CHAPTER 8

Thermal radiation modeling in flames and fires

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Abstract

An overview of thermal radiation models for different combustion processes is presented. The pertinent constitutive equations and associated radiative property models are discussed. Various solution techniques for the radiative transfer equation are described. Finally, the implications for flames and fires are discussed in the context of the role of different thermal radiation models.

1 Introduction

Radiation is the dominant energy transport mechanism to surrounding surfaces during many combustion processes, particularly when entrained particles are present. It plays an important role in practical systems such as furnaces [1], during fundamental flame phenomena, such as the radiation-induced extinction of flames at low stretch [2], radiation-turbulence interactions [1], and in fires [3]. Typically, the radiation intensity on a wall becomes very significant when the combustion length scale approaches a meter [4].

Thermal radiation is strongly coupled with soot kinetics and the flame structure through the local temperatures. Characterizing radiative energy transport is therefore a crucial element in modeling combustion systems. However, this is also a very complex problem. For example, in a typical coal fired furnace, radiation includes contributions from particulates (like coal/char, soot, ash) as well as from gases (such as CO₂, H₂O). The accuracy of a radiation simulation depends on a combination of the accuracy of the calculation method and the accuracy with which the radiative properties of the media and surfaces are known [5].

The current focus for radiative heat transfer models is on describing radiative interactions with a participating medium. The process is characterized by absorption, emission, and scattering of radiant energy, and mathematical models and computer codes are necessary to solve various radiation problems. Products of combustion gases, such as carbon dioxide, water vapor, and their mixtures with soot are considered within these radiation problems. An important issue of gas radiation is the description of the radiative properties of these gases (or the so-called nongray gases) [6].
2 Basic equations

2.1 Energy conservation equation

The mass, momentum, energy, and species balance equations must be solved to address combustion problems. These equations retain their usual form, while the energy equation addresses thermal radiation in a participating medium through an appropriate term, i.e. [6]

\[ \rho \frac{\partial h}{\partial t} + \nabla \cdot (\rho \mathbf{v} h) = -\nabla \cdot \mathbf{q} + \dot{S}, \]

where \( h \) denotes the enthalpy of the fluid and \( \dot{S} \) the sources of heat generation, viscous heat dissipation, pressure, and body force work. The heat flux vector

\[ \mathbf{q} = -K \nabla T + \rho \sum_{i=1}^{N} h_i \omega_i \mathbf{v}_i + \mathbf{F}. \]

The terms on the right-hand side represent heat conduction, inter-species heat diffusion, and radiative heat flux that can be written as:

\[ \hat{F}(\hat{r}, t) = \int_{0}^{\infty} I_{l\lambda}(\hat{r}, \hat{s}, t) \hat{s} \, d\Omega \, d\lambda. \]

2.2 Radiative transfer equation

The spectral intensity of radiation, \( I_{l\lambda}(\hat{r}, \hat{s}, t) \), at wavelength \( \lambda \) is found from the radiative transfer equation (RTE). The interaction of electromagnetic radiation with matter that absorbs, emits, and scatters thermal radiation is described by the RTE. For the sake of brevity the derivation of RTE has not been repeated here, since it is well explained in the literature [7].

If we consider the local thermodynamic equilibrium of a medium capable of absorbing, emitting, and scattering radiation, the spectral radiation intensity \( I_{l\lambda}(\hat{r}, \hat{s}, t) \) of the radiation field is [7]

\[ \hat{s} \cdot \nabla I_{l\lambda} = k_{l\lambda} I_{l\lambda} - \beta_{l\lambda} I_{l\lambda} + \frac{\sigma_{l\lambda}}{4\pi} \int I_{l\lambda}(\hat{s}, \hat{s}) \Phi_{l\lambda}(\hat{s}, \hat{s}) \, d\Omega, \]

where \( k \) denotes the absorption coefficient, \( \beta \) the extinction coefficient, \( \sigma \) the scattering coefficient, and \( \Phi \) the scattering phase function that can be interpreted as the ratio of scattered radiative intensity in a given direction to the scattered radiative intensity in the same direction by isotropic scattering. The time dependent term for the radiation intensity can be usually neglected (as we have done).

Equation (4) is the radiation balance for an infinitesimal pencil of rays in which absorption, extinction and scattering terms are considered. Thus, in order to obtain a volume balance, the equation must be integrated over all solid angles, i.e.

\[ \int_{4\pi} \hat{s} \cdot \nabla I_{l\lambda} \, d\Omega = \int_{4\pi} k_{l\lambda} I_{l\lambda} \, d\Omega - \int_{4\pi} \beta_{l\lambda} I_{l\lambda} \, d\Omega + \int_{4\pi} \frac{\sigma_{l\lambda}}{4\pi} \int I_{l\lambda}(\hat{s}, \hat{s}) \Phi_{l\lambda}(\hat{s}, \hat{s}) \, d\Omega \, d\Omega. \]
After rearranging, this relation can be written in the form [7]

\[
\nabla \cdot q_{j} = 4\pi k_{j} I_{b,j} - \beta_{j} \int I_{j}(\hat{\delta})d\Omega + \sigma_{j} \int I_{j}(\hat{\delta}) d\Omega,
\]

where

\[
\beta_{j} = \sigma_{j} - \sigma_{j}^{l},
\]

and

\[
\nabla \cdot q_{j} = k_{j} \left( 4\pi I_{b,j} - \int I_{j} d\Omega \right) = k_{j} \left( 4\pi I_{b,j} - G_{j} \right),
\]

where \( G_{j} \) denotes the incident radiation. Integration over the entire spectrum can be carried out to obtain the divergence of radiation heat flux, \( F \).

