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Application of the full-spectrum *k*-distribution method to photon Monte Carlo solvers

L. Wang, J. Yang, M.F. Modest*, D.C. Haworth

The Pennsylvania State University, Department of Mechanical and Nuclear Engineering, University Park, PA 16802, USA

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Abstract

Accurate prediction of radiative heat transfer is key in most high temperature applications, such as combustion devices and fires. Among the various solution methods for the radiative transfer equation (RTE), the photon Monte Carlo (PMC) method is potentially the most accurate and the most versatile. The implementation of a PMC method in multidimensional inhomogeneous problems, however, can be limited by its demand for large computer storage space and its CPU time consumption. This is particularly true if the spectral absorption coefficient is to be accurately represented, due to its irregular behavior. On the other hand, the recently developed full-spectrum *k*-distribution (FSK) method reorders the irregular absorption coefficient into smooth *k*-distributions and, therefore, provides an efficient and accurate scheme for the spectral integration of radiative quantities of interest. In this paper the accuracy of the PMC method in solving the RTE and the efficiency and storage advantage provided by the FSK method are combined. The advantages of the proposed PMC/FSK method is described in detail. The accuracy and the efficiency of the method are demonstrated by sample calculations that consider inhomogeneous problems.

Keywords: Radiative heat transfer; Inhomogeneous problems; Full-spectrum *k*-distribution; Combustion; Fire modeling

1. Introduction

Thermal radiation plays an important role in fires and combustion applications due to its usually fourth power dependence on temperature. In fires, fire growth and spread and containment are strongly influenced by radiative heat transfer. In combustion applications, flame structure and pollutant emission, such as NO_x and soot, are intimately coupled with radiative heat transfer. The determination of thermal radiation is thus of great importance in fire and pollutant emission control.

Computational fluid dynamics (CFD) has been commonly used in fire and combustion simulations. Accurate and efficient modeling of thermal radiation, however, has been an issue in these simulations [1,2]. One of the major difficulties is the solution to the radiative transfer equation (RTE). Various solution methods [3–5] have been employed and commonly used methods include the spherical harmonics (P_1) method (e.g. [6]),

*Corresponding author. Fax: +1 814 863 4848.
E-mail address: MFModest@psu.edu (M.F. Modest).

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the discrete ordinates (S_N) method (e.g. [7]), and the discrete transfer method (e.g. [8]). These methods transform the RTE into a set of simultaneous partial differential equations that can be readily solved in a CFD program. Each of these methods, however, has drawbacks, for example, the discrete ordinates method suffers from the so-called "ray effect" and "false scattering" [9], and the P_1 method is not suitable for quantitative radiation modeling in jet flame configurations [10]. In cases where accurate determination of temperature is important, for example, in the prediction of NO_x emission, the use of these method is not sufficient. In other cases where turbulence radiation interactions become important, the use of these methods inevitably invokes the employment of the "optically thin eddy" approximation [3,6,7].

The photon Monte Carlo (PMC), or Monte Carlo ray tracing method, is well suited for radiative transfer problems since radiative energy travels in discrete photons over relatively long distance along a straight path before interaction with participating media. It also can be applied to problems of arbitrary difficulty with relative ease [3]. PMC calculations yield answers with statistical fluctuations about the "exact" answer and, in general, the results are reliable if a sufficient number of photon bundles are utilized. In the case of turbulent combustion, PMC methods facilitate the treatment of turbulence-radiation interactions without any approximation [11]. The disadvantages of the method are that it is computationally expensive and memory demanding, as well as subject to statistical noise. The computational cost and the memory requirements derive partly from the fact that the absorption coefficient of participating media (e.g., water and carbon dioxide) varies irregularly across the spectrum and this variation must be accurately represented in a PMC method for spectral integration. In addition, tracing a large number of photon bundles in a CFD mesh is also time consuming. For these reasons the PMC method has seldom been employed in CFD simulations of fires and flames.

With continuous improvements in numerical methods and computer capabilities, photon tracing in complex three-dimensional unstructured CFD meshes is no longer a concern. For instance, parallel computing and multi-grids scheme [12] have greatly reduced the cost of photon tracing. The spectral integration of radiative properties, on the other hand, is still a time-consuming task. Simplified spectral models, e.g., a gray model, may be employed but may lead to large errors.

