A Comparison of Electromagnetic Wave and Radiative Transfer Equation Analyses of a Coal Particle Surrounded by a Soot Cloud

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The electromagnetic wave analysis of scattering from a two-component, stratified sphere has been applied to the physical situation consisting of a coal particle surrounded by a soot cloud. The analysis enables definition of emission coefficients for the coal and soot components. Comparisons are made with models based upon solutions to the radiative transfer equation, and agreement is found to be excellent for coal particle diameters six to seven times larger than the wavelength of radiation.

INTRODUCTION

Accurate prediction of the radiative properties of particulates in pulverized-coal (PC) flames is essential to both the determination of heat transfer rates and the interpretation of optical diagnostic data obtained from such flames. Determination of the radiative behavior of the individual particulate components, i.e., coal, soot, and fly ash, is a relatively straightforward process involving the application of Lorenz–Mie or Rayleigh theory and has been carried out by several investigators [1, 2]. Net radiative behavior can be obtained from the summation of the individual properties provided that the distances between particles are large compared to the particle dimensions and the particles are distributed uniformly in space. However, images of devolatilizing coal particles indicate that soot, formed during the gas-phase combustion of volatile matter, can form a concentric "mantle" about the parent coal particle [3, 4]. Under this situation, the validity of simply adding the radiative contributions of coal and soot is questionable.

Recently, analytical methods involving an appropriately formulated radiative transfer equation (RTE) have been applied to the composite coal particle–soot cloud system [5, 6]. Results of these investigations indicate that the overall radiative properties of the coal–soot system can indeed be different from the sum of the individual components. However, application of the RTE to physical systems having dimensions comparable to the wavelength of radiation, as can be the case with PC, is in itself questionable [7].

Macroscopically defined radiative properties utilized in the above investigations [5, 6], such as the surface emittance of the coal particle, are not invariant with respect to particle size in the small-particle limit. Indeed, the spectral emission coefficient of a particle, which under Kirchhoff's law is equal to the absorption efficiency [8], can exceed unity for particle diameters on the order of the wavelength. An approach valid for all particle sizes, and in particular the small-size regimes where the RTE approach fails, involves application of electromagnetic wave (EMW) scattering theory to the coal–soot system [7]. Such an application and the determination of the size
regime below which the RTE formulation fails is the objective of the work presented herein.

**RADIATIVE MODEL**

Assuming the soot to be uniformly distributed between the coal particle surface and an outer boundary, the coal–soot system is represented for radiative transfer analysis as a two-component, stratified sphere (Fig. 1) for which the coal particle core and soot cloud layer, having respective diameters of \( D_c \) and \( D_1 \), are characterized by size parameters \( x_c = \pi D_c / \lambda \) and \( x_l = \pi D_1 / \lambda \) and refractive indices \( m_c \) and \( m_l \). The refractive index of the soot layer, \( m_l \), is not the actual soot particle refractive index, \( m_s \), but rather an "effective" refractive index of the medium; a formula for \( m_l \) is discussed below, but in general, \( m_l \) is function of \( m_s \) and the soot volume fraction, \( f_v \). The complex index of refraction here will be written as \( m = n + ki \) following Bohren and Huffman [10].

Although this model, along with the assumptions that follow, is an admittedly simple one, adoption of it allows us to make direct comparison with the results of others who employed it [5, 6] and to avoid practical complications that would make application of EMW analysis, or RTE analysis for that matter, intractable. The resulting simple problem is a first approximation to sorting out the radiative behavior of the complicated phenomena that occur in the vicinity of a burning coal particle.

The solution of Maxwell’s equations yielding the electric and magnetic fields for the stratified sphere has been presented by others [9, 10]. These fields can be used to derive relationships to allow emission, absorption, and scattering coefficients to be determined. The solution technique is similar to that for the scattering by a homogeneous sphere in that the expansion of the incoming, internal, and scattered waves in terms of infinite series of spherical vector harmonics enables a separation-of-variables solution of the governing differential equations. The resulting expressions for overall radiative properties of the composite particle, i.e., the scattering and extinction efficiencies and the differential scattering cross sections, are identical to those obtained from Lorenz–Mie theory for homogeneous spheres.

Of interest here is the application of the EMW formulation to the prediction of radiant emission from the composite particle system. Under isothermal conditions, the spectral emission coefficient of the system can be equated to the absorption efficiency. In actual situations, however, the coal particle, because of the endothermic devolatilization process or exothermic surface oxidation, is likely to be at a different temperature than the surrounding soot cloud. It is not possible to define a temperature-independent emission coefficient of the composite particle system under nonisothermal situations, and yet we expect Kirchoff’s law, when applied to the locally isothermal regions inside the system, still to be valid. That is, \( \int dC_{abs} \, dV = \int dC_{emis} \, dV \), where \( dC_{abs} \) and \( dC_{emis} \) are the respective differential absorption and emission cross sections of an isothermal volume element \( dV \) within the system. Expressions for \( dC_{abs} \) can be obtained from analysis of the electric (\( E \)) and magnetic (\( H \)) fields, which are obtained as part of the solution of Maxwell’s equations for this particular situation as developed in Ref. 10.

The rate of radiant energy transfer at a particular location is given by the Poynting vector,

\[
S = \frac{1}{2} \text{Re} (E \times H^*),
\]

where the superscript "*'" indicates the complex conjugate. Integration of \( S \) over the boundary
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enclosing \( dV \) will yield the net rate of energy absorption within the element. For the problem at hand, only the radial variation in absorption need be considered. Thus the rate of absorption within a spherical boundary located a distance \( r \) from the particle center is

\[
W_{\text{abs}}(r) = \frac{1}{2} \Re \left( \int_0^{2\pi} \int_0^\pi (E_{1\theta} H_{1\theta}^* - E_{1\phi} H_{1\phi}^*) \sin \theta \, d\theta \, d\varphi \right).
\]

(2)

Using the series expressions for the internal field components [10] and the orthogonality properties of Legendre functions, the above integrals can be analytically evaluated to yield \( W_{\text{abs}}(r) \) in terms of Ricatti-Bessel functions and the internal field coefficients. Details of the analysis are given elsewhere [11]. The absorption cross section of the particle at radius \( r \), \( C_{\text{abs}}(r) \), is defined as the ratio of \( W_{\text{abs}}(r) \) to the incident intensity falling on the particle. The absorption cross section of the core is obtained from evaluation of \( C_{\text{abs}}(r = r_c) \). From conservation of energy, the absorption cross section of the layer is the difference between the total and core absorption cross sections. In terms of efficiencies, \( Q \), the core and layer absorptions are

\[
Q_c = \frac{C_{\text{abs}}(r_c)}{\pi r_c^2},
\]

(3)

\[
Q_l = \frac{1}{\pi r_l^2} \left[ C_{\text{abs}}(r_l) - C_{\text{abs}}(r_c) \right].
\]

(4)

Assuming that the soot and coal are at separate but uniform temperatures, the radiant flux at the outer surface of the soot layer is

\[
E_\lambda = Q_c E_{\text{bl}}(T_c) + \frac{r_c^2}{r_l^2} Q_c E_{\text{bl}}(T_c),
\]

(5)

where \( E_{\text{bl}} \) is the Planck blackbody function.

\( Q_c \) and \( Q_e \) can be viewed as effective emission coefficients of the coal particle and soot cloud, respectively. As the soot cloud becomes more tenuous, \( m_1 \) will approach unity, and \( Q_c \) will approach the value given for a single, homogeneous sphere by Lorenz–Mie theory. An increase in \( \text{Im}(m_1) \) will generally result in a decrease in \( Q_c \), although a nonabsorbing (real \( m_1 \)) layer can actually result in an increase in \( Q_c \), because the layer acts as a "lens" and tends to focus more radiant energy upon the core particle [9].

An appropriate formulation for the effective refractive index of the soot cloud, \( m_1 \), is obtained from Maxwell–Garnett theory, as discussed in Ref. 10. The theory considers a medium within which is imbedded a distribution of uniformly spaced, Rayleigh-sized inclusions. The effective refractive index of the medium, in this case the soot cloud, is given by

\[
m_1^2 = 1 + 3f_v \left[ \frac{m_s^2 - 1}{m_s^2 + 2} \right] \left[ 1 - \frac{m_v}{m_s^2 + 2} \right]^{-1},
\]

(6)

where \( m_s \) is the refractive index of the soot particles and \( f_v \) is the volume fraction of the soot within the cloud layer.

The formulation of \( m_1 \) in this manner results in physically reasonable limiting behavior. If \( C_{\text{abs}}[x, m_1(m_s, f_v)] \) is the absorption cross section of a spherical particle computed for a size parameter \( x \) and effective refractive index \( m_1 \), then as \( f_v \) goes to zero, \( C_{\text{abs}} \) approaches the value given in the Rayleigh limit multiplied by \( f_v \). Therefore, for small values of \( f_v \), (which will correspond to small \( Q_c \)) the coal–soot model should yield essentially the results given by separate analysis of the soot and coal particles.

In the large soot-particle concentration limit, i.e., \( f_v \rightarrow 1 \), the near-field interactions, or dependent scattering, among the soot particles will become important. For this situation, it has been shown that the "net" radiative behavior of the soot particles is well-approximated by the Maxwell–Garnett effective refractive index analysis of the soot particle cloud [12].

RESULTS

Calculation of results was accomplished through a slight modification of the BHOAT Fortran code listed in Ref. 10. For typical values of soot and coal refractive indices [13, 14] and volume fractions on the order of \( 10^{-4} \), the upper bounds on \( x_c \) and \( x_l \) in the code are approximately 100 and 500, respectively.
Comparisons are made with the RTE analysis given by Choi and Kruger [6]. The STaR (Spherically Translucent and Radiating) model developed in Ref. 6 allows for definition of effective soot cloud and coal particle emission coefficients corresponding to Eq. 29. For an assumed coal particle emittance of unity and an isothermal soot cloud, the effective coefficients are given as

\[ Q_e = 2R[E_3(\tau_\text{sd}) - \tau_\text{sd}E_4(\tau_\text{sd}) - E_5(\tau_\text{sd})] \]

\[ + \tau_1^*E_4(\tau_1^*) - E_5(\tau_1^*)], \quad (7) \]

\[ Q_1 = \frac{2}{\tau_\text{sd}} \int_{\tau_\text{cl}}^{\tau_\text{c}} \left[ \tau_\text{sd}E_2(\tau_\text{c} - \tau) + E_3(\tau_\text{c} - \tau) \right. \]

\[ - \tau_1^*E_2(\tau_1^* + \tau) - E_3(\tau_1^* + \tau* \right) dt. \quad (8) \]

where \( \tau \) is the optical depth of the soot cloud \((= \kappa^2 p)\), \( \tau_\text{sd}^* = \tau^2 - \tau_\text{c}^2 \), \( R = r_\text{c}/r_1 \), and \( E_n \) is the exponential integral function of order \( n \). The absorption coefficient of the soot, \( \kappa^2 \), is given in the Rayleigh limit as

\[ \kappa^2 = \frac{6\pi f_\nu}{\lambda} \text{Im} \left[ \frac{m_s^2 - 1}{m_s^2 + 2} \right]. \quad (9) \]

The soot layer optical depth in the STaR model, \( \tau_\text{sd} \), is related to the two parameters in the EMW model, \( x_c \) and \( f_\nu \), by

\[ f_\nu = \frac{R\tau_\text{sd}}{3x_c(1 - R) \text{Im}(m_s^2 - 1)/(m_s^2 + 2)} \quad (10) \]

Comparisons between the STaR and EMW model effective emission coefficients are given in Figs. 2–5, in which \( Q_e \) and \( Q_1 \) are presented as a function of \( \tau_\text{sd} \) for \( R = 0.5 \) and 0.25 and \( x_c \) ranging from 1 to 100. The \( R \) values used in the calculation were chosen to be consistent with experimentally observed values [15]. Agreement between the two formulations is seen to improve with increasing \( x_c \); for the index of refraction values used here for \( x_c > 20 \) there is around a 5% difference in \( Q_e \) and a negligible difference in \( Q_1 \) regardless of the value of \( \tau_\text{sd} \). The correspondence between the two models in a large-particle limit is to be expected, but the value of \( x_c \) beyond which this correspondence obtains could not have been determined without the EMW analysis.

Significant departures between the EMW and STaR results occur in the prediction of \( Q_e \) for relatively small values of \( x_c \) (i.e., \( x_c < 5 \)). The source of the disparity lies mainly in the fact that the emission coefficient of coal particles in this size parameter range can significantly exceed unity [10].
On a physical basis, the existence of a detached flame about the coal particle may be limited to particles having diameters in excess of 60 μm \([16, 17]\), but the diameter can be much smaller than this in fuel-rich systems \([17]\). For radiant heat transfer, which occurs mostly within the 1–3-μm wavelength region, the corresponding size parameters of the soot-producing coal particles may be in excess of 60, for which the RTE formulation appears entirely appropriate. However, for diagnostic techniques employing longer wavelengths, e.g., a CO₂ laser at 10.6 μm, the size parameter of a sooting coal particle, particularly in a fuel-rich environment, can be substantially smaller than 20. It should also be noted that the maximum \(\tau_{cl}\) values presented can correspond, for the smaller \(x_c\) values, to unrealistically large \((> 0.1) f_v\) values.

Numerical results indicate that the variation in soot-layer absorption from refractive index variation is practically identical to that predicted from Rayleigh theory, i.e., the functional dependence on \(m\) is approximately that of Eq. 10. For the range of quoted soot \(m\) values \([13]\), the results presented in Figs. 2 and 4 can be shifted by around 25% with the maximum variation occurring for the smaller \(\tau_{cl}\) values. The effect of coal refractive index variation is minimal for relatively large coal particle size parameters, as is the case here. This latter point has been made before \([1]\).

**CONCLUSIONS**

The electromagnetic wave analysis of a two-component, stratified sphere has been applied to a coal particle surrounded by a soot cloud. Results indicate that, for coal particle size parameters in excess of 20, the radiative transfer equation formulation of the problem is in excellent agreement with the EMW analysis.

**REFERENCES**


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