3 Solution of the RTE

The solution of the RTE can be substituted in the thermal energy equation to determine the temperature distribution in a reacting flow. This requires knowledge of the spectral radiative properties of the gases and an efficient method to solve the RTE. The evaluation of the radiative flux vector \( F \) or its divergence represents a fundamental problem that is related to the treatment of the spectral radiative properties of gases, the solution of the RTE, and integration over the spectrum.

3.1 Radiative property models

The accuracy of any solution of the RTE depends upon an accurate knowledge of the radiation properties of the combustion product gases and the entrained/generated particles. Models used to define the radiative properties of combustion gases in radiation calculations can be roughly sorted in three groups [8], i.e.

1. Spectral line-by-line (LBL) models;
2. Spectral band models; and

Each has its merits and drawbacks that prescribe its area of application. Historically, the oldest and the simplest concept for the prediction of radiation by a gas is the gray gas model [9]. It assumes that the gas absorption coefficient is constant and therefore, when compared with other models, provides predictions with poorer accuracy [10].

The LBL model provides the best accuracy. With this method the RTE is integrated over the detailed molecular spectrum for the gases [11]. Because of the enormous computational requirements, this model is used mainly for benchmark solutions. It has two main disadvantages. First, the required spectral resolution should be smaller than the line width (i.e. \( 10^{-3} \text{--} 10^{-2} \text{cm}^{-1} \)), which corresponds to roughly 106 spectral discretization intervals to cover the entire infrared spectrum. Second, at higher temperatures, accurate descriptions of a large number of lines associated with high energy levels and their quantum states are required.

Recent developments in gas molecular spectroscopy have improved the database of radiative properties. Rothman et al. [12] have successfully implemented the LBL method to predict radiative transfer in the low temperature atmosphere. The 1992 version of the HITRAN database [12] contains information about spectroscopic transition line parameters for 32 molecules at the reference
temperature of 296 K. The molecules included in the database are H$_2$O, CO$_2$, O$_3$, N$_2$O, CO, CH$_4$, O$_2$, NO, SO$_2$, NO$_2$, NH$_3$, HNO$_3$, OH, HF, HCl, HBr, ClO, OCS, H$_2$CO, HClO, N$_2$, HCN, CH$_3$C, HCl, H$_2$O$_2$, C$_2$H$_6$, C$_2$H$_4$, PH$_3$, COF$_3$, SF$_6$, H$_2$S, and HCO$_2$H. It covers a spectral range from $10^{-6}$ to 22,656 cm$^{-1}$ (i.e. 0.4414–1.010 µm). LBL calculations have been reported for H$_2$O–CO$_2$–CO semitransparent gas mixtures up to 2,000 K [13, 14]. In this model the spectral absorption coefficient for a gas mixture

$$k_j = \sum_i \sum_j k_{ij},$$

where the subscript $i$ refers to the absorbing species and subscript $j$ to all the lines of all the bands in these species. The line mixing and collision effects can be considered using phenomenological functions [12, 15]. The key problem is to obtain all center locations, lower level energy, and intensities of all lines contributing to absorption. The HITRAN database [12] is available for atmospheric and higher temperatures [16, 17].

Approximate models that have been developed to characterize the spectral structure of radiation can be classified into two groups, namely, (1) band models and (2) global or total models. In band models, the entire spectrum is divided into a number of bands. Thereafter, radiative properties, averaged over each band, are calculated from the absorption spectra or statistical properties of a line. These bands are assumed to be sufficiently narrow such that variations of radiative properties can be neglected.

When a narrow band model is used, the RTE must be averaged over a band to yield the band-averaged radiation intensity. To obtain spectrally-averaged or narrow band values of the absorption coefficient, some information must be available on the spacing of individual lines within the group and their strengths. A number of models have been proposed for this purpose and the statistical model is most widely used. It assumes that the spectral lines are not equally spaced within a narrow band. This can be a true representation for complex molecules for which lines from different rotational modes overlap in an irregular fashion [18].

An extensive description of narrow band models can be found in refs [15, 18]. These models require a database containing the measurements of both the reciprocal mean line spacing parameter and the mean absorption coefficient over the entire infrared spectrum at different temperatures. The most complete set, of measured narrow band parameters for H$_2$O and CO$_2$ is that of Ludwig and coworkers. Improved narrow band parameters have been published by Taine and coworkers [13, 14, 19] and Phillips [20, 21]. To date, the general dynamic database enables radiative property calculations for H$_2$O, CO$_2$, CO, OH, NO, HF, and CN. For CH$_3$, C$_2$H$_4$, and soot, a narrow band model calculation can be performed using the approaches outlined by Brossmer and Tien [22, 23] and Ludwig et al. [18].

The statistical narrow band (SNB) model is more accurate for predictions of radiative transfer in high temperature gases. It provides the spectral transmissivity averaged over a narrow band. However, because of this it is difficult to couple the model with a solution methodology such as the finite volume method (FVM), which requires values of spectral (monochromatic) absorption coefficients or their averages over wavelength intervals. Another disadvantage is that the model requires a large number of bands and is therefore computationally very expensive. The wide band model (WBM) is a simplification of the SNB model. Instead of spectral lines, it considers bands and so is more economical but less accurate. It yields wideband absorptance while the solution of RTE by FVM operates either with spectral or averaged absorption coefficients. Therefore the WBM cannot easily and simply be incorporated in a FVM. In addition, WBM requires knowledge of the path length in the model as well as the associated spectral parameters.
The concept underlying the exponential wide band model (EWBM) [24, 25] stems from the experimental observation that absorption by gases is mainly due to four or five strong absorption bands located in the near infrared and infrared regions (1–20 µm). The EWBM does not look at a narrow band but rather at the whole absorption band. This model provides fairly simple mathematical expressions to predict the temperature and pressure dependence of the most important absorption bands of H$_2$O, CO$_2$, CO, CH$_4$, NO, SO$_2$, N$_2$O, NH$_3$, and C$_2$H$_2$. The EWBM can also be utilized to predict the homogeneous total emissivity of gas-soot mixtures provided the soot concentration is known. This model could be utilized to calculate radiation in nonhomogeneous gas mixtures.

