Radiation in an Emitting and Absorbing Medium: a Gridless Approach†

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† This work was performed at Sandia National Laboratories, a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U. S. Department of Energy under Contract DE-AC04-94AL85000.

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Abstract

A gridless technique for the solution of the integral form of the radiative-heat flux equation for emitting and absorbing media is presented. Treatment of non-uniform absorptivity and gray boundaries is included. As part of this work, we have developed fast multipole techniques for extracting radiative heat flux quantities from the temperature fields of one-dimensional and three-dimensional geometries. Example calculations include those for one-dimensional radiative heat transfer through multiple flame sheets, a three-dimensional enclosure with black walls, and an axisymmetric enclosure with black walls.

1. Introduction

Combustion systems and fire environments represent important examples of reacting flows where computational modeling yields the promise of a priori prediction of performance (in the case of combustion systems) or thermal hazard (in the case of fires). The challenge of conventional grid-based modeling of these systems is increased due to the complexity of gridding domains that are very large relative to the scale required to resolve the important transport phenomena. Multiple, or cumbersome grids may also be required to resolve gradients in different transported quantities. A logical alternative is the Lagrangian-based approach employed in vortex methods to represent fluid flows. These techniques have been used successfully to simulate turbulence dynamics in internal and external flows, mixing flows, and in buoyant jets and plumes. The same strategy has been employed by Ghoniem et al. [1][2][3] in formulating the transport element method to solve the species transport equation and the energy equation in conjunction with vortex methods.

In many cases, such as in large fires, the velocity is sufficiently low and the temperature and species fields are such that a significant fraction of the energy is transported by participating media radiation. Coupled solutions of radiative heat, momentum and scalar
transport therefore become increasingly important. Challenges associated with obtaining these coupled solutions include significant differences in the form of the radiative heat flux equation and the governing equations for momentum and scalar transport. Radiative heat transfer in participating media has been modeled using a variety of methods. Traditional techniques such as zonal and Monte Carlo techniques have existed for decades. Other methods that have more recently become popular include the discrete ordinates (SN), spherical harmonics (PN), and discrete transfer methods. New methods that have appeared within the last decade include the generalized zonal method (GZM), discrete exchange factor (DEF), YIX, and finite volume techniques. These radiative transfer modeling techniques require the use of a grid and are therefore not compatible with the transport element method. Other principal features, strengths, and shortcomings of these techniques are described in reviews by Viskanta and Menguc [4], and Howell [5].

In this work we develop an approach that is compatible with gridless solution techniques that is not subject to simplification of the governing equations. This approach may also be of use for direct analysis of radiative transfer at length scales smaller than the control volumes in present field models of fire and combustion systems. An important part of this work is to make use of fast multipole methods to compute radiation flux quantities from the temperature field.
2. **Radiation Integral Equations**

Radiant energy transported in a participating medium along a line of sight in the $s$ direction can be attenuated by absorption and out-scattering, and supplemented by emission and in-scattering. If the participating medium is primarily comprised of small (relative to the wavelength of the energy, i.e. $\pi D/\lambda << 1$) spherical soot particles with limited agglomeration, then the scattering of radiant energy, as predicted by the Rayleigh limit of the Mie theory [6], is negligible. The size of the primary soot particles present within small flames [7] and assessments of the effect of agglomeration on the radiative properties for energy transfer within the relevant infrared wavelength regime [8] tend to support this assumption. More recent, limited data from larger heavy hydrocarbon fires [9][10] show larger particle sizes that may call the validity of this assumption into question.