Several methods have been proposed to improve the efficiency of the spectral integration of radiative quantities. These include the weighted-sum-of-gray-gases (WSGG) model [3], the spectral-line-based weighted-sum-of-gray-gases (SLW) model [13,14], the absorption distribution function (ADF) method [15,16], and the recent full-spectrum *k*-distribution (FSK) method [17]. Whereas the SLW and ADF methods are weighted-sum-of-gray-gases approaches (i.e., the—assumed to be correlated—absorption coefficient is reduced to a few discrete values) the FSK method distinguishes itself in that it is an *exact* method for a correlated absorption coefficient, utilizing a continuous *k*-distribution over the whole spectrum, allowing a quadrature scheme of arbitrary order of accuracy to be employed. Compared to the SLW/ADF/WSGG models, the FSK method is exact for homogeneous problems. The FSK method achieves line-by-line (LBL) accuracy for homogeneous media with only a tiny fraction of LBLs computational cost. Since its introduction, the FSK method has undergone several major developments [18–23], and has become one of the most promising spectral model for radiative transfer in participating media.

Up to date nobody has attempted a LBL PMC implementation because of the accompanying difficulties that will be discussed in the following. It appears that the first nongray PMC simulation for molecular gas radiation with spectral line structure was done by Modest [24] in 1992, who employed a statistical narrow-band model in the simulation. Recently, the PMC method has been coupled with other spectral models and used in a couple of CFD simulations of combustion. In his study of buoyant turbulent nonpremixed flames, Snegirev [25] incorporated a PMC method into a CFD code using the WSGG model for spectral integrations. Tessé et al. [26,27] proposed two Monte Carlo methods that are coupled with a parameterized narrow-band CK model using more than 1000 pseudo-spectral points. They employed their PMC methods to model radiation heat transfer as a post-process in their study of a turbulent sooty flame. In the coupling of their PMC methods with the spectral models, a discrete representation of the spectral variation was used.

Here we propose a PMC method that is coupled with the state-of-the-art FSK method for spectral integration of radiative quantities in CFD simulations of fires and flames. The FSK method provides a smooth and continuous representation of spectral variations. It not only preserves the accuracy of the LBL model but

also facilitates the implementation of a PMC method in a CFD code by increasing the efficiency of the PMC method and greatly decreasing the memory requirements.

2. Photon Monte Carlo method for nongray gases

2.1. Line-by-line considerations

The only difference between the PMC method applied to gray and to nongray media is the need to determine wavenumbers for every emitted photon bundle according to a representative random number relationship for the nongray case. The random number relationship to find the spectral location of an emitted photon is written as [3]

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

Here the spectral variable is wavenumber η, σ is the Stefan–Boltzmann constant, κ_p is the Planck-mean absorption coefficient, κ_η is the spectral absorption coefficient, $I_{b\eta}$ is the Planck function or spectral blackbody intensity, and T is the temperature at the point of emission. The quantity R_η is a random number and the upper limit of the integral η is the wavenumber being sought.

For combustion gases this random number relationship is rather cumbersome to use because of the strongly irregular behavior of the absorption coefficient κ_η. As an example, Fig. 1 shows the spectral variation of the absorption coefficient κ_η for a mixture containing 10% CO_2 and 20% H_2O at 1500 K and 1 atm. The absorption coefficient is obtained from the HITEMP [28] (for H_2O) and CDSD [29] (for CO_2) spectral databases. This seemingly random variation raises several issues in implementing the spectral PMC method in a CFD program considering that the inversion of the random number relation must be carried out many times for every computational cell/grid and for every time/iteration step during a CFD run.