From a practical perspective, the requirement of an almost insignificant database is the main advantage of EWBM as compared to SNB models. The model does not require excessive computational power and possesses all the generality required for the radiation simulations in combustion at atmospheric and elevated pressures. Its major shortcoming is in treating radiation problems in enclosures, since it does not readily account for wall interactions. This problem originates from the formulation, which requires the calculation of the total band absorptance prior to those of the band transmissivity and bandwidth. Since the width of each absorption band varies with temperature, pressure, and pathlength, a different division of the infrared spectrum is required for each path along which the RTE is solved. However, to properly account for gas-wall interactions, the same spectral division for the wall and the gas phase should be used. The division of the spectral emissivity at the wall can only be setup once the RTE is solved along each path within the gas volume. This procedure requires a larger computational memory than narrow band models and is more computationally expensive. Some of the main impediments to the coupling of the EWBM with classical solution methods for the RTE have been discussed by Edwards [26].

In correlated-\(k\) (CK) methods, for any radiative quantity that is solely dependent on the gas absorption coefficient (which is true for a narrow band over which the blackbody function can be treated as a constant), the integration over wavenumber can be replaced by integration over the absorption coefficient. When integration over wavenumber is replaced with one over the gas absorption coefficient, the spectral gas absorption coefficient \(k\) is denoted by \(k\), since it now plays the role of an independent variable that is no longer a function of wavenumber. This is equivalent to the concept of the reordered absorption coefficient introduced by Lee et al. [27]. The distribution function \(f(k)\) can be determined in two ways. One is by analyzing the HITRAN database [28] and another by performing the inverse Laplace transformation of the gas transmissivity of a narrow band model, as in the SBN-based correlated-\(k\) (SNBCK) method described by Lacis and Oinas [29].

Denison and Webb [30–32] have developed polynomial correlations to calculate the cumulative distribution functions for water vapor and carbon dioxide. A set of 30 correlations was developed for H$_2$O. The \(k\)-distributions were selected to cover the spectral range 400–12,000 cm$^{-1}$ (0.83–25 µm) with intervals of 400 cm$^{-1}$. The correlations were obtained by fitting spectral line predictions of the cumulative distribution in the temperature and volumetric ranges 400–2,500 K and 0–1, respectively. The \(k\)-distribution model suffers from the disadvantage that new correlations must be computed whenever the total pressure or the temperature is changed (unlike narrow band models and EWBM).

The most widely used global model method is the weighted sum of gray gases (WSGG). The concept was first presented by Hottel and Sarofim [9]. In this method, the nongray gas is replaced by a number of gray gases. For the gray gases, the heat transfer rates can be calculated independently. The total heat flux is then found by summing these heat fluxes with appropriate weights.
This approach can be used in a directional equation of transfer, as shown by Modest [33], and can therefore be used with any solution technique for the RTE.

3.2 Radiative properties of entrained and generated particles

The evaluation of radiative properties of entrained and generated particles is important in combustion processes, since in almost all the cases, the flow is laden with particles like soot, coal, or ash. The radiative properties required for an entrained particle phase are the absorption coefficients and the scattering phase function which depend on the particle concentration, size distribution, and effective complex refractive indices. However, the optical properties of particulates, such as soot and coal, are not well characterized [34, 35] and considerable uncertainties exist, e.g. regarding the size and concentration of soot and the refractive index of ash. The absorption and scattering efficiencies are strongly dependent on the concentration and size distributions. Generally, to simplify the calculation of radiative properties, particles are assumed to be spherical and homogeneous, which is an oversimplification, although the radiative characteristics of a cloud of irregularly shaped particles are not very sensitive to the geometric shapes of the particles (as for pulverized coal) [4].

Given these assumptions, the absorption cross-sections can be calculated using Mie theory [36, 37] based on a specified particle size distribution, wavelength of radiation, and the complex refractive index. Once the absorption and scattering efficiencies for individual particle sizes are known from Mie theory, the absorption and scattering coefficients of the particulates can be evaluated [5]. Unfortunately, Mie theory is strictly applicable only to isolated particles interacting with plane waves. Because of this limitation and due to the highly forward-scattering properties of entrained or combustion-generated particulates, scattering intensities are often approximated by phase functions. The scattering phase function can be modeled using the Dirac-delta approximation [38]. The overall absorption coefficient for the volume can then be obtained as

\[ k = k_p + k_g, \]

where \( k_p \) and \( k_g \) are the absorption coefficients for particle and gas, and the total radiative source for the gas enthalpy equation can be written as

\[ \hat{F} = k \int_{4\pi} Id\omega - 4E_b \],

\[ \int_{4\pi} \]

where \( E_b \) denotes the blackbody emission of the gas. For a gray analysis, the blackbody emissive power for the gas is provided by Stefan–Boltzmann law of radiation [39]. Particle radiative properties and radiative emission can be determined using the source-in-cell technique [40] for Eulerian radiation field calculations.