If scattering is neglected, the change in radiant intensity (i.e. the energy transfer rate per area per unit solid angle) at wavelength $\lambda$ along a line of sight in the $s$ direction in an absorbing and emitting medium, is governed by:

$$\frac{dI_\lambda}{ds} = \alpha_\lambda(s)(-I_\lambda + i_{b\lambda}(T)),$$

where $\alpha_\lambda(s)$ is the path-dependent absorption coefficient and $i_{b\lambda}(T)$ is the blackbody spectral emitted intensity given, for temperatures representative of fire and combustion environments (i.e. $\exp(C_2/\lambda T) >> 1$), by:

$$i_{b\lambda}(T) = \frac{2C_1}{\lambda^5 \exp(C_2/(\lambda T))},$$

where $T$ is the local temperature. The constants are given by $C_1 = 5.9544 \times 10^7$ W-μm$^4$/m$^2$ and $C_2 = 14388$ μm-K.
As given by Tan [11], integration over all wavelengths and solid angles yields the 3-D integral form of the equation for the vector heat flux field \( \bar{q}(\vec{r}) \) radiating from a volume of absorbing medium at \( \vec{r}' \) to the point \( \vec{r} \) in terms of the temperature field \( T \):

\[
\bar{q}(\vec{r}) = \frac{\sigma}{4\pi} \int \alpha(\vec{r}') I^4(\vec{r}') \frac{e^{-\alpha|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|^3} \left( \vec{r} - \vec{r}' \right) dV(\vec{r}').
\]

Here \( \sigma \) is the Boltzmann constant (5.67x10^{-8} W/m^2-K) and \( \alpha(\vec{r}') \) is the Planck-mean absorption coefficient at the source. The variable \( \bar{\alpha} \) is the Planck-mean average absorptivity along the line of sight between the source element and target point given by

\[
\bar{\alpha}(\vec{r}, \vec{r}') = \frac{1}{s} \int \alpha(s') ds' \text{ for } s \text{ defined by the path from } \vec{r}' \text{ to } \vec{r}.
\]

If gray boundaries are also present, there is additional heat flux from the boundaries to the point \( \vec{r} \) given by:

\[
\bar{q}(\vec{r}) = \int \left( \frac{\sigma T^4(\vec{r}')}{4\pi} - \frac{1 - \varepsilon}{\varepsilon} q_s(\vec{r}') \right) \frac{e^{-\bar{\alpha}|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|^4} \left( \hat{n}' \cdot (\vec{r} - \vec{r}') \right) (\vec{r} - \vec{r}') dA(\vec{r}'),
\]

where \( \varepsilon \) is the emissivity of the boundary, \( q_s(\vec{r}') \) is the magnitude of the net heat flux out of the boundary, and \( \hat{n}' \) is the inward unit vector at \( \vec{r}' \) which is normal to the surface.

The thermal response of a participating medium is defined by the net deposition of radiative energy per unit volume. Accordingly, the source term in the energy equation due to radiative heat transfer is equal to the difference between the total incident energy, i.e. the irradiance \( G(\vec{r}) \), and the local emission as given by the divergence of the heat flux:

\[
\nabla \cdot \bar{q}(\vec{r}) = -\alpha(\vec{r}) \left( 4\sigma T^4 - G(\vec{r}) \right).
\]
The irradiance \( G(\vec{r}) \) (also called the integrated intensity) may be expressed as:

\[
G(\vec{r}) = \frac{\sigma}{\pi} \int \alpha(\vec{r}') \frac{r'^4}{|\vec{r} - \vec{r}'|^2} dV(\vec{r}') + \int \left( \frac{\sigma T^4(\vec{r}')}{\pi} \frac{1 - \varepsilon}{\varepsilon} q_s(\vec{r}') \right) e^{-|\vec{r} - \vec{r}'|} (\hat{r}' \cdot (\vec{r} - \vec{r}')) dA(\vec{r}')
\]

\[\text{Multipole Expansions}\]

By inspection, it can be seen that the various volume integrals given in Section 2 can be expressed in the following general form:

\[
f(\vec{r}) = g(\vec{r}) \int h(\vec{r}') \frac{e^{-|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|^n} dV(\vec{r}').
\]

The discrete form of Equation (7) can be written as:

\[
f(\vec{r}) = g(\vec{r}) \sum_{i=1}^{N_s} h(\vec{r}') S(\vec{r}') \frac{e^{-|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|^n} = g(\vec{r}) \sum_{i=1}^{N_s} S(\vec{r}') \frac{e^{-|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|^n},
\]

where \( S(\vec{r}') \) is some source strength and \( N_s \) is the number of sources in a particular source domain. The surface or boundary integrals can be represented in a similar manner.

