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The Effect of Scattering by Soot Aggregates on Radiative Transfer In Large-Scale Hydrocarbon Pool Fires

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**THE EFFECT OF SCATTERING BY SOOT AGGREGATES ON
RADIATIVE TRANSFER IN LARGE-SCALE HYDROCARBON
POOL FIRES**

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ABSTRACT

The modeling of large-scale hydrocarbon fuel fires is under investigation at Sandia National Laboratories. This work is being pursued as part of a program to determine energy transfer rates to weapon systems during fuel fire accident scenarios. Radiant energy transfer through the fire and at its boundaries contributes significantly to the energy transfer to a weapon system exposed to a fuel fire. The majority of the thermal radiation in a pool fire comes from hot soot aggregates. The purpose of this report is to document calculations performed to examine the effects of scattering by soot aggregates on the radiative transfer in large-scale hydrocarbon pool fires. The intent of this work is to determine whether the effects of soot aggregate scattering need to be included in large-scale 3-dimensional finite element radiative heat transfer models of fires. The approach followed was to develop a model for the optical properties of soot aggregates that included scattering. The soot optical property model was then used in a one-dimensional discrete ordinate radiative transfer model of a fire. The radiative transfer model was executed with and without the inclusion of scattering for a typical range of soot and fire parameters to determine the significance of including scattering in the calculations.

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THE EFFECT OF SCATTERING BY SOOT AGGREGATES ON RADIATIVE TRANSFER IN LARGE-SCALE HYDROCARBON POOL FIRES

1.0 Introduction

The modeling of large scale hydrocarbon fuel fires is under investigation at Sandia National Laboratories [1]. This work is being pursued as part of a program to determine energy transfer rates to weapon systems during fuel fire accident scenarios. Radiant energy transfer through the fire and at its boundaries plays a significant role in determining the energy transfer to a weapon system exposed to a fuel fire. The majority of the thermal radiation in a pool fire comes from soot aggregates. The purpose of this memo is to document calculations performed to examine the effects of scattering by soot aggregates on the radiative transfer in large scale hydrocarbon pool fires. The intent of the work is to make a recommendation as to whether or not the effects of soot aggregate scattering need to be included in pool fire radiative transfer models such as the Syrinx code [2]. If the effects of scattering can be neglected, then the additional complexity of adding scattering to such an analysis can be avoided, and the amount of computational effort required to compute the radiative transfer in the fire can be reduced.

The approach followed in this work was to develop a model for the optical properties of soot aggregates that included the effects of scattering. The soot optical property model was then used in a one-dimensional discrete ordinate radiative transfer model of a fire. The model accounts for the directional nature of the radiation field, soot scattering and absorption, and the wavelength dependence of the soot optical properties. The radiative transfer model was executed with and without the inclusion of scattering for a typical range of soot and fire parameters to determine the significance of including scattering in the calculations. Results from the model were compared on the basis of radiative heat flux and its divergence. The radiative heat flux is the important parameter in determining thermal radiation energy transfer to the exposed weapon system. The divergence of the radiative heat flux appears as a source term in the thermal energy equation that is solved as part of the fluid mechanics model of the fire.

2.0 Analysis

The transport of radiant energy within the fire is governed by the equation of radiation transfer as given in Equation (1).

$$\vec{s} \cdot \nabla I_\lambda(r) = -(\sigma_\lambda + \kappa_\lambda) I_\lambda(r) + \kappa_\lambda I_{b,\lambda}(T(r)) + \frac{\sigma_\lambda}{4\pi} \int_{4\pi} I_\lambda(\vec{s}_i) p_\lambda(\vec{s}_i \rightarrow \vec{s}) d\Omega_i \quad (1)$$

Equation (1) is the equation of radiative transfer [2] including absorption, emission, scattering, and multiple scattering. In Equation (1) $I_\lambda(r)$ is the monochromatic intensity at position r where the subscript λ denotes wavelength. The absorption coefficient, κ_λ , scattering coefficient, σ_λ , and phase function, $p_\lambda(s_i \rightarrow s)$, are monochromatic optical properties which depend on the size, complex refractive index, and concentration of soot in the fire. The phase function represents the probability that a beam moving in the direction s_i and confined to a solid angle $d\Omega_i$, will be scattered into a solid angle $d\Omega$ about the direction s . The term, $I_{b,\lambda}(T(r))$, is Planck's function and account for thermal emission from the soot.

