

ly the carbon to hydrogen ratio of the fuel) and the local equivalence ratio and temperature. Tien and Lee (1982) and Blokh (1988) provide in depth discussions of soot particle characteristics and summaries of measurements and predictions of soot radiation properties. Menguc and Viskanta (1987) and Modest (1993) also provide summaries of correlations commonly used to predict soot absorption properties.

6.2 Soot Radiative Property Models

A significant amount of research has been conducted to develop a general method for predicting soot formation and radiative properties (Dalzell and Sarofim, 1969, Chippett and Gray, 1978, Lee and Tien, 1980, Haynes and Wagner, 1981, Felske, Hsu and Ku, 1986, Glassman, 1988, Dobbins, Santoro and Semerjian, 1990, Syed, Stewart and Moss, 1990, Sivathanu, Kounalakis and Faeth, 1990). To date, however, there is still no single theory accepted for general use. Current methods for predicting radiative properties are decoupled from soot formation models and thus require soot particle concentrations, size, shape and complex refractive index as known inputs. These techniques then use Mie theory or statistical relations correlated with measured data to estimate radiative properties. Because these techniques are commonly employed to predict only a few properties at a time, they are not very efficient and greatly increase the computational overhead of a CFD-based combustion program which may require properties to be calculated at a half-million node points. A reasonable alternative to these methods seems to be a method based on experimental correlations that takes into account local furnace properties (including turbulence), but that does not require the amount of soot formation detail and computational time of more precise techniques.

Three such methods involve correlations presented by Blokh (1988), Felske and Tien (1977) and Sarofim and Hottel (1978). Blokh's method is applicable only for sooting liquid and gaseous fuels and is based on the flame temperature, stoichiometric

ratio, and relative content of carbon and hydrogen in the working mass of the fuel. This correlation has shown good agreement in the temperature range 1000 - 2000 K with the experimental data of several authors (see Sato, Kunitomo, Nakashima and Fujii, 1969) and is also independent of wavelength and therefore very computationally efficient. Unfortunately, this correlation is based on the optical thickness across the entire sooting flame and is thus difficult to apply at specific points in the flame as required by the discretization approach used in this research.

The approach used by Felske and Tien (1977) is based on Rayleigh scattering theory for small particles. This theory results in the commonly referenced relation

$$k_{soot, \lambda} = \frac{C_0 f_v}{\lambda} \quad (6.1)$$

where C_0 is a variable representing the effects of the soot complex refractive index, f_v is the soot volume fraction and λ is the incident wavelength. The variable C_0 is written

$$C_0 = \frac{36\pi n \kappa}{(n^2 - \kappa^2 + 2)^2 + 4n^2 \kappa^2} \quad (6.2)$$

where n and κ are the real and imaginary parts of the complex index of refraction, $m = n - i\kappa$, respectively.

Values for the complex refractive index of different fuels have been presented by several authors, including Lee and Tien (1980), Stull and Plass (1960), Dalzell and Sarofim (1969), Howarth, Foster and Thring (1966) and Felske, Charalmpopoulos and Hura (1984). Siegel (1976) has summarized these results and found that C_0 is between 3.7 and 7.5 for coal flames, 6.3 for oil flames, 4.9 for propane flames and 4.0 for acetylene flames.

The results of Lee and Tien (1980) and Siegel (1976) indicate that n and κ depend only weakly on wavelength. Therefore, appropriate spectral average values for n and κ may be chosen which eliminate the wavelength dependence of C_0 in Equation

(6.1). This means the absorption coefficient has a $1/\lambda$ dependence. This allows Planck and Rosseland mean absorption coefficients, respectively, to be calculated from Equation (6.1) as

$$k_P = 3.83f_v C_0 T / C_2 \quad (6.3)$$

and

$$k_R = 3.60f_v C_0 T / C_2 \quad (6.4)$$

where $C_2 = 0.014388$ m-K is the second Planck function constant. Felske and Tien (1977) have noted that the difference between the Planck and Rosseland means differs by only six percent and have suggested using an average of the two means. Their relation is

$$k_{soot, F-T} = 3.72f_v C_0 T / C_2 \quad (6.5)$$

Because Equation (6.5) was derived from Rayleigh scattering theory, it is valid only for very small soot particles, i.e., it is not appropriate for soot agglomerates.