The first issue is the computer memory requirement. It is impractical to store the absorption coefficient κ_η for every computational cell and it is inefficient to invert the random number relation using the local absorption coefficient for every cell and every time/iteration step. The issue of storing absorption coefficients may be managed by pretabulating pressure-based absorption coefficients at specified temperatures and species concentrations. Linear interpolation may then be used to obtain absorption coefficients at arbitrary

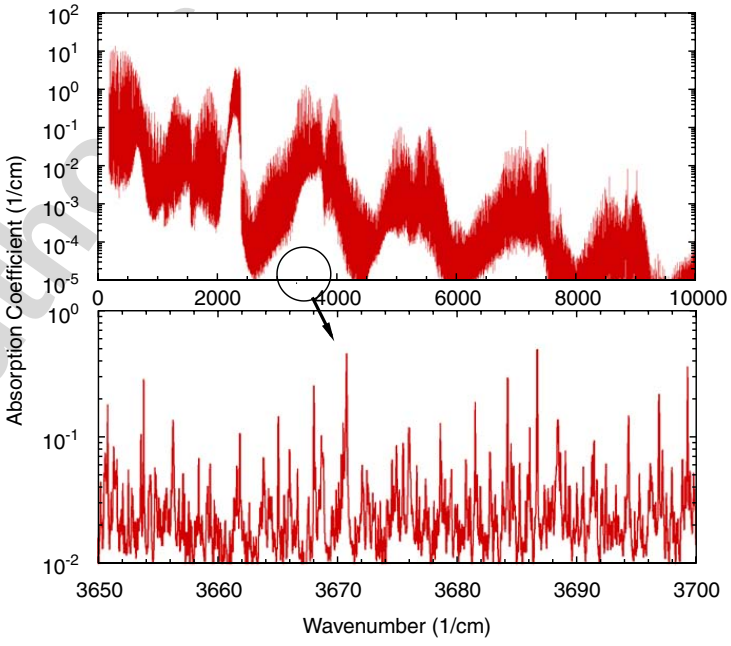

Fig. 1. Absorption coefficient of a mixture of 20% H_2O and 20% CO_2 at 1500 K.

conditions. If pressure-based absorption coefficients are pretabulated for 25 temperatures from 300 to 2700 K, 3 mol fractions from 0 to 0.5, and 3 species including CO_2, H_2O, and CO, then somewhat more than 1 GB memory is needed for single precision storage.

For the inversion of the random number relation a table may also be established for the η vs. R_η relation as a function of temperature, species, and species mole fraction. Given a random number, linear interpolation may then be used to obtain the wavenumber according to the local condition. If one total pressure is considered, then one more gigabyte of memory is required for the pretabulation of the random number relationship. The total requirement of more than two gigabyte memory is high, since radiation calculations usually constitute only a small part of an overall CFD simulation of fires and flames.

Another issue of implementing the LBL/PMC method is efficiency. First of all, the data arrays for the pretabulated absorption coefficients and random number relation are very large and, therefore, the multiple interpolations needed to find local absorption coefficients and the wavenumbers of emitted photons are relatively slow. Secondly, the minimum number of photons emitted during one PMC test/trial must be on the order of several million to adequately resolve the irregular variation of absorption coefficient. Thus, the computational overhead resulting from multiple interpolations and tracing photons is substantial.

2.2. The PMC method coupled with the FSK method

The various issues that arise in a spectral PMC method can be addressed effectively by the FSK method without much compromise in accuracy even for inhomogeneous problems. The essence of the FSK method is a reordering process. It has been observed that the oscillatory absorption coefficient attains the same value k many times at different wavenumbers even across a very small portion of the spectrum (narrow band), each time resulting in identical radiative intensity if the RTE is solved for a homogeneous medium. This observation has led to the reordering of the absorption coefficient across such small wavenumber intervals into a monotonic absorption coefficient distribution against normalized artificial wavenumber. This is known as the narrow band k-distribution approach [30,31]. The continuous k-distribution can also be obtained for the entire spectrum [18], leading to the FSK method and, therefore, facilitating the application of the k-distribution approach to practical engineering problems.

Fig. 2 shows the full-spectrum k-distribution generated by reordering the absorption coefficient shown in Fig. 1. Unlike the irregular absorption coefficient in wavenumber space, the k-distribution in g-space, which is the cumulative distribution function of the absorption coefficient and serves as the Planck-function-weighted normalized spectral variable, is smooth and monotonically increasing. The tedious spectral integration over