To assess the importance of scattering by soot in computing the radiative transfer in fires, Eq. (1) was applied to compute the radiative transfer in a plane parallel layer of hot soot as shown in Figure 1.

Figure 1. Diagram of system for radiative transfer analysis.

For the one-dimensional soot layer shown in Figure 1, Eq. (1) reduces to the form

$$\begin{aligned} \cos \theta \frac{dI_{\lambda}}{dy}(y, \theta, \phi) = & -(\sigma_{\lambda} + \kappa_{\lambda})I_{\lambda}(y, \theta, \phi) + \kappa_{\lambda}I_{b,\lambda}(T(y)) \\ & + \frac{\sigma_{\lambda}}{4\pi} \int_0^{2\pi} \int_0^{\pi} I_{\lambda}(y, \theta', \phi') p_{\lambda}(\theta', \phi' \rightarrow \theta, \phi) \sin \theta' d\theta' d\phi' \end{aligned} \quad (2)$$

For the purposes of the analysis it is convenient to introduce the dimensionless parameters $\omega_{\lambda} = \sigma_{\lambda}/\beta_{\lambda}$ and $d\tau_{\lambda} = \beta_{\lambda} dy$, where the extinction coefficient, β_{λ} , is the sum $(\sigma_{\lambda} + \kappa_{\lambda})$. The quantity ω_{λ} is the single scattering albedo and is a measure of the relative importance of scattering to absorption. The albedo ranges from a value of zero for a purely absorbing soot, to a value of one for soot that only scatters radiation. The quantity τ_{λ} is termed the optical thickness, and the total optical thickness of the soot layer is defined as

$$\tau_{\lambda} = \int_0^L \beta_{\lambda} dy \quad (3)$$

where L is the thickness of the soot layer. The forward (for) and backward (bac) components of the local spectral radiation heat flux are given by the following expressions:

$$F_{\lambda,for}(y) = \int_0^{2\pi} \int_0^{\pi/2} I_{\lambda}(y, \theta, \phi) \cos \theta \sin \theta d\theta d\phi \quad (4)$$

$$F_{\lambda,bac}(y) = \int_0^{2\pi} \int_{\pi/2}^{\pi} I_{\lambda}(y, \theta, \phi) \cos \theta \sin \theta d\theta d\phi \quad (5)$$

The total spectral radiative flux, F_{λ} , is the sum

$$F_{\lambda} = F_{\lambda,for} + F_{\lambda,bac} \quad (6)$$

The net local volumetric radiation absorption rate, is the divergence of the total spectral radiative flux, F_{λ} and was determined from the expression

$$\frac{dF_{\lambda}(y)}{dy} = \kappa_{\lambda} (4\pi I_{b,\lambda}(y) - G(y)), \quad (7)$$

where G_{λ} the radiative energy, is defined as

$$G_{\lambda}(y) = \int_0^{2\pi} \int_0^{\pi} I_{\lambda}(y, \theta, \phi) \sin \theta d\theta d\phi. \quad (8)$$

The total radiative flux and net volumetric absorption rate are determined by integrating the monochromatic values over the entire spectrum; that is

$$F(y) = \int_{all \lambda} F_{\lambda}(y) d\lambda \quad (9)$$

$$\frac{dF}{dy} = \int_{all \lambda} \left(\frac{dF_{\lambda}(y)}{dy} \right) d\lambda \quad (10)$$

The net volumetric absorption rate and the radiation heat flux are the two major parameters important in a radiation heat transfer simulation of a fire. The net volumetric absorption rate appears as a source term in the energy equation in a fully coupled simulation of a fire that includes fluid mechanics. The radiative heat flux is applied as part of a boundary condition to determine the heat transfer to a weapon system in the fire. The goal of this study is to determine the importance of scattering from the soot aggregates in determining these two parameters.