Almost all the soot models assume that the soot number density decreases as a result of particle agglomeration into spherical aggregates. The only exception is perhaps the study of Ezeoye and Zhang [41] who investigated the effect of particle agglomeration. It has been established that soot aggregates consist of more or less identical primary soot particles but the primary soot particle number density remains almost constant in the growth region. For either a Mie or a Rayleigh–Debye–Gans calculation, the overall properties must be integrated over either particle or aggregate size distribution. However, the fractal aggregate nature of soot has not found its way into most computational studies.
3.3 Solution methodologies

The RTE is an integro-differential equation for which exact solutions are not available for practical engineering applications. Multi-dimensionality, nonhomogeneous media, and the spectral variation of radiative properties make solutions of the RTE quite difficult. However, reasonably accurate numerical solutions can be obtained by introducing certain approximations. Because it is not possible to develop a single solution method that is equally applicable to a wide variety of different systems, several methods with varying degrees of approximation have been developed according to the nature of the physical systems, characteristics of the medium, degree of accuracy required, and the availability of computer facilities [4].

The major approaches are: (1) statistical or Monte Carlo methods; (2) zonal methods; (3) flux methods including the discrete-ordinates approximation; (4) moment methods; (5) spherical harmonics approximation; and (6) hybrid methods. Description of the statistical methods for radiative heat transfer calculations have been provided by Modest [7] and Haji-Sheikh [42]. These can be used for complex geometries and spectral effects can be accounted for without much difficulty. In its simplest form, a statistical approach simulates the histories of a finite but very large number of photons which originate from specified volume/surface elements, propagate in all directions, and are absorbed and scattered based on local values for absorption and scattering coefficients. Different researchers have applied these methods to combustion problems [43–45].

The zonal method (usually referred to as Hottel’s zonal method) is a widely employed model for calculating radiative transfer in enclosures such as combustion chambers. Hottel and Sarofim [9] and Hottel and Cohen [46] first described this approach. In this method, the surface and volume of the combustion chamber are divided into a number of zones, each of which has a uniform temperature and radiative properties. An energy balance is written for each zone, which leads to a set of simultaneous equations for the unknown heat fluxes or temperatures. The radiative heat flux generated by the exchange between the zones is determined using a radiosity method based on appropriate shape factors. The radiosities of the zones are determined by solving simultaneous equations. When an absorbing-emitting medium is involved, the calculation of direct exchange areas becomes complicated by the attenuation of radiation along a path connecting two zones. Because the approach is practical and powerful, it is attractive for many engineering calculations. This method is not however computationally efficient when coupled with finite-volume reactive fluid flow approaches usually used in comprehensive combustion models [47, 48].

Flux methods are based on separating the angular dependence of the radiation intensities, which arise from the spatial dependence of the in-scattering source term. By employing the assumption that intensities are uniform over defined intervals of the solid angle, the integro-differential equation can be simplified into a series of coupled, linear, differential equations expressed in terms of average radiative intensities or fluxes. Different flux models arise based on the number of solid angles used to approximate the directional dependence of the radiant intensity, such as two-flux approach (i.e. forward and backward scattering) for a one-dimensional approximation, four-flux for two dimensions, or six-flux models for three dimensions. Within each of the different flux models, various approximations and simplifications are employed to relate the angular dependence of the fluxes and characterize scattering phase functions to arrive at a closed set of solvable equations.

The flux methods have been particularly effective for simultaneous use with reacting flow field solutions. The discrete-ordinates approach is a particular case of a flux method that was originally developed by Chandrasekhar [49] for astrophysical applications. It has also been used extensively in analyzing neutron transport [50, 51]. In the discrete-ordinates model, a quadrature scheme is used to integrate the in-scattering term. The quadrature set consists of ordinates...
(radiant energy directions) and weights which are chosen by applying appropriate constraints, such as symmetry and moments matching, as well as conserving radiant energy within a control angle and the total control volume. One quadrature scheme commonly used is the \( SN \) approach, in which the entire solid angle is divided into \( N(N + 2) \) angular divisions, where \( N \) can be evaluated on the basis of the order of the quadrature scheme.

Applications of the \( SN \) approach have been shown by Fiveland \[48, 52, 53\] to produce accurate and computationally efficient results as compared with other approaches. Raithby and Chui \[54, 55\] and Chai et al. \[56\] have presented quadrature approaches based on a control volume scheme for fluid mechanics and convective heat transfer calculations. Control volumes can be based on either structured or unstructured grids. Because of its capabilities to consider common control volumes and grid structures to couple the radiation and reactive fluid flow solutions, the discrete ordinates method is the method of choice in comprehensive combustion models where thermal radiation has an important role.

In other approximations of the RTE, the radiative intensity is expressed as a series of products of angular and spatial functions. With it, the integral part of the equation can be eliminated and a series of equations in terms of different orders of moments can be generated. A moment is defined as the integral of intensity multiplied by a power of a directional cosine over a predetermined solid angle division. If the angular dependence is expressed using a Taylor power series expansion, then the method is called the moment method, and if spherical harmonics are used to express the intensity, the spherical harmonics (PN) approximation results. The first moment, the first order spherical harmonics (P1), and the S2 discrete ordinates approximation are essentially identical. Applications of the moment method have been discussed by several researchers \[57–60\].

The general equations for the solution of the P1 and P3 approximations for absorbing, emitting, and anisotropically scattering in cylindrical and three-dimensional rectangular enclosures were developed by Menguc and Viskanta \[61, 62\]. The P1 approximation is particularly simple, since it can be cast as a single, second-order differential equation, but this simplicity is at the expense of accuracy. The prediction error can be as large as 50% for media with small optical thicknesses. Finally, combinations of various methods for solving the RTE (described above) have been used to formulate hybrid methods, which attempt to compensate for the flaws of one approach with the strengths of another. Several of these hybrid approaches have been summarized by Viskanta and Menguc \[4\]. As an example of a hybrid approach, the 'discrete transfer' model proposed by Lockwood and Shah \[58\] combines the advantages of the zonal, Monte Carlo, and discrete ordinates methods. Although designed for computing radiation in absorbing, emitting, and scattering media, no results have been reported for scattering in media in multi-dimensional enclosures. This method has been applied in furnace simulations \[63, 64\] and has been adapted for coupling with complex fluid mechanics and heat transfer grid topologies \[65\].