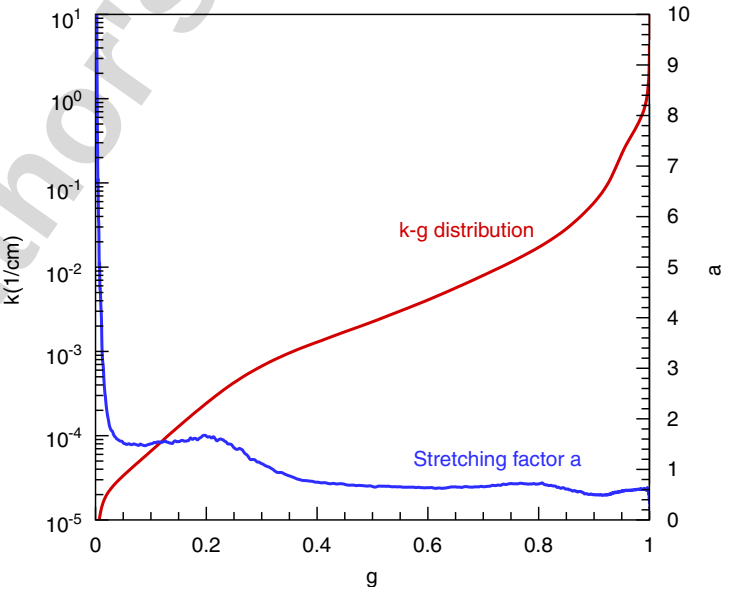

Fig. 2. k–g distribution and "a" function of the mixture of 20% H_2O and 20% CO_2 at 1500 K.

wavenumber space can then be replaced by integration over g-space using a much smaller number of data points. This is the virtue of the k-distribution method.

Within the FSK method, the radiative transfer equation [3],

$$\frac{\mathrm{d}I_\eta}{\mathrm{d}s} = \kappa_\eta[I_{b\eta} - I_\eta] - \sigma_{s\eta}\left[I_\eta - \frac{1}{4\pi}\int_{4\pi} I_\eta(\hat{s}')\Phi_\eta(\hat{s},\hat{s}')\,\mathrm{d}\Omega'\right], \tag{2}$$

is reordered into g-space [18] as

$$\frac{\mathrm{d}I_g}{\mathrm{d}s} = k(T_0,\underline{\phi},g)\left[a(T,T_0,g)I_b - I_g\right] - \sigma_s\left[I_g - \frac{1}{4\pi}\int_{4\pi} I_g(\hat{s}')\Phi(\hat{s},\hat{s}')\,\mathrm{d}\Omega'\right], \tag{3}$$

where I_g is the radiative intensity being solved in g-space, k is the reordered local absorption coefficient κ_η using a reference temperature (T_0) for the Planck function weight, I_b is the total blackbody intensity evaluated at local temperature (T), and a is a nongray stretching factor accounting for the difference of local temperatures (T) from the reference temperature (T_0) in the Planck function that is used to construct the k–g distributions [18]. The vector $\underline{\phi}$ contains state variables that affect κ_η, which include temperature T, total pressure P, and gas mole fractions $\underline{x}$: $\underline{\phi} = (T, P, \underline{x})$. Here in the equations σ_s is the scattering coefficient, Φ is the scattering phase function, and Ω is the solid angle.

In Eq. (3) the first term in the first bracket on the right hand side represents the augmentation of I_g due to local emission. In terms of k–g distributions, the random number relationship in g-space is written as the ratio of the partial integration of the emission term from 0 to g to the full integration of the emission term across the entire g-space (from 0 to 1):

$$R_g = \frac{\int_0^g k(T_0,\underline{\phi},g)a(T,T_0,g)I_b\,\mathrm{d}g}{\int_0^1 k(T_0,\underline{\phi},g)a(T,T_0,g)I_b\,\mathrm{d}g} = \frac{\int_0^g k(T_0,\underline{\phi},g)a(T,T_0,g)\,\mathrm{d}g}{\int_0^1 k(T_0,\underline{\phi},g)a(T,T_0,g)\,\mathrm{d}g}, \tag{4}$$

since I_b does not depend on g. Here R_g is a random number and the upper limit g in the numerator is the spectral location being sought in g-space. This equation is the g-space counterpart of Eq. (1). The denominator is the local Planck-mean absorption coefficient.