3.0 Method of Solution

A discrete ordinate method was used to solve for the radiative transfer. Briefly, the method divides the radiation field at any location in the layer into a finite number of discrete streams (M), thereby transforming the radiative transfer equation into the same number of simultaneous, integrodifferential equations. Each of these equations is then transformed into a linear differential equation by expanding the phase function in a series of Legendre polynomials and replacing the multiple scattering integral by a quadrature formula. The size of the resulting equation set is determined by the number of discrete streams (M) used in the quadrature approximation.

The solution to this system of simultaneous, linear, differential equations was obtained in two steps. First, a homogeneous solution was found by substituting an assumed solution, consisting of the sum of M exponentials, into the homogeneous equations. This results in an eigenvalue problem that can be solved using efficient numerical algorithms to compute eigenvalues and eigenvectors of the coefficient matrix. A particular solution to the nonhomogeneous equations is then obtained by using the homogeneous solution in conjunction with the variation of parameters method. The general solution to the equations is the sum of the particular solution plus the homogeneous solution times an array of undetermined coefficients. The boundary conditions of the problem are then applied to the general solution to determine the unknown coefficients. The spectral fluxes and radiative energy defined in Eqs. (4), (5), and (8) are then computed by using quadrature formulas to integrate the discrete intensities.

Integrations over wavelength were performed by dividing the spectrum into a finite number of discrete wavelength bands and assuming the optical properties of the soot to be constant within each band. Monochromatic calculations of the radiation field were performed for each band and the total flux and volumetric absorption rates were computed by summing the results over the total number of bands.

4.0 Soot Optical Property Model

The optical properties of soot are required to compute the radiative transfer in a fire. Transmission electron microscope (TEM) photographs of soot collected from pool fires [3] as well as other flames indicate that soot forms aggregates that appear as long wispy chains. Quantitative examination of the soot aggregates indicate that aggregates consist of nearly spherical primary particles having relatively uniform diameters at given flame conditions.

A suitable model for the optical properties of soot aggregates is presented by Koylu and Faeth [4]. The extinction coefficient is the sum of the absorption and scattering coefficients and is given by an expression of the form

$$\beta_{\lambda} = (\sigma_{\lambda} + \kappa_{\lambda}) = \kappa_{\lambda}(1 + \rho_{sa,\lambda}^a) \quad (11)$$

where $\rho_{sa,\lambda}^a$ is the ratio of the scattering to absorption cross section for the soot aggregate. The single scattering albedo is given by the expression

$$\omega_{\lambda} = \frac{1}{1 + 1/\rho_{sa,\lambda}^a} \quad (12)$$

The absorption coefficient is given by the expression

$$\kappa_{\lambda} = \frac{6\pi E(m)}{\lambda} f_v \quad (13)$$

where f_v is the soot volume fraction and $E(m)$ is imaginary part of the complex number $(m^2 - 1)/(m^2 + 2)$, with $m = m_r + im_i$ representing the complex refractive index of soot. The ratio of scattering to absorption for the aggregate is given by the expression

$$\rho_{sa,\lambda}^a = \rho_{sa,\lambda}^p Ng(kR_g, D_f) \quad (14)$$

where $\rho_{sa,\lambda}^p$ the ratio of the scattering to absorption cross section for primary particles in the aggregate, N is the number of primary particles in the aggregate, g is the aggregate total scattering factor, k is the wave number ($2\pi/\lambda$), R_g is the radius of gyration, D_f is mass fractal dimension. Initially the ratio of scattering to absorption for the aggregate increases with the number of primary particles in the aggregate, however,

as the size of the aggregates increases, $\rho_{sa,\lambda}^a$ saturates at a maximum value independent of N . At this large aggregate limit the value of $\rho_{sa,\lambda}^a$ is given by the expression

$$\rho_{sa,\lambda}^a = \rho_{sa,\lambda}^p k_f (4x_p)^{-D_f} (3/(2-D_f) - 12/((6-D_f)(4-D_f))) \quad (15)$$