4 Radiation from flames

Although the importance of radiation heat transfer as a flame heat-loss mechanism is recognized, the radiation absorption and nongray radiation models have not been adequately implemented in combustion simulations. It has become almost common practice, mainly due to computational constraints, to assume (often without justification) that the optically thin approximation (OTA) is valid to simulate various laboratory (sooting or nonsooting) flames due to their relatively small optical dimensions \[66\]. In fact, several numerical calculations of such flames using detailed chemistry and the OTA for radiation heat transfer have been performed \[67–72\].
Kennedy et al. [67] developed a model for a laminar soot-laden ethylene diffusion coflow flame and compared it with measurements in sooting and nonsooting flames, studied by Santoro et al. [73]. They incorporated the divergence of the radiative heat flux term in the energy equation and calculated it using an optically thin model for emission from soot alone [74, 75]. They ignored the gas radiation in view of the strong luminosity of the soot particles and compared calculated-temperature values for the nonsooting flame with experimentally obtained data [76]. This comparison shows good agreement at a lower height above the burner. At a large distance above the burner, their model predicts a higher temperature. Since the model considers radiation from only soot, it predicts a smaller radiation loss than if gas radiation had also been included.

Smooke et al. [68] included an optically thin radiation model in their calculations of laminar coflow flames. They assumed that for methane–air mixtures the significant radiating species are H₂O, CO, CO₂, and soot. The OTA method was also employed by Hall [77, 78] whose results predict the general shape and structure of flames (e.g. locations of peak flame temperatures) reasonably well. Temperature is a critical flame parameter since it has a direct influence on virtually all the other flame properties. The Hall model underpredicts experimental measurements along the centerline by about 100 K at all heights within the flame. While the location and value of the peak temperature are reasonably well-described by the model up to a certain height for a flame, temperatures are overpredicted at the outside flame edge (i.e. predicted temperatures do not fall off as rapidly as the data with increasing radius). In addition, the laboratory flame closes to the centerline more rapidly than their model predicts. Figure 1 shows the temperature profiles at different heights in the flame from ref. [68].

![Temperature Profiles](image-url)
One possible explanation for the low centerline temperatures is the lack of inclusion in the model of absorption by methane of the energy radiated from the flame front. This lack of participation by different components induces a smaller radiation loss from the outer surface of the flame. Without this additional radiation component, the predicted peak temperatures are higher by an increment that is large enough to affect predicted soot levels and species concentrations. The significance of thermal radiation in a lightly sooting coflow flame arises from residence times that are relatively long compared to those for counterflow diffusion flames, in which radiation effects are significant only for extremely low strain rates [79].

In nonbuoyant flames, radiation plays an important role since it is the major heat transfer mechanism (in absence of convection). Walsh et al. [71] performed a numerical and experimental investigation of an axisymmetric laminar diffusion flame to assess the role of buoyancy and dilution on various flame properties, such as temperature, fuel, and oxygen concentration, and soot volume fraction. Their predicted temperature profiles are in excellent agreement with measurement in both normal gravity and microgravity flames for low dilution levels. Kaplan and Kailashnath [70] investigated flowfield effects on soot formation in normal and inverse methane–air diffusion flames. Because methane is a relatively low sooting fuel, the radiation transport submodel is based on the simplifying assumption that the medium is optically thin. The absorption coefficient for soot was assumed based on Kent and Honnery [80], while that for CO₂ and H₂O was derived from Magnussen and Hjertager [81]. These were combined to provide an overall Planck mean absorption coefficient.

Microgravity experiments on flame spread over thermally thick fuels have been important for assessments of fire hazards in orbiting spacecraft [82]. Such experiments on flame spread have been conducted over thermally thick foam fuels (that have relatively low densities and thermal conductivities, and thus higher spread rates as compared to dense fuels such as PMMA [83]). These experiments suggest that steady spread can occur over thick fuels in quiescent microgravity environments, especially when a radiatively active diluent such as CO₂ is employed. This is due to the dominance of radiation transfer from the flame to the fuel surface over conduction heat transfer from the flame to the fuel bed. Radiative effects become more significant at microgravity due to a larger flame thickness volume of radiating combustion products.

Liu et al. [84] investigated an atmospheric coflow laminar moderately sooting ethylene-air diffusion flame. They calculated radiation heat transfer using both the optically thin model and the discrete-ordinates method coupled with a SNB model. The radiation source term in the energy equation was obtained using the discrete-ordinates method in an axisymmetric cylindrical geometry as described by Truelove [85]. The J3 quadrature [86] was used for the angular discretization. Spatial discretization of the transfer equation was achieved using the FVM along with the central difference scheme. The SNBCK-based WBM developed by Liu et al. [87, 88] was employed to obtain the absorption coefficients of the combustion products containing CO, CO₂, and H₂O at each wide band. They assumed the spectral absorption coefficient of soot to be 5.5f streamline (f being the soot volume fraction and λ the wavelength). The wide bands considered in the calculations were formed by lumping 10 successive uniform narrow bands of 25 cm⁻¹ to obtain a bandwidth of 250 cm⁻¹ for each wide band. The blackbody intensity at each wide band was evaluated at the band center. The SNB parameters for CO, CO₂, and H₂O were those compiled by Soufiani and Taine [89] based on LBL calculations. At overlapping bands, the approximate treatment based on the optically thin limit developed by Liu et al. [90] was employed. To further speed up the calculations without losing accuracy, the 4-point Gaussian–Legendre quadrature was used to invert the cumulative distribution function to obtain the absorption coefficients based on Liu et al. [91]. The radiation source term was calculated by summing up contributions of all the 36 wide bands (from 150 to 9,150 cm⁻¹) considered in the calculations.
To evaluate the results of the optically thin model using those of the WBM discussed above, numerical calculations were also conducted [84] using the optically thin radiation model. Under OTA, the radiation source term