In contrast to the oscillatory variation of κ_η, shown in Fig. 1, the variations of k and a with g are much smoother as shown in Fig. 2. A number of data points on the order of 100 is sufficient to represent these smooth k- and a-distributions. Memory requirement is thus no longer an issue if the FSK method is used in the PMC method. In addition, the number of photons needed to resolve the spectral variation during one PMC trial is greatly reduced. The much smaller storage and the fewer photons needed greatly reduce the CPU time spent on the PMC simulation.

Other components of the PMC method, such as emission direction, photon tracing, and scattering, are unaffected by the differences between the gray/PMC, FSK/PMC, and LBL/PMC methods.

3. Sample calculations

In order to verify the results of the PMC calculations, a one-dimensional layer of an inhomogeneous gas mixture contains CO_2, H_2O, and N_2 is considered. A parabolic profile is taken for both mole fraction and temperature variations across the layer. The maximum temperature and H_2O and CO_2 mole fractions at the center of the layer are 1500 K, 30%, and 20%, respectively. The minimum temperature and H_2O and CO_2 mole fractions at the two boundaries of the layer are 500 K, 3%, and 2%, respectively. The analytical solution for this one-dimensional medium has been formulated using both LBL and FSK approaches. In both the LBL and FSK calculations, the absorption coefficients of the mixture are obtained from the HITEMP [28] (for H_2O) and CDSD [29] (for CO_2) spectral databases. In the FSK calculations, the correlated-k approach (FSCK) [18] has been taken.

The PMC method coupled with the FSK method was implemented in a three-dimensional unstructured CFD code [10]. A one-dimensional mesh with 21 cells is used to model the one-dimensional problem, which, with the parabolic temperature and species distributions, mimics a radial temperature and species distribution of a jet flame at a certain downstream axial location. In the PMC simulations 10 tests/trials were carried out,

and for each test 30,000 photon bundles were used. This number of photon bundles was chosen such that the standard deviations of the ten tests were within 1.5% of the averaged values. An energy partition scheme [3] is employed to increase efficiency, in which the energy content of a photon bundle is depleted due to gradual absorption and no random number is drawn for photon absorption. The k–g distributions were represented by 128 data points. The normalized mean radiative heat sources are shown in Fig. 3 and their standard deviations are shown as error bars.

The radiative heat sources calculated by the analytical LBL and FSK approaches are also shown in Fig. 3. There are two kinds of LBL analytical solutions: one considers the continuous parabolic profile by using Simpson's rule for spatial integration and is denoted "LBL theoretical" in the figure; the other discretizes the parabolic profiles into 21 step values similar to the homogeneous cells considered by the PMC calculations and is denoted "LBL step 21" in the figure. The FSK analytical solution also used the 21-step discretized parabolic profiles, in order to isolate the error made by the FSK approximation in the PMC calculations. The heat sources are normalized by the maximum emitted energy, which occurs at the center of the medium. It can be seen by comparing step LBL and step FSCK solutions that the FSCK method, which is exact for homogeneous problems, performs very well for this inhomogeneous medium (the error is less than 1% for a large part of the domain). Comparisons of the LBL and FSCK analytical solutions also show that the error caused by spatial discretization (inevitable in mesh generation) is larger than the error caused by the FSCK method. This is still true when the number of cells is doubled.

It is also shown that the PMC/FSCK results follow closely the FSCK analytical solution. The relatively small number of $10 \times 30,000$ photon bundles is sufficient to achieve good accuracy for this inhomogeneous problems. In a LBL/PMC implementation, the number of photon bundles used for each test would have to be at least a few million in order to resolve the spectral absorption coefficient. This demonstrates that coupling the FSK method with the PMC method not only greatly reduces the memory requirement but also the number of photon bundles needed in a PMC simulation. Both reductions greatly decrease the CPU time spent on the PMC solver in a CFD program.