where x_p is the primary particle size parameter ($\pi d_p/\lambda$) and k_f is the fractal prefactor. The value of $\rho_{sa,\lambda}^p$ is given by the expression

$$\rho_{sa,\lambda}^p = \frac{2F(m)}{3E(m)} x_p^3 \quad (16)$$

where $F(m)$ is the square of the magnitude of the complex number $(m^2 - 1)/(m^2 + 2)$. Equation (12) together with Eq. (15) can be used to calculate the scattering albedo for a given set of soot fractal parameters and soot complex refractive index data. The large aggregate limit expression yields the maximum amount of scattering that would be expected to occur for this range of soot parameters. This maximum value of the scattering albedo was used in the radiative transfer simulations to assess whether or not the effects of scattering are significant in determining the radiative heat transfer in pool fires.

Koylu and Faeth [4, 5, 6] as well as other researchers have measured the properties of soot fractals from flames of different types of fuels. Values of D_f are reported to be in the range from 1.6 to 1.8. Values of the prefactor k_f in Eq. (15) are less well known and are in the range from approximately 5.8 to 9.0. Values for the diameters of primary particles, d_p , in the soot aggregate range from approximately 30 to 50 nm.

Some of the highest scattering albedos reported from the work of Faeth [5, 6] are for acetylene, where the primary particle diameter d_p was reported to be 47nm and the mass fractal dimension D_p was reported to be 1.79. These values of d_p and D_p as well as the value of $k_f = 5.8$ reported by Dobibins and Megaridis [7] and Koylu and Faeth (1992) [5] were used as values of the soot fractal properties in Eqs. (12), (15), and (16) to compute the scattering albedo for the radiative transfer calculations. In addition, the well known soot refractive index data of Dalzell and Sarofim [8] was used to compute the values of $E(m)$ and $F(m)$ used in the equations.

Figure 2 shows a plot of the scattering albedo computed from the soot model as a function of wavelength. Plotted along with the curve are data for the single scattering albedo available from the literature. These include the data of Gritz [3] for soot from a Sandia pool fire, the data of Dobbins, Mulholland, and Bryner [9] for soot from a fuel fire, and the data of Koylu and Faeth [6] for soot from acetylene, propylene, ethylene, propane, toluene, and benzene flames. The figure shows that the model provides a good upper bound for the albedo compared to data available from the literature. It is interesting to note that some authors suggest that a value of fractal prefactor, k_f , should be approximately 8.1. If a value of $k_f = 8.1$ is used in Eq. (15) then the value of the single scattering albedo in Figure 2 would be approximately 25% higher at $1.0 \mu\text{m}$ and approximately 33% at $10 \mu\text{m}$. The value of $k_f = 5.8$ seems to adequately bound the available data.

Figure 2 also displays plots of the blackbody intensity and blackbody energy fraction for a nominal fire temperature of 1500 K. Figure 2 shows that for a 1500K fire the intensity peaks at approximately $2.0 \mu\text{m}$, however, the fraction of energy radiated between 0 and $2.0 \mu\text{m}$ is only approximately 25% of the total. It should be noted that no data for the single scattering albedo of soot could be found in the literature for wavelengths beyond $2.0 \mu\text{m}$, yet Figure 2 shows that approximately 75% of the energy from a 1500 K fire is radiated at wavelengths greater than $2.0 \mu\text{m}$.

Figure 2. Comparison of single scattering albedo computed from soot model with available data.

The final soot optical property needed for the analysis is the phase function, $p_\lambda(s_i \rightarrow s)$, shown in Equation (1). The phase function gives the directional distribution of energy scattered by a soot fractal. For this study the phase function will be assumed independent of wavelength and approximated by an expression of the form

$$p(\xi) = 1 + \sum_{k=1}^{100} (2k+1)g^k P_k(\cos \xi) \quad (17)$$

where P_k are Legendre polynomials of order k , and ξ is the angle between the incident (θ', ϕ') and scattered intensity (θ, ϕ) . The value g is an asymmetry factor which may be varied from -1 (strictly backward scattering) to 1 (strictly forward scattering) in order to alter the shape of the scattering function. A value of g equal to zero corresponds to an isotropic scattering distribution. A nominal value of $g=0.75$ was used for the

scattering study and the value of g was varied in order to assess the sensitivity of the calculations to the phase function. Figure 3 shows a plot of the phase function for different values of g as compared to measured data for the phase function of soot fractals[10].