In order to develop a multipole expansion for the discrete form of the radiation integral equations we only need to be concerned with expansion of the kernel:

\[
K(\vec{R}) = e^{-|\vec{r}|} |\vec{R}|^n,
\]

where \( |\vec{R}| = |\vec{r} - \vec{r}'| \) is as indicated in Figure 1.

Strickland, Gritzo, Baty, et al. [12] have constructed a multipole expansion in spherical coordinates for the three dimensional kernels of Equation (9) which is given by:

\[
K(\vec{R}) = \frac{e^{-|\vec{r}|}}{r^n} \left\{ \sum_{m=0}^{p} \sum_{l=0}^{m} \sum_{k=-m}^{m} \sum_{l=0}^{m} \frac{4\pi}{2m + 1} g_{(m,l,n)} Y_{m,k}^*(\theta', \phi') Y_{m,k}(\theta, \phi) \left( \frac{r'^n}{r^n} \right) \right\}.
\]
Here, \( Y_{m,k} \) is the spherical harmonic function as defined by Jackson [13]. The values for the coefficients \( g_{(m,i,l,n)} \) for \( p = 0 \) to 3 are given in Table 1. It should be noted that the \( g_{(i,j,k,n)} \) coefficients are equal to zero for \( m + i \) equal to an odd integer or for \( i < m \).

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Table 1. \( g_{(m,i,l,n)} \) Coefficients for \( p = 0 \) to 3

We are now in a position to write the multipole expansion for sources near the expansion center. The multipole expansion can be written in terms of coefficients that are a function of the strengths \( S_j (\vec{r}_j) \) and locations of the sources.

\[
\sum_{j=1}^{N_x} S_j (\vec{r}_j) K(|\vec{R}|) = \frac{e^{-\alpha r}}{r^n} \sum_{l=0}^{p} \sum_{m=0}^{l} \sum_{i=0}^{m} A_{(i,m,k)} \alpha^{i-l} g_{(m,i,l,n)} Y_{m,k} (\theta, \phi) r^{-l} + \varepsilon, \tag{11}
\]

\[
A_{(i,m,k)} = \sum_{j=1}^{N_x} \left[ \frac{4\pi \alpha r^i}{2m+1} Y_{m,k}^{**} (\theta', \phi') \right].
\]

By rearranging the sums, Equation (11) may be rewritten more compactly as:
\[
\sum_{j=1}^{N_r} S_j (\vec{r}') K(|\vec{R}|) = e^{-ixr} \sum_{l=0}^{P} \sum_{m=0}^{P} \sum_{k=-m}^{m} \chi_{m,k} (\theta, \phi) r^{-l} + \epsilon,
\]

(12)

We note that in the special case where \( \bar{z} = 0 \), one of the sums in Equation (11) can be removed since \( i = l \) yields the only nonzero values of \( \bar{z}^{i-l} \). For the additional special case where \( n = 1 \), we find that \( g_{(m,i,n)} \) is equal to 1 for \( m = i \) and zero otherwise. This allows removal of yet another sum to yield the familiar multipole expansion for the vector potential associated with the vortex method in fluid mechanics. The number of \( \lambda_{i,j,k} \) coefficients for this special case is \( N_{Ac} = (p + 1)^2 \). It can be shown that for the general case, the number of \( \lambda_{i,j,k} \) coefficients is equal to \( N_{Ac} = (p + 1)(p + 2)(p + 3)/6 \) which is exactly the number of coefficients that would be required if one were to use a Cartesian coordinate system as would be expected. As long as \( p \) is less than 8, \( N_{Ac} \) is never more than twice \( (p + 1)^2 \) which is the number of coefficients required for the multipole expansion of \(|\vec{R}|\).