\[ \tilde{F} = -Cf_T T^5 - k_p 4\sigma T^4, \]  

where \( C \) is a constant that is calculated based on the spectral absorption coefficient of soot, \( \sigma \) the Stefan–Boltzmann constant, and \( k_p \) the Planck mean absorption coefficient of the gas mixture including contributions from CO, CO\(_2\), and H\(_2\)O. The Planck mean absorption coefficients of these three species were calculated based on the SNB model given by Ju et al. [92].

The predicted temperature field with both gas and soot radiation accounted for (using SNBCK) was in qualitative agreement with measurements, as shown in Fig. 2. However, the predicted peak flame and centerline temperatures were more than 100 K lower than the corresponding measured values. In addition, the predicted maximum temperature annulus was found to be thinner than the measurement. The causes of these discrepancies were attributed to the use of a simplified soot model. The peak temperature predicted using the optically thin model was only about 5 K lower than that of the band model. The centerline temperatures were also underpredicted due to neglect of radiation absorption by CO\(_2\) (and to a lesser degree by CO), especially in CO burnout regions just above the flame tip where the concentration of CO\(_2\) is high. The optically thin model underpredicted the temperatures in these regions by more than 50 K compared to the band model. When radiation by gases was neglected, the predicted temperature levels were in reasonably good agreement with experimental values. However, the peak flame temperature was now higher, indicating that radiation by gases is also important and should be accounted for. The results [84] suggest that soot radiation is more important than gas radiation in such a flame, since its inclusion has a greater impact on the predicted temperature distributions. The comparison of measured and predicted soot volume fraction is shown in Fig. 3.

![Figure 2: Comparison of measured and predicted temperature distributions with the peak values indicated. (Reprinted with permission from Elsevier [84]. Copyright 2002 Elsevier.)](image-url)
Sivathanu and Gore [93] investigated the effect of gas band radiation on soot kinetics in a laminar coflow methane-air diffusion flame. The local radiative heat loss fraction was obtained using the solution of the energy equation including soot and gas-band radiation [94]. They concluded that the contribution of the participating gases (CO$_2$ and H$_2$O) dominates the soot radiation by an order of magnitude in their methane/air flames and the local radiative heat loss/gain strongly influences the soot nucleation, formation, and oxidation rates. The measurements and predictions of area-integrated soot volume fractions as a function of axial distance using three different methods of estimating the local temperatures are shown in Fig. 4 from ref. [93]. The calculations are offset by 20 mm so that soot growth starts at approximately the same location for both the measurements as well as the predictions. These three sets of calculations correspond to: (1) a fully coupled calculation where the local temperatures are obtained by considering the local energy loss or gain by radiation from gas molecules and soot particles, (2) an uncoupled calculation where adiabatic flame temperatures are prescribed at all locations as a function of the local mixture fraction, and (3) an uncoupled calculation where the radiative heat loss fraction was assumed to be constant at 19% (close to the experimentally observed value) and temperatures are prescribed at all locations as a function of the local mixture fraction.

Qin et al. [95] characterized gravity and radiation effects on the structure of laminar methane-air partially premixed flames through detailed simulations. They modeled radiation using an optically thin assumption that provides a limiting value for the radiation heat transfer. The overall effect of radiation on the structure of 1-g flame is less significant than for the corresponding 0-g flame. Due to radiation effects, the flame heights of 0-g flames increase, and the heat release rate intensity near the premixed reaction zone tip decreases. When radiation effects are not included in the simulations, the peak temperatures are nearly the same for the 1-g and 0-g flames. With radiation the difference in these temperatures is significant. The decrease in the peak temperature due to radiation for their 0-g flame is nearly five times larger than for the 1-g flame. The value of the radiation loss fraction for 0-g flames without coflow can be as large as 50%, although
it drops significantly in the presence of a coflow. While the flowfields upstream of the inner premixed reaction zone are nearly identical for 1-g and 0-g double flames, they are markedly different in the regions between the two reaction zones as well as downstream of the outer nonpremixed reaction zone. Lock et al. [96] also discussed important aspects of thermal radiation effects in microgravity flames.

Gas radiative properties vary strongly with wavelength so that use of the gray-gas model or the OTA often introduces large errors. Although LBL models provide very accurate results of spectral radiation heat transfer, they are not practical for coupled multi-dimensional calculations of radiation, fluid flow, and chemical reactions due to large computational time required. In the absence of LBL results, results of the SNB model are often sufficiently accurate, even for benchmark solutions for the evaluation of other approximate nongray-gas radiation models. Direct implementation of the SNB model in multiple dimensions is computationally very demanding since it is formulated in terms of the transmissivity instead of the absorption coefficient [97].