Figure 3. Comparison of phase function from Eq. (17) for different values of g with data for phase function from soot fractals.

5.0 Parametric Study

A parametric study was performed with the soot layer model discussed in Section 2.0 and the soot fractal optical property model discussed in Section 4.0 to assess whether the effects of scattering are important in determining the radiation heat transfer in pool fires. The soot layer was considered to be isothermal and the soot volume fraction, layer thickness, soot scattering phase function, and temperature were varied over reasonable ranges typical of pool fires. Calculations for the case where scattering was included were performed using the single scattering albedo curve shown in Figure 2. Results without scattering for the identical conditions were generated by setting the albedo to zero for all wavelengths. Calculations were performed on a nongray basis by dividing the wavelength range between 0.4 μm and 50 μm into 16 bands and performing monochromatic calculations for each band. The results for radiative flux and its divergence from each band were then summed to compute the total flux and divergence over the full spectrum. The wavelength bands were grouped more tightly in regions where the albedo varied strongly with wavelength. A total of 16 ordinate directions distributed according to the weights of Gaussian quadrature were used for the discrete ordinate calculations.

Table 1 gives a summary of the range of physical parameters varied in the study. Two values of the soot temperature (T_{soot}) were used; the nominal value of 1500 K and the adiabatic flame temperature of approximately 2300 K [12]. Three values of the soot layer thickness were used; 1.0, 5.0, and 10.0 meters. The soot volume fraction for the fire was varied between the minimum value of 10^{-8} and the maximum value of 10^{-4} . The shape of the scattering function was varied by changing the g value in Eq. (17) between values of 0.6, 0.75, and 0.85. Nominal conditions for the study were $T_{\text{soot}} = 1500$ K, $f_v = 10^{-6}$, and $g = 0.75$.

Table 1. Fire parameters for parametric study.

Soot Temperature (T)	Soot Layer Thickness (L)	Soot Volume Fraction (f_v)	Phase Function Factor (g)
1500 K, 2300 K	1.0, 5.0, 10.0 m	10^{-8} , 10^{-6} , 10^{-4}	0.6, 0.75, 0.85

Figure 4. Radiative heat flux through soot layers of different thickness (1.0m, 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=1500$ K, $f_v=10^{-8}$, $g=0.75$.

Figure 4 shows results for the radiative heat flux (Eq. (9)) through the soot layer for the case where the soot volume fraction is $f_v=10^{-8}$, the soot layer temperature is 1500 K, and a value of $g=0.75$ was used to represent the scattering distribution (see Figure 3). Results are shown for three layer thicknesses of $L = 1.0$ m, 5.0 m, and 10.0 m. The y-coordinate shown on the abscissa is nondimensionalized by the total thickness of the layer L , while the radiative heat flux shown on the ordinate is nondimensionalized by the blackbody emissive power at the soot layer temperature. Results for the cases where scattering is included in the calculation are shown as lines in the plot where the corresponding cases without scattering ($\omega_\lambda=0$) are shown as points. The results indicate that there is little difference between the radiation heat flux in the layer with or without the inclusion of scattering.

Figure 5 shows the divergence of the radiative flux (Eq. (10)) for the same conditions as Figure 4. The divergence of the radiative heat flux shown on the abscissa is nondimensionalized by the blackbody emissive power at the soot layer temperature and the total thickness of the layer, L . The results also show that for the divergence of the radiative heat flux there is little difference between the cases where scattering is included or not included.

Figure 5. Divergence of the radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=1500$ K, $f_v=10^{-8}$, $g=0.75$.