Gritzo, Strickland, and DesJardin [14] have used Equation (12) to develop a parallelized fast multipole method. Multipole expansions and associated fast solution techniques for planar radiation (one-dimensional) have also been developed by Gritzo and Strickland [15]. Examples using these fast solution techniques for three-dimensional and one-dimensional problems will be given in Section 5.

4. Variable Absorptivity

We note that for a case in which the absorptivity is spatially non-uniform one must find the average absorptivity \( \bar{\alpha}(\vec{r}_1, \vec{r}_2) \) along a line connecting the center of a source with a target
point as indicated in Figure 2. The source may be either a single source element or a source box associated with the fast multipole method. The average absorptivity from source to target can be obtained from the absorptivity $\alpha(\vec{r})$ along the path as:

$$\bar{\alpha}(\vec{r}_1, \vec{r}_2) = \int_0^1 \alpha(\vec{r}_p) d\xi.$$  \hspace{1cm} (13)

When using a gridless technique it is convenient to use Gaussian basis functions (core functions) to represent the absorptivity field $\alpha(\vec{r})$. The absorptivity field is thus represented by the superposition of Gaussian elements located at points $i$ such that:

$$\alpha(\vec{r}) = \sum_i c_i \text{Exp} \left( -\frac{|\vec{r} - \vec{r}_i|^2}{\sigma_i^2} \right), \hspace{1cm} (14)$$

where $\vec{r}_i$ is the center of the $i^{th}$ element and $\sigma_i$ represents a measure of the core size of the element. It is assumed that the core size and the coefficients $c_i$ are chosen so as to faithfully represent the absorptivity field with suitable smoothness and amplitude. The absorptivity at any point $p$ on the path indicated in Figure 2 is therefore:

$$\alpha(\vec{r}_p) = \sum_i c_i \text{Exp} \left( -\frac{|\vec{r}_p - \vec{r}_i + \zeta(\vec{r}_2 - \vec{r}_1)|^2}{\sigma_i^2} \right). \hspace{1cm} (15)$$

Equation (15) may be recast into the following form:

$$\alpha(\vec{r}_p) = \sum_i c_i \text{Exp} \left[ -(a + 2b\zeta + c\zeta^2) \right], \hspace{1cm} (16)$$

where

$$a = \frac{1}{\sigma_i^2} (\vec{r}_i - \vec{r}_1) : (\vec{r}_1 - \vec{r}_i),$$

$$b = \frac{1}{\sigma_i^2} (\vec{r}_i - \vec{r}_1) : (\vec{r}_2 - \vec{r}_i), \hspace{1cm} (17)$$
The average absorptivity may now be obtained by inserting Equation (16) into Equation (13) and performing the indicated integration:

\[ \bar{\alpha}(\vec{r}_1, \vec{r}_2) = \frac{\sqrt{\pi}}{2} \sum_i \frac{c_i}{\sqrt{c}} \text{Exp} \left( -a + \frac{b^2}{c} \right) \left[ \text{Erf} \left( \frac{b}{\sqrt{c}} \right) - \text{Erf} \left( \frac{b+c}{\sqrt{c}} \right) \right] \] (18)

Here, \( \text{Erf}(x) \) is the error function of \( x \).

We note that the application of Equation (18) to compute the value of \( \bar{\alpha}(\vec{r}_1, \vec{r}_2) \) between each pair of \( N \) radiation elements will require on the order of \( N^3 \) operations if the fast multipole method is not used. The operation count can be reduced the order of \( N^2 \) by noting that the elements where the ratio \( c/b \) is small may be neglected. A small value of \( c/b \) simply means that the \( i^{th} \) element is not close to the path of integration. Furthermore, if the fast multipole method is being used, the operation count will be reduced significantly since \( \bar{\alpha}(\vec{r}_1, \vec{r}_2) \) will not be required between every individual source element. In summary, this approach has the advantage that it is completely gridless and is consistent with the rest of the 3D gridless radiation method.