Goutière et al. [98] have shown that the SNBCK method is an efficient alternative to the SNB model with essentially the same accuracy. The computational time for the standard SNBCK method (using a bandwidth of 25 cm$^{-1}$ and seven-point Gauss–Lobatto quadrature), though substantially smaller than for the SNB model (6 times), is still quite large, especially in multi-dimensional problems involving two or more radiating gases. In several subsequent studies, Liu et al. [88, 90, 91] considerably improved the computational efficiency of the SNBCK method with only minimal loss of accuracy by developing approximate treatments for overlapping bands, introducing the band-lumping strategy, and using an optimized quadrature set. Band models of different band-widths can be formulated by easily lumping different numbers of narrow bands. In addition, the order of Gauss quadrature used in SNBCK calculations can also be readily changed. The improved SNBCK

Figure 4: Axial variation of the measured and predicted soot volume fraction in a methane/air diffusion flame using different radiation models. (Reprinted with permission from Elsevier Science [93]. Copyright 1997 by The Combustion Institute.)
method also offers greater flexibility to accommodate different levels of compromise between efficiency and accuracy without reformulation of the model. Recently, Goutière et al. [99] proposed the so-called optimized band-lumping (regrouping) strategy based on the four large absorbing bands of CO₂. This band-lumping method offers better computational efficiency than the uniform lumping strategy originally proposed by Liu et al. [87, 100]. The spectral-line-based weighted-sum-of-gray-gases model developed by Denison and Webb [31, 32], though computationally more efficient, can be less accurate than the SNBCK methods in two-dimensional gas radiation calculations [98, 99].

The effects of radiative transfer on the structure and extinction limits of counterflow H₂/O₂/N₂ diffusion flames have been investigated [101]. The radiative properties of the main emitting species, H₂O and OH in these flames were computed using an SNB model. As expected radiative losses decrease the flame temperature and width, and significantly reduce the minor species (such as NO) that are sensitive to temperature. The amplitude of the radiative effects increases with the ratio of the global radiative loss to chemical heat release. Quick estimation of this parameter is useful for determining whether radiative transfer can be neglected in the prediction of small-scale flames. No effect of radiation on the extinction of high-strain rate extinction limit was found in the study, but suggested a value for the radiation-limited extinction for low strain rate flames.

An early review of radiation from turbulent flames [102] suggests that the calculation of thermal radiation in turbulent combustion involves three key factors: the solution of the RTE, the spectral variation of radiative properties, and the evaluation of turbulence–radiation interactions. Because of the inherent difficulties in radiation calculations, the common practice for turbulent flames has been to neglect turbulence–radiation interactions and to use the OTA or a gray-medium assumption, even for luminous sooting flames [103–105]. Although the OTA is useful, its application produces errors, since it neglects self-absorption effects [106, 107]. Radiation, along with soot, is such a complex and nonlinear phenomena that gray or OTA models generally are inadequate to describe it, particularly in oxygen-enriched flames. Wang et al. [108] implemented two radiation models with self-absorption effects (one that accounts for nongray-gas properties and the other that does not) for an oxygen-enriched, propane-fueled, turbulent, nonpremixed jet flame.

One important aspect for combustion studies is the prediction of radiative transport due to particles and gases within flames. The RTE is generally used to solve for the radiative heat transfer in a semi-transparent media. In order to make proper calculations, information regarding the radiative properties of the medium must be calculated. Soot, or the polycyclic aromatic hydrocarbon particulates formed during coal combustion, can be a major contributor to radiative transport. Some calculations indicate that soot can contribute as much as 15% to the total radiative flux [109]. Other research indicates that temperature predictions in certain combustor locations can vary by as much as several hundred kelvin based on the inclusion of soot predictions [110, 111]. While this may not be important for the overall energy balance in a combustor, it could be significant for pollutant calculations. Minor changes in temperatures can make a substantial impact on pollutant formation predictions, which tend to be highly temperature-dependent. Since the near burner region is of great interest for pollutant prediction calculations (and also tends to be the region of maximum soot concentration), predicting the radiative contribution of soot becomes even more important.

Adams and Smith [110] developed a simple empirical model for turbulent soot formation that related the soot volume fraction to the local equivalence ratio. Soot was assumed to exist where the local equivalence ratio was unity and above, increasing linearly to a maximum value at an equivalence ratio of 2.0 and above. The maximum soot concentration value was calculated as a
direct function of the amount of volatile carbon calculated to exist at that point. The soot volume fraction was then related to the radiative properties. They concluded that the inclusion of a soot radiation model increases predicted radiative transfer; however, the maximum local temperature difference between predictions with and without the soot model was lower than expected (about 50 K). Ahluwalia and Im [109] developed a similar model, and reported that soot significantly enhanced the radiative heat transfer. Both models use an empirical survivability constant of 0.1 which serves to reduce the predicted soot concentrations. A detailed discussion on coal combustion and gasification can be found in ref. [112]. Another important aspect is study of the flames immersed in porous media. There are many interesting radiation problems in such system. Interested readers can consult the excellent review paper by Howell et al. [113].

5 Radiation from fires

Two types of fire analyses are mainly found in the fire safety literature: for compartment fires (also called enclosure fires) and for outdoor fires (such as forest or wildland fires). Although thermal radiation plays a significant role in these phenomena, radiative mechanisms are often only grossly accounted for in the associated models [3]. Fire simulations use fluid dynamic models for chemically reacting and radiating flows. Due to the complexity of the phenomena, fire modeling has been carried out with different degrees of simplification ranging from strictly empirical models to correlations that are variously based on dimensional analysis, semi-empirical models, and theoretical models.

The trend in fire simulations is to use software packages based on CFD codes for chemically reacting flows. A number of fire simulation codes were developed in the 1980s of which some are based on commercially-available codes [114, 115]. In fire modeling, the spread of heat and smoke in a complex geometry is required. The complex structure of the combustion products, composed of molecular gases and soot particles, makes the treatment of radiative transport very difficult. Hence, researchers initially used grossly simplified models for combustion and/or radiation [116].