Figure 6 shows radiative heat flux results for the same conditions ($T_{\text{soot}}=1500$ K, $g=0.75$) but with the soot volume fraction increased to $f_v=10^{-4}$. Because of the increased soot loading the layer becomes optically thick and the net radiative heat flux is zero except near the edges of the layer where it radiates to the environment. As with the previous cases the results with and without the inclusion of scattering show very little difference.

Figure 7 shows results for the divergence of the radiative heat flux for the same conditions as Figure 6. The divergence of the radiative heat flux is zero in the optically thick center of the layer where emission is balanced by absorption. Near the edges of the layer where radiation is lost to the environment the divergence becomes nonzero. As in the previous cases the results with and without the inclusion of scattering show very little difference.

Figure 6. Radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=1500$ K, $f_v=10^{-4}$, $g=0.75$.

Figure 7. Divergence of the radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=1500$ K, $f_v=10^{-4}$, $g=0.75$.

The sensitivity of the results to variations in the phase function or scattering distribution was evaluated by altering the value of g from the nominal value of 0.75 to values of 0.60 and 0.85. These values were picked because they alter the shape of the phase function (see Figure 3) to values that are above and below the reported scattering distribution for soot. Again, the soot albedo curve shown in Figure 2 was used for the calculations.

Figure 8 shows a comparison of the radiative heat flux with the inclusion of scattering for different values of the scattering distribution ($g=0.60, g=0.85$). Results for $g=0.60$ are shown as lines while results for $g=0.85$ are shown as points. The results show that the shape of the scattering distribution does not appreciably effect the value of the radiative heat flux in the layers for this scattering albedo (Figure 2).

Similar trends are observed for the divergence of the radiative heat flux (not shown) for these conditions.

Figure 8. Radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=1500$ K, $f_v=10^{-8}$, $g=0.60$, $g=0.80$.

As a final evaluation of the importance of scattering, the temperature of the soot layer was increased to a value close to the adiabatic flame temperature ($T_{\text{soot}}=2300$ K). This represents an upper bound on what the expected temperature for the soot in the fire

might be. Increasing the soot temperature shifts the emitted radiation to shorter wavelengths where the scattering albedo is higher (see Figure 2). For a temperature of 2300 K the peak emission occurs at approximately $1.25 \mu\text{m}$.

Figure 9. Radiative heat flux through soot layers of different thickness (1.0m, 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}}=2300 \text{ K}$, $f_v=10^{-8}$, $g=0.75$.

Figure 9 shows results for the radiative heat flux through soot layers for the conditions of $g=0.75$, $f_v = 10^{-8}$, but with a soot temperature of 2300 K. Results for the case where scattering is included are shown as lines where results without the inclusion of scattering are shown as points. The results again show that even at an elevated temperature of 2300 K the effect of scattering has little effect on the radiative heat flux through the soot. Results for the divergence of the radiative heat flux (not shown) show similar trends.

6.0 Constant Albedo Analysis

The calculations of Section 5.0 showed that the effects of scattering on radiative heat transfer in hot soot layers are minimal when the Koylu and Faeth soot optical property model is used to determine the single scattering albedo for the calculations. Although it is felt that this soot optical property model is reasonable, based on comparisons with available data, a series of simulations were performed for higher values of the single scattering albedo to try and determine the range where scattering would become important. In this case the soot layer problem studied in Section 5.0 was solved but the ratio of scattering to absorption was specified instead of calculating it from the soot albedo model given by Eqs. (14) and (15). As a first approach, the ratio of scattering to absorption, $\rho_{sa,\lambda}^a$, was set to a constant value of 9.0. This amounts to fixing the single scattering albedo to a value of $\omega = 0.9$ for all wavelengths. The absorption coefficient was again calculated from Eq. (13) using the refractive index data of Dalzell and Sarofim [8]. For this study the soot volume fraction was set to the value of $f_v = 10^{-6}$ which is close to the value measured in large scale pool fires at Sandia [12]. Calculations were performed with 24 ordinate directions.

Figure 10. Radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{soot} = 1500$ K, $f_v = 10^{-6}$, $g = 0.75$ and a constant albedo of $\omega = 0.9$.