5. Numerical Results

In this section we present example calculations for one-dimensional radiative heat transfer through multiple flame sheets, a three-dimensional enclosure with black walls, and an axisymmetric enclosure with black walls.

To investigate radiative transfer within multiple flame sheets, we consider a case that has 150 flame sheets equally spaced over a domain of 3 optical thicknesses (\( k = 2, x = 3 \)). For a uniform absorption coefficient of \( 10 \text{ m}^{-1} \), the domain corresponds to a physical distance of 0.3 m, which is typical of the smallest control volume size used in fire field model.
calculations for large fires [16]. This case also provides some interesting insight into subgrid radiative transfer modeling for grid-based methods. No sources are present at the boundary or outside the domain. Each flame sheet is represented by 50 discrete sources. Twenty target points were located between each flame sheet resulting in a field of 13,350 target points and 7,500 source points. Combined computational time to calculate $\vec{q}_r$, $\nabla \cdot \vec{q}_r$, and $\nabla (\nabla \cdot \vec{q}_r)$ for this highly-resolved temperature field was reduced from 4,590 s to 290 s using the one-dimensional fast multipole solver described in Reference [15].

The results for $\vec{q}_r$ and $\nabla \cdot \vec{q}_r$ are provided in Figure 3. The normalized net heat flux at the boundary is approximately 0.11 implying that the temperature of a surface in radiative equilibrium at the boundary (i.e. $q_r = \sigma T^4$) of the domain would be 58% of the maximum temperature in the flame sheet. The trend in the results is consistent with data from measurements in large fires. Due in part to radiative transfer within a field of flame sheets (such as the example presented here) to practical devices such as thermocouples, typically cited fire temperatures are much lower than the expected temperature at the center of the flame sheets.

Figure 3 also shows the calculated normalized divergence of the net heat flux throughout the domain. Sharp peaks can be observed at locations corresponding to the flame sheets. The lower limit of the results is consistently less than zero due to deposition of energy within the medium between the flame sheets. As expected, the largest rate of energy deposition occurs farthest from the boundaries of the domain (i.e. near $\kappa = 1.5$). With the exception of the peaks, overall variation in $\nabla \cdot q_r$ is small.

An enlarged view of the results for 2 of the 150 flame sheets near the center of the domain is provided in Figure 4. Note that the value of $\nabla \cdot q_r$ between the flame sheets remains
essentially constant and hence $\nabla(\nabla \cdot q_\alpha)$ is zero in this region. It is therefore possible to focus on the results within the flame sheets thus eliminating the need for target points between each set of source points. A further reduction in computational time to 165 s is achieved by evaluating the variables of interest only at the locations of the sources. Thus, the application of this technique to the transport element method that only tracks gradients in temperature should prove to be highly efficient. In that application, source locations would only be located in regions of temperature gradients. It is important to emphasize, however, that radiative energy transport will generate new temperature gradients and hence new sources, which must be accounted for in any transport element formulation.

The simulation chosen for the 3D case consists of the rectangular enclosure shown in Figure 5. This enclosure contains a uniform concentration of emitting and absorbing medium at a uniform temperature $T_\alpha$ with black boundaries at temperature $T_w=0$. Cross sections in the x-z plane are square with unit length. The length in the y direction is 5 units, to allow for comparison of solutions at the midplane with the exact and other numerical solutions provided in the literature [17], [18].

Heat transfer into the wall at $(x=0, y=2.5)$ as indicated in Figure 5 is given in Figure 6. Solutions were obtained for optical thicknesses, given by $\kappa = \alpha z_{\text{MAX}}$, of 0.1, 1.0 and 10.0. In this example, $z_{\text{MAX}} = 1.0$. Results of the net heat flux are superimposed on the solutions presented by Shah [17] and Fiveland [18], [19] for a 2D square enclosure. Solutions were obtained with elements filling the entire domain. Element densities of $20 \times 20 \times 100$ were employed for optical thicknesses of 0.1. Increased discretization of $40 \times 40 \times 200$ and $60 \times 60 \times 300$ was required to represent the transport for optical thicknesses of 1.0 and 10.0 respectively. Excellent agreement is observed between Shah's exact (2D solution) and the 3D solution for the walls at the midplane of the enclosure. Some deviation from the exact
solution is observed near the edges due to the sharp gradients in radiative emission. It is expected that increasing the level of discretization in these regions would eliminate such deviations. Fast solvers were used to reduce run times to the order of a few minutes.