The fire dynamics simulator (FDS) is most popular among these codes. It uses the large eddy simulation (LES) FVM with improved radiation and combustion models [117−119]. An FVM submodel solves the RTE by using a narrow band gas radiation model (RADCAL). There have been many enhancements to RADCAL after its earlier development, e.g. Fuss et al. [120, 121] incorporated high temperature flammable gases into RADCAL.

A more sophisticated radiative submodel is available in the JASMINE code [114], which is based on the discrete transfer method (DTM) combined with a simplified model of gas radiative properties. The radiation model works in conjunction with a SIMPLE pressure correction algorithm and the standard $k−\varepsilon$ method to compute turbulence. The simulation of fires in enclosures (SOFIE) code was developed to predict fire propagation in enclosures [122]. It uses either a gray six-flux algorithm or a DTM combined with a WSGG to solve the RTE [123].

A Monte Carlo solution method for the gray-formulated RTE has been implemented in a 3D CFD model to investigate compartment fires. Consalvi et al. [124] developed a CFD FVM code to simulate fires in enclosures with internal obstacles or partitions. They used a modified Chai et al. blocked-off discrete ordinates model [56] to solve a gray formulation of the RTE. The FDS code has also been used recently with some modifications in the combustion and soot models [125] and by incorporating the computation of the radiative flux emitted towards the fuel surface and upstream of it [126].

The structure of soot and its radiative properties are important parameters for analyses of fires. These radiative properties have been extensively investigated by Faeth and coworkers in the
context of fire modeling [127–131]. The work by Sivathanu et al. [132] on the in situ determination of the absorption coefficient of soot particles represents another contribution. The estimation of optical and radiative properties of soot can be carried out using the Rayleigh–Debye–Gans theory for fractal aggregates with acceptable accuracy [133].

Gas radiative properties are also important parameters for fire modeling. The use of LBL calculations is formidable for fire applications since the absorption spectra of most combustion gases contain a large number of spectral lines for evaluating gas radiative properties. Modak [134, 135] proposed a method for computing gray gas radiative properties for isothermal, homogeneous mixtures of carbon dioxide, water vapor, and soot. This method is popular due to its simplicity and reasonable accuracy and is still being used in a number of fire simulation codes. Since the isothermal assumption is not valid in large-scale fires, Modak’s model might not provide highly accurate results for such cases [136]. Grosshandler [137] proposed remedial corrections to Modak’s simplified method and suggested an SNB model based upon the Goody approach [15] and the Curtis–Godson approximation to deal with nonhomogeneous effects. His code uses the data of Ludwig et al. [18] and the parameters for the primary infrared bands of water vapor and carbon dioxide are computed according to Malkmus [138, 139].

Grosshandler’s SNB approach used in conjunction with the DTM were recently evaluated together with three other gas radiative property models, Modak’s approach [135], Truelove’s mixed gray gas model [85], and Edward’s WBM [24]. The test cases were an idealized 1D case with parabolic profiles of temperature, CO₂, and H₂O concentrations, and two experimental cases, i.e. a laboratory-scale flame and a field-scale natural gas jet fire [140]. The comparison in terms of radiative fluxes shows a satisfactory level of agreement. However, the performances of all models are diminished when compared to the narrow band model while dealing with complex non-Cartesian meshes. Encouraged by this, researchers have developed ‘fast narrow band models (FASTNB)’ [141, 142]. Used in conjunction with the DTM, FASTNB [143] is 20 times faster than RADCAL for comparable results (and deviations smaller than 1%).

Other useful alternatives to SNB approaches that are based on the absorption coefficient concept are the WSGG model, CK model, and their recently improved versions (SLW, ADF, ADFFG, FSCK). Detailed presentations of these models can be found in Modest [7]. Most of these predict small/medium scale fire behavior (like that of compartment fires) satisfactorily. The large number of grid points required for large/outdoor fires requires a large amount of computational time and this, in turn, limits the complexity of the radiation model that is employed [144]. Discrete Transfer Models are therefore less attractive to solve the RTE for large fires and thus simplifications are required in the associated radiation models. Usually, the radiation models employed in case of large fires are gray and scattering is generally neglected [3].

An overview of the recent research on wildland and forest fires has been provided by Albini [145] and regarding which Grishin and coworkers have made noteworthy contributions [146–148]. Radiation has been unsurprisingly identified as the controlling heat transfer mechanism that fixes the rate of spread of wildland fires [149–153]. Fire growth models are now being used in campaign fire strategic planning. Research is also being performed to develop a gray nonscattering DOM for solving the RTE and couple it to a CFD model for wildland fire propagation [154, 155].

Research is also focused on developing radiation models to simulate fire spread in urban areas. Mainly due to the complex geometries, most such models are zonal. Radiative transfer is approximated by means of gray gas, gray surface emissivities, and radiative exchange areas or view factors between the cells [156]. The urban–wildland interface fire is another subject of concern. Again, radiative transfer is mostly treated through rough simplified models. Predictions of the impact of fire on structures in the urban–wildland interface have been obtained using sophisticated simulation
tools, such as DOM with SLW or gray nonscattering gas models, that have been coupled with CFD codes [157, 158]. The gray gas model (as compared to SLW) has been found to be reasonably accurate. On the other hand, savings in computational time (six times faster than SLW) allow the use of this model as a fire operational tool [157, 158]. Simeoni et al. [159] reached a compromise between rapidity and accuracy, by developing a semi-physical model of fire spread across a fuel bed, which is unsteady and two-dimensional along the ground shape. In this model, they assumed that radiation is the prevailing heat transfer mechanism involved in fire spread [160]. Nevertheless, it was unable to correctly predict the high wind effects on the rate of spread.

6 Summary

Thermal radiation is an important and often dominant heat transfer mode during many combustion processes. However, the complexities of the RTE and the associated radiative properties have made the