Figure 10 shows results of the soot layer calculations for layer thicknesses of 1.0, 5.0, and 10.0 meters with values of $\omega = 0.9$, $f_v = 10^{-6}$, and $T_{\text{soot}} = 1500$ K. The results without scattering are indicated in the legend with the “ns” (no scattering) designation. The results show a large difference between the radiative heat flux with and without scattering for this high value of albedo.

To further assess the importance of scattering, the ratio of scattering to absorption, $\rho_{\text{sa},\lambda}^a$, was lowered to 1.0. This amounts to fixing the single scattering albedo to a value of $\omega = 0.5$ for all wavelengths. Figure 11 shows results of the soot layer calculations for layer thickness of 1.0, 5.0, and 10.0 meters with values of $\omega = 0.5$, $f_v = 10^{-6}$, and $T_{\text{soot}} = 1500$ K. The difference between the radiative heat flux with and without scattering is much smaller than in the case where $\omega = 0.9$.

Figure 11. Radiative heat flux through soot layers of different thickness (1.0m , 5.0m, 10.0m) with and without scattering for the case where $T_{\text{soot}} = 1500$ K, $f_v = 10^{-6}$, $g = 0.75$ and a constant albedo of $\omega = 0.5$.

Table II shows a comparison of the normalized radiation heat flux at the boundary of the soot layer ($Y=0.0$) for the constant albedo cases of $\omega = 0.5$ and $\omega = 0.9$, for soot layer thicknesses of 1.0, 5.0, and 10.0 meters. For the case where the albedo is 0.9

the boundary radiation heat fluxes with and without the inclusion of scattering differ by a maximum of about 25%. For the case where the albedo is lowered to 0.5 the maximum difference in the boundary heat flux with and without scattering was observed to be about 5%.

Table II. Comparison of normalized boundary radiation heat flux ($F/\sigma T^4$) for different soot layer thicknesses and constant values of the single scattering albedo. The case where $\omega = 0.0$ is the nonscattering case. Results are for the cases shown in Figures 10 and 11 ($T_{\text{soot}}=1500$ K, $f_v=10^{-6}$, $g=0.75$).

Soot Layer Thickness (M)	$(F/\sigma T^4)$ $\omega = 0.0$	$(F/\sigma T^4)$ $\omega = 0.5$	$(F/\sigma T^4)$ $\omega = 0.9$
1.0 M	0.9068	0.8804 (2.9%)	0.7205 (20.5%)
5.0 M	0.9932	0.9504 (4.3%)	0.7480 (24.7%)
10.0 M	0.9982	0.9539 (4.4%)	0.7488 (25.0%)

7.0 Verification of Discrete Ordinates Model

To verify the accuracy of the discrete ordinate calculations a comparison with an analytical solution for isotropic scattering was performed. If the intensity is assumed to be isotropic (uniform in all directions) and the phase function is assumed to be isotropic ($g=0$) then the 1-dimensional radiative transfer equation given by Eq. (2) can be solved to obtain an analytical solution for the radiative heat flux through the one-dimensional layer shown in Figure 1. This analytical solution provides a means for checking the accuracy of the discrete ordinates model used for the calculation. The analytical solution for the total heat flux through the layer is given by an expression of the form

$$F(\tau) = 2\sigma T^4 (E_3((1-\omega)(\tau_L - \tau)) - E_3(\tau(1-\omega))) \quad (18)$$

where $E_3(t)$ is the exponential integral function [11]. The analytical solution is valid when the product of the scattering albedo (ω) and the total optical thickness of the layer (τ_L) is much less than one (ie. $\omega\tau_L \ll 1$) [11]. As a first approach comparisons between the analytical solution and discrete ordinates model were made for fixed values of the albedo (ω) and total layer optical thickness (τ_L) in order to assure that the condition ($\omega\tau_L \ll 1$) was maintained. This is different than the parametric studies performed in Section 5.0 where the albedo and total optical thickness varied with wavelength according to the soot optical property model previously presented.