Fig. 4 shows a comparison of nongray and gray PMC calculations for the same inhomogeneous problem considered in Fig. 3. The nongray PMC curve in Fig. 4 is the same as that in Fig. 3. The gray PMC calculations employs the Planck mean absorption coefficient for radiative properties. The large difference between gray and nongray simulations illustrates the importance of taking nongray properties into account in radiation modeling of combustion gases. The gray analytical solution is also shown in the figure as a black solid line. In the gray PMC simulation, 10 tests were carried out and a total number of $10 \times 3,000$ photons

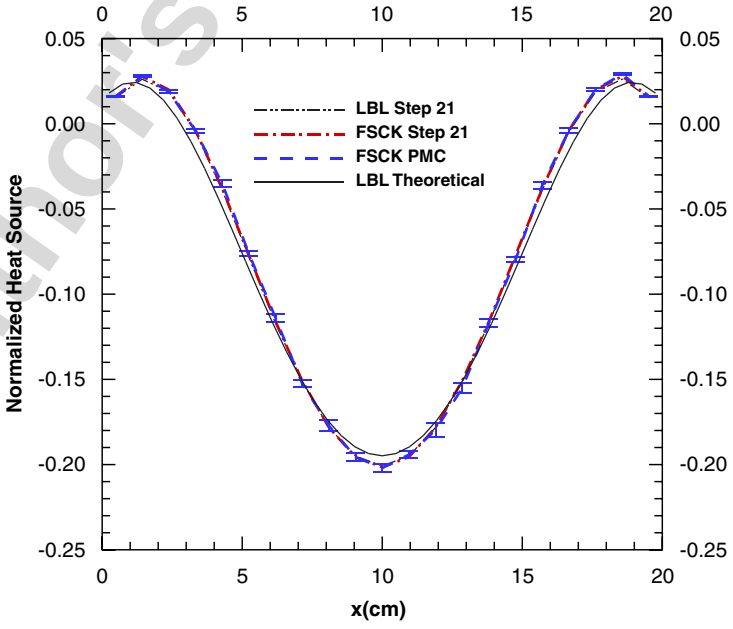

Fig. 3. Normalized radiative heat sources for the one-dimensional layer.

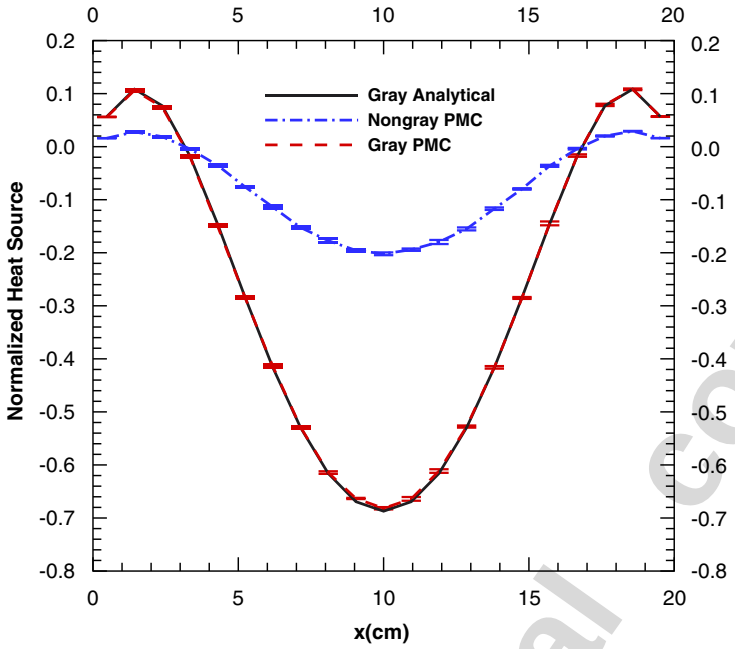

Fig. 4. Normalized radiative heat sources for the one-dimensional layer.

were traced. This number of photons was chosen such that both the nongray and gray PMC calculations have roughly the same standard deviations. The 10 times fewer photons used in the gray PMC simulation than in the nongray FSK/PMC simulation reflect the fact that one less (but well-behaved) variable needs to be resolved in the gray PMC simulation.

4. Conclusions

A spectral photon Monte Carlo method was devised to use the full-spectrum k-distribution method, in order to increase the efficiency of the nongray PMC method in CFD simulations of fires and combustion. The major advantages of using the FSK method in a PMC implementation were discussed in detail. A coupled FSK/PMC method was implemented in a three-dimensional unstructured CFD code and sample calculations were conducted to show the performance and the accuracy of the coupled method. The coupled method greatly reduces the memory requirements to store spectral radiative properties, simplifies the procedure to determine spectral locations of emitted photons, and reduces the number of photons needed in a PMC simulation. These, in turn, greatly reduce the CPU time spent on the PMC solver.

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