The simulation chosen for the axisymmetric calculation is from the benchmark problem of Chui et al. [20] for a cylinder. A sketch of the geometry, a 2 m diameter cylinder with a length of 2 m, is provided in Figure 7. The temperature inside the cylinder was chosen to be 100 K with a wall temperature of 0 K. This choice of wall temperature allows for the effects of the boundary conditions to be neglected.

Due to the limitations of the axisymmetric formulation described in Reference [14] (i.e. constant absorptivity, no fast solver), the three-dimensional formulation was also used for this problem. In the code developed for axisymmetric cases, elements are automatically generated in the azimuthal direction given a field of $r$ and $z$ radiation elements. The resulting discretization of a cylindrical domain is shown in Figure 8. The core diameters of the radiation elements are all assumed to be equal.

The computational requirement of using a 3D solver for the axisymmetric domain is more than balanced by the calculation savings that the 3D formulation provides through the use of multipole expansion fast solvers and parallelization. Calculations using core diameters of $\delta = 0.05$ and 0.025 m were conducted for three different values of absorptivities of $\alpha^{*} = 0.1, 1.0, \text{and } 5.0$ where $\alpha^{*} = \alpha r_{\text{MAX}}$. Here, $r_{\text{MAX}} = 1.0$. The total number of elements for the two core sizes was 54,530 and 419,013 for $\delta = 0.05$ and 0.025 m, respectively. Figure 9 shows the radial component of the radiation heat flux vector along the length of the cylinder as compared to the exact solution from Chui et al. [20].

The results show that the code converges to the exact answer with decreasing core size. The simulation results converge slower to the exact solution for larger values of
absorptivity due to the resolution required to capture the heat flux gradients near the edge and ends of the cylinder. Additional calculations (not shown) indicated the overall heat flux to the cylinder wall is highly sensitive to the resolution of the heat flux gradients near the wall. No special treatment for these gradients was pursued in this study. As in the 3D simulations, further improvement in accuracy and computational efficiency may be achieved by clustering elements near the boundary for the higher absorptivity cases. In a grid free flow simulation, some of this adaptivity will automatically be included as part of the solution for the fluid and reactive element flow fields.

6. Summary and Conclusions

A gridless method for treating radiation heat transfer in a non-uniform absorbing medium with gray boundaries is presented. The numerical results included herein, as well as those found in References [12], [14], and [15], indicate that fast and accurate results are obtainable with this method.

Additional development will be required in order for this methodology to become a useful and well-understood simulation tool. At this point, we have very limited experience with calculations in which the absorptivity is variable and the boundaries are gray instead of black. The multipole expansions of the boundary integral kernels must eventually be used in conjunction with an appropriate quadrature formulation for the boundary integrals. Our present representation of these integrals assumes piecewise constant integrands. Finally, issues regarding element core size versus accuracy must be resolved.
References


Figure 1: Multipole Expansion Geometry in Spherical Coordinates

Figure 2: Absorptivity Integration Path
Figure 3: Radiative Heat Transfer for 150 Equally Spaced Planar Flame Sheets

Figure 4: Radiative Heat Transfer Results for 2 of 150 Flame Sheets
Figure 5: Enclosure at Temperature $T$ with Walls at Temperature $T_W$

Figure 6: Wall Heat Flux at Midplane of Rectangular Enclosure
Figure 7: Axisymmetric Problem

Figure 8: Cross Sections of Axisymmetric Problem Showing Element Discretization.

Figure 9: Axisymmetric Problem Results