Figure 12 shows a comparison of results between the analytical solution and the discrete ordinates model for an albedo of $\omega = 0.1$, a total layer thickness of $\tau_L = 1.0$, and a layer temperature of 1500 K. Figure 13 shows a comparison of results between the discrete ordinates model and analytical solution for the same case but with an albedo of $\omega = 0.5$. Figures 12 and 13 show that the discrete ordinates model and the analytical solution are in very good agreement.

As an additional verification of the discrete ordinate model the nongray soot layer problem of Section 5.0 was solved by replacing the scattering model of Eqs. (14) and (15) with a constant value of $\rho_{sa,\lambda}^a = 9.0$ for all wavelengths. This amounts to fixing the value of the single scattering albedo to a value of $\omega = 0.9$. The absorption coefficient was calculated as before from Eq. (13) and the phase function was assumed

Figure 12. Comparison of discrete ordinates and analytical solution for an albedo of $\omega = 0.1$, a total layer thickness of $\tau_L = 1.0$, and a layer temperature of 1500 K.

Figure 13. Comparison of discrete ordinates and analytical solution for an albedo of $\omega = 0.5$, a total layer thickness of $\tau_L = 1.0$, and a layer temperature of 1500 K. to be isotropic ($g=0.0$).

Figure 14 shows a comparison of the discrete ordinates calculation with the analytical solution of Eq. (18) for layer thickness of 1.0m, 5.0m, and 10m with a soot volume fraction of $f_v=10^{-8}$. Excellent agreement between the analytical solution and the discrete ordinates model is obtained for the 1.0m and 5.0m thick soot layers and a slight amount of disagreement is seen for the 10.0m thick layer. The total optical thickness of the layer is not constant in this case as in the previous two verification cases because the absorption coefficient given by Eq. (13) varies with wavelength. For the 10.0m thick layer the total optical thickness of the layer starts to become large (approximately 6.0 at a wavelength of 1.0 μm) and disagreement between the discrete ordinate model and analytical solution can probably be attributed to the fact that the analytical solution is beyond it's range of validity (ie. $\omega\tau_L \ll 1$).

Figure 14. Comparison of discrete ordinates and analytical solution for radiative heat flux through soot layers of different thickness (1.0m, 5.0m, and 10m) for the case of a constant albedo of 0.9, $T_{\text{soot}} = 1500 \text{ K}$, $f_v=10^{-8}$, and isotropic scattering ($g=0$).

8.0 Summary and Conclusions

Results of the parametric study discussed in this report indicate that including the effects of soot scattering are not important in determining the radiative heat flux and the divergence of the radiative heat flux in pool fires. The study assumed that the scattering from soot in a pool fire is bounded by the single scattering albedo curve shown in Figure 2. The single scattering albedo curve was generated based on the theory of Koylu and Faeth in the limit of large aggregates where the amount of scattering is expected to be the largest. The soot refractive index data used in the model was taken from the measurements of Dalzell and Sarofim.

Only a limited amount of data could be found to directly verify the soot single scattering albedo curve (Figure 2) used in the model. Although the single scattering albedo curve agreed well with available data, all of the data were taken at wavelengths less than approximately $2.0\ \mu\text{m}$ where only about 25% of the energy emitted by a 1500 K soot layer would occur. The validity of the study would be improved if data for the single scattering albedo curve (Figure 2) used in the model were available at wavelengths greater than $2.0\ \mu\text{m}$ where the majority of the energy is radiated.

Because of the uncertainty in measured values of the soot albedo at longer wavelengths, some nongray bounding calculations were performed with wavelength independent (constant) values of the single scattering albedo. For an albedo of 0.5 approximately 5% difference in the radiation heat flux at the boundary of the soot layer was observed with and without the inclusion of scattering. For an albedo of 0.9, the radiation heat flux at the boundary differed by approximately 25% with and without the inclusion of scattering.

The discrete ordinates model was verified against an analytical solution that assumed isotropic intensity and isotropic scattering. The discrete ordinate model (with and without scattering) was found to be in good agreement with the analytical solution for a parameter set within the range of validity of the analytical solution.

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