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Monte Carlo methods for radiative transfer in quasi-isothermal participating media

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ABSTRACT

Based on the superposition principle, we propose in this study a Monte Carlo (MC) formulation for radiative transfer in quasi-isothermal media which consists in directly computing the difference between the actual radiative field and the equilibrium radiative field at the minimum temperature in the medium. This shift formulation is implemented for the prediction of radiative fluxes and volumetric powers in a combined free convection–radiation problem where a differentially heated cubical cavity is filled with air with a small amount of H_2O and CO_2. High resolution spectra are used to describe radiative properties of the gas in this 3D configuration. We show that, compared to the standard analog MC method, the shift approach leads to a huge saving of required computational times to reach a given convergence level. In addition, this approach is compared to reciprocal MC formulations and is shown to be more efficient for the prediction of wall fluxes but slightly less efficient for volumetric powers.

1. Introduction

The Monte Carlo (MC) method for radiative heat transfer calculation appears to be the most efficient way to take into account some complex aspects of radiation, like spectral gas properties, complex geometries or scattering effects, without further approximations. A review of MC application to radiative transfer may be found for instance in Ref. [1]. In the case of very weak temperature gradients, the standard analog MC method suffers from slow convergence rate due to the small differences between emitted and absorbed powers that are calculated separately and, thus, must be computed very accurately to capture their difference. Such small temperature gradients are encountered for instance in atmospheric studies and in thermal building applications where radiation and natural convection are strongly coupled.

Based on the reciprocity principle, Cherkaoui et al. [2,3] developed a net-exchange formulation suited to nearly isothermal applications. They use the MC integration technique to calculate the exchanged power between each couple of cells of the discretized medium, as in the zonal method [4]. Despite an acceleration of convergence rate compared to conventional approaches, and the ability to allow a deep analysis of exchange mechanisms for each cell, the method exhibits an important drawback. Indeed, each net-exchange power has to be calculated separately, which involves a number of MC calculations equal to the square of the total number of cells, and may require very important computer time and storage capacities. Therefore, this formulation has mainly been applied to one-dimensional problems or for validation purposes in multidimensional geometries, like in Ref. [5], to compute the radiative power in some selected cells. Tessé et al. [6] proposed an alternative implementation of the reciprocity principle, using the same optical paths as in the standard

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analog MC method and without recourse to independent calculations for each couple of cells. In this way, they could carry out three-dimensional calculations but they only applied their formulation to combustion applications.

This paper presents an original approach, called shift method, based on the linearity of the Radiative Transfer Equation (RTE). As the ratio between exchanged and emitted power is very small in quasi-isothermal media, we strongly increase it by transforming the problem to an equivalent one where the equilibrium radiative field at the minimum temperature in the medium is subtracted from the actual radiative field. Thus, exchanged powers are computed more accurately. The shift method is implemented for the calculation of radiative fluxes and volumetric powers, based on a temperature field representative of coupled free convection and radiation in a differentially heated cubical cavity filled with an air/H_2O/CO_2 mixture. High resolution absorption spectra (line by line calculations) of H_2O and CO_2 are used for the simulations.

The paper is organized as follows. In Section 2, the shift formulation is presented (Section 2.1), then the reciprocal formulation of Tessé et al. [6] is recalled (Section 2.2), and numerical details of MC algorithms are provided (Section 2.3). In Section 3, results are analyzed and compared to those obtained with the standard analog MC method (Section 3.1) and with the reciprocity MC methods (Section 3.2). The influence of the temperature difference level on the efficiency of the shift method and on the spectral radiative properties is finally discussed in Section 3.3.

2. Monte Carlo methods

2.1. Shift formulation

First, we define the shifted intensity $i_\nu(\mathbf{r},\mathbf{u})$ at point $\mathbf{r}$ and along the direction $\mathbf{u}$, by subtracting to the actual intensity $I_\nu(\mathbf{r},\mathbf{u})$ the uniform equilibrium intensity calculated at the minimum temperature in the medium $I_{b\nu}(T_{min})$

$$i_\nu(\mathbf{r},\mathbf{u}) = I_\nu(\mathbf{r},\mathbf{u}) - I_{b\nu}(T_{min}). \tag{1}$$

In the same manner, we define the shifted equilibrium intensity $i_{b\nu}(T(\mathbf{r}))$ by

$$i_{b\nu}(T(\mathbf{r})) = I_{b\nu}(T(\mathbf{r})) - I_{b\nu}(T_{min}). \tag{2}$$