The dependence of Equations (6.2) and (6.5) on κ is illustrated in Figure 6.1. The results shown are based on a constant value of 2.0 for the real part of the refractive index, a constant temperature of 1600 K and a soot volume fraction of 1.0×10^{-7} . The real part of the refractive index was held constant because it is less dependent on wavelength than the imaginary part. Values for the variable C_0 range from 3.5 to 7.0, a range which compares well with the values of Siegel (1976). The linear dependence of the absorption coefficient on C_0 causes the k_{soot} values to track C_0 . If the axes of Figure 6.1 are adjusted correctly, the two curves will be identical since in this case they differ only by a constant. The roll over at high κ values is caused by the constant n assumption. When κ reaches values near 2.0, n has actually increased to around 2.5. The

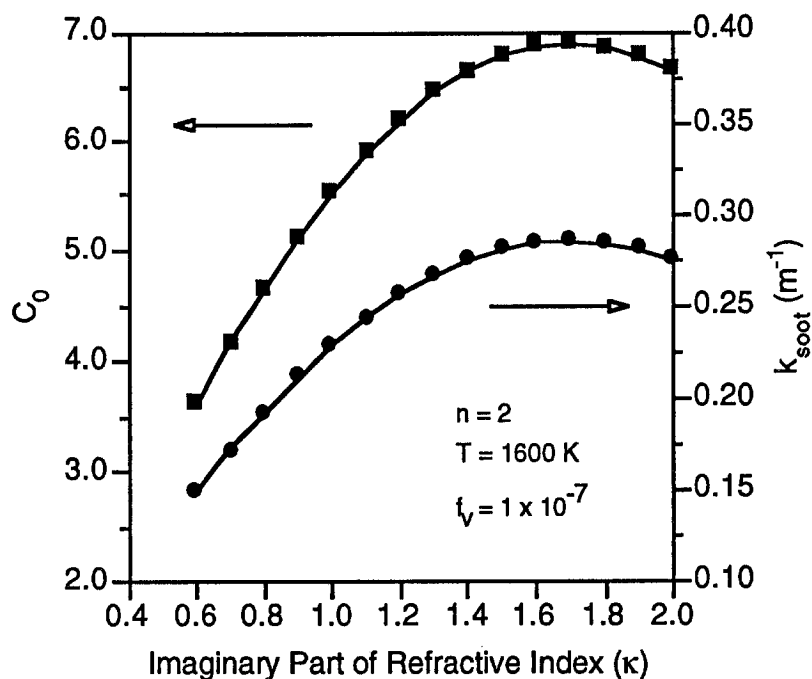


Figure 6.1 Dependence of Soot Absorption Coefficient on Imaginary Part of the Complex Refractive Index As Given by Equations (6.2) and (6.5).

soot absorption coefficient in this model is linearly dependent on soot volume fraction and temperature as indicated by Equation (6.5).

The correlation for the emissivity of a sooting flame presented by Sarofim and Hottel (1978) is applicable to gas or coal flames and is more readily adapted to calculating radiative properties for the discrete-ordinates method than the correlation of Blokh. Sarofim and Hottel's correlation may be written as

$$\epsilon_{soot} = 1 - (1 + 350f_v T L_e)^{-4} \quad (6.6)$$

where ϵ_{soot} is the flame emissivity due to soot, f_v is the soot volume fraction, T is the gas or soot temperature in Kelvin, and L_e is the mean beam length of the furnace. This relation can be rewritten in terms of the absorption coefficient as

$$k_{soot, S-H} = \frac{-4}{L_e} \ln(1 + 350f_v TL_e) \quad (6.7)$$

Like the gas emissivity relations, this relation has an undesirable dependence on beam length. However, the effect is relatively minor. If the soot volume fraction and temperature are assigned values of 1×10^{-7} and 1600 K, respectively, the absorption coefficient is found to change less than ten percent as the beam length is varied from 1 - 5 m.

The accuracy of this correlation is illustrated in Figure 6.2 which compares the results of Equation (6.6) with spectral-based calculations of Felske and Tien (1973). Results shown are for temperatures of 1000 and 1600 K and a mean beam length of 1 m, however agreement is consistent for other temperatures and pathlengths. The agreement between Equation (6.6) and the spectral data is excellent. Figure 6.2 also illustrates the sensitivity of the soot emissivity to soot volume fraction and temperature.

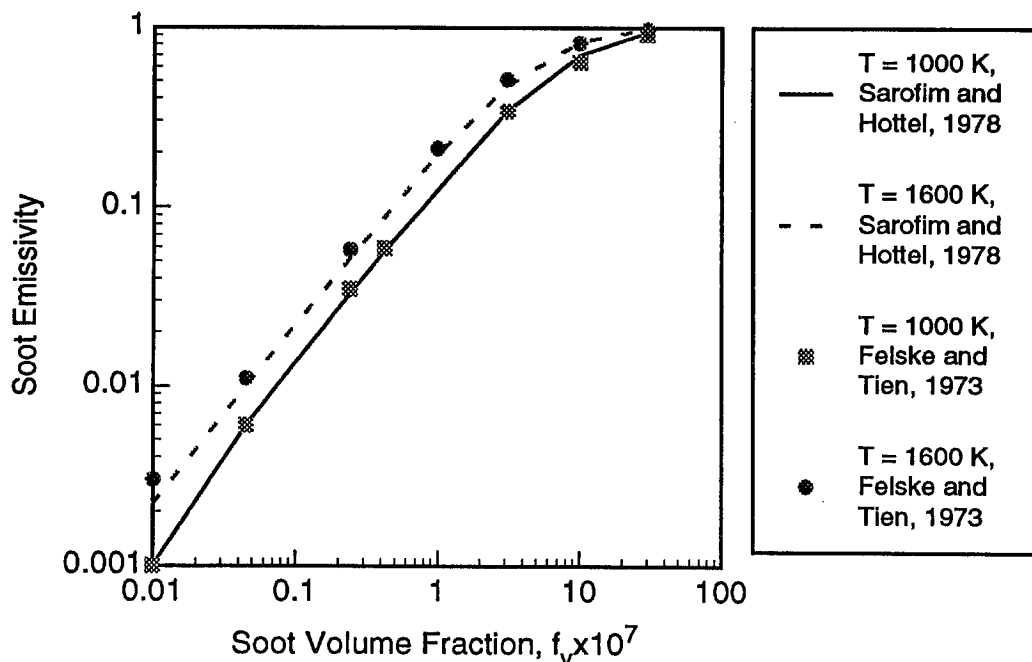


Figure 6.2 Comparison of Predicted Soot Emissivities Based on Spectral Calculations of Felske and Tien (1973) and Equation (6.6).

Based on the similarity of the two correlations and the agreement between Equation (6.6) and the spectral data of Felske and Tien (1973), the correlation of Sarofim and Hottel (1978) was selected for use in this research.

6.3 Soot Formation Model

The parameter with the greatest degree of uncertainty in Equations (6.5) and (6.7) is the soot volume fraction. As mentioned above, no general model has been developed to allow specification of this quantity. Sarofim and Hottel (1978) suggest that the volume fraction is fundamentally composed of two components, soot formation and destruction. The magnitude of these two mechanisms determines the amount of soot available for radiation. In this research, soot formation is calculated from the relation

$$f_{v,formed} = \frac{C_1 b_c M_c}{\rho_{soot}} \quad (6.8)$$

where C_1 is the mass fraction of volatile fuel carbon which forms soot, M_c is the molecular weight of carbon, b_c is the mass-atoms of carbon per mass of reactant mixture, and ρ_{soot} is the soot (carbon) density. The constant C_1 has been experimentally found to range between 0.0 - 0.2 (Sarofim and Hottel, 1978). This research assumes a value of 0.1. The value for b_c is calculated as a function of the local gas density and mixture fraction and basically determines the amount of volatile fuel carbon which is available to form soot. Several researchers (Felske and Tien, 1973, Smyth, Miller, Dorfman, Mallard and Santoro, 1985, and Sato, Tree, Hodges and Foster, 1990) have suggested that the main temperature region for soot formation and burnout is approximately 1000 - 2000 K. For this reason, soot formation in the current research model is limited to temperatures greater than or equal to 1000 K.

The amount of soot destruction may also be thought of as the fraction of soot formed which survives to radiate. This quantity is calculated from the relation

$$C_2 = \frac{\text{MAX}(0.0, \text{MIN}(E - E_{cr}, E_{inf} - E_{cr}))}{(E_{inf} - E_{cr})} \quad (6.9)$$

where C_2 is the fraction of soot formed which survives to radiate, E is the equivalence ratio, E_{cr} is the critical equivalence ratio where soot formation begins, E_{inf} is the equivalence ratio where all soot formed remains to radiate (i.e., no burnout), and MIN and MAX represent FORTRAN minimum and maximum functions, respectively. The critical equivalence ratio varies with fuel type and flame type, but for most lower order hydrocarbons, a single value of 1.0 is sufficiently representative (see Glassman, 1987). A value of twice the critical equivalence ratio was used for E_{inf} . Thus when the local equivalence ratio is less than 1.0, C_2 is 0.0 and no soot survives to radiate; when the equivalence ratio is 2.0 or greater, C_2 is 1.0 and all soot formed survives to radiate. C_2 varies linearly between equivalence ratios of 1.0 and 2.0 as shown in Figure 6.6.

The final expression for soot volume fraction as used in Equation (6.7) is a combination of the soot formation and destruction and may be written as

$$f_v = \frac{0.1 C_2 b_c M_c}{\rho_{soot}} \quad (6.10)$$

Equations (6.7) and (6.10) account for what are believed to be the major factors affecting soot contributions to radiative absorption and emission - temperature, stoichiometric ratio and fuel type. Several characteristics can be observed which relate correlation behavior to a physical basis. First, the coefficient C_2 , and hence the absorption coefficient, go to zero as the stoichiometry becomes lean. This is indicative of a lack of excess carbon to form soot. Second, increases in temperature produce increases