray analysis the absorption coefficient would be very large over small parts of the spectrum, where absorption TRI would be expected to be appreciable. However, after integration over the entire spectrum, the effect would still be expected to be minimal, as pointed out by Hartick [19]. Similarly, Fig. 3 shows that heat source contours of the full-TRI and the partial-TRI treatments are very close to each other, while the contours of the no-TRI treatment show considerable differences from those of the other two treatments. Compared to the other two treatments, the no-TRI treatment results in considerably less emission and relatively unaffected local absorption, which leads to larger local heat sources (absorption minus emission) as observed in Fig. 3.

5. Summary

For Monte Carlo simulations of radiative heat transfer in highly inhomogeneous media represented by particle fields, frequently encountered in combustion modeling, an efficient emission scheme to limit ray energies to a small range and to minimize the statistical error has been presented. A method to evaluate the radiative heat source, as required by the overall energy equation, was also developed.

In a turbulent jet flame represented by a particle field, tracing the same number of rays, it was shown that the proposed emission scheme greatly reduces statistical errors with little increase of CPU time, compared to the scheme in which particles emit identical numbers of rays. The standard Monte Carlo method requires less CPU time but has higher statistical error than the energy-partitioning Monte Carlo method.

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