The linearity of the RTE allows us to write for a non-scattering medium

$$\frac{\partial i_\nu(\mathbf{r},\mathbf{u})}{\partial s} = \kappa_\nu (i_{b\nu}(T(\mathbf{r})) - i_\nu(\mathbf{r},\mathbf{u})), \tag{3}$$

where κ_ν designates the absorption coefficient and s is the abscissa along the direction $\mathbf{u}$. The shifted intensity leaving a surface element along the direction $\mathbf{u}$ such that $\mathbf{u}\cdot\mathbf{n} > 0$, $\mathbf{n}$ being the normal to the surface directed towards the gas, is given for a diffuse reflecting wall of emissivity ε_ν by

$$i_\nu(\mathbf{r},\mathbf{u}) = \varepsilon_\nu i_{b\nu}(T(\mathbf{r})) + \frac{1-\varepsilon_\nu}{\pi} \int_{\mathbf{u}'\cdot\mathbf{n}<0} i_\nu(\mathbf{r},\mathbf{u}') |\mathbf{u}'\cdot\mathbf{n}| \, \mathrm{d}\mathbf{u}'. \tag{4}$$

The volumetric radiative power is equal to the difference between shifted emitted and shifted absorbed volumetric powers

$$\nabla\cdot\mathbf{q}^R = 4\pi \int_0^\infty \kappa_\nu i_{b\nu}(T(\mathbf{r})) \, \mathrm{d}\nu - \int_0^\infty \int_{4\pi} \kappa_\nu i_\nu(\mathbf{r},\mathbf{u}) \, \mathrm{d}\mathbf{u} \, \mathrm{d}\nu, \tag{5}$$

and, in the same manner, the wall flux is given by

$$\mathbf{q}^R\cdot\mathbf{n} = \pi \int_0^\infty \varepsilon_\nu i_{b\nu}(T(\mathbf{r})) \, \mathrm{d}\nu - \int_0^\infty \varepsilon_\nu \int_{\mathbf{u}'\cdot\mathbf{n}<0} i_\nu(\mathbf{r},\mathbf{u}') |\mathbf{u}'\cdot\mathbf{n}| \, \mathrm{d}\mathbf{u}' \, \mathrm{d}\nu. \tag{6}$$

It appears then that the shifted intensity obeys exactly the same equations as the actual one and allows to calculate radiative fluxes and volumetric powers from the same expressions. The forward analog MC method can thus be applied to $i_\nu(\mathbf{r},\mathbf{u})$ instead of $I_\nu(\mathbf{r},\mathbf{u})$. It is implemented here with energy partitioning, i.e., deterministic treatment of absorption along the stochastically generated optical paths. We designate by Forward Method (FM) and Shifted Forward Method (SFM) this algorithm, depending on whether the RTE is shifted or not. A large number of bundles N is emitted from the medium discretized in surface and volume isothermal cells. The random determination of the position $\mathbf{r}$ inside a cell, the direction $\mathbf{u}$ and the frequency ν of bundles is described in Section 2.3. The number N_i of bundles emitted by the cell i (of volume V_i, temperature T_i) is deterministic and proportional to the power emitted by the volume cell i, P_i^e, given by

$$P_i^e = 4\pi V_i \int_0^\infty \kappa_{i\nu} i_{b\nu}(T_i) \, \mathrm{d}\nu \tag{7}$$

and similarly for surface elements. The power emitted by the volume cell i and absorbed by volume cell j may be written as

$$P_{ij}^{ea} = \int_0^\infty \kappa_{i\nu} i_{b\nu}(T_i) \int_{V_i} \int_{4\pi} \mathcal{A}_{ij\nu} \, \mathrm{d}\mathbf{u}_i \, \mathrm{d}\mathbf{r}_i \, \mathrm{d}\nu, \tag{8}$$

where $\mathcal{A}_{ij\nu}$ denotes the density of the absorbed power relative to the elementary power emitted in $\mathrm{d}\mathbf{u}_i \, \mathrm{d}\mathbf{r}_i \, \mathrm{d}\nu$. It accounts for transmission to the cell j and absorption by this cell, following all possible optical paths including reflections by diffuse walls and possible multiple crossings of cell j. Similar expressions can be derived for surface–surface or surface–volume exchanges. The exchanged radiative power of the cell i is finally calculated in the SFM method according to

$$P_i^{SFM} = P_i^e - \sum_{j=1}^{M} P_{ji}^{ea}, \tag{9}$$

where M is the total number of volume and surface cells. In the FM method, P_i^{FM} is obtained by replacing $i_\nu(\mathbf{r},\mathbf{u})$ with $I_\nu(\mathbf{r},\mathbf{u})$ in the previous expressions.

2.2. Reciprocal formulation

We briefly recall here the reciprocity MC formulations given in [6,7]. Like in the FM method, a large number of bundles are emitted from the medium but the evaluation of radiative powers is based on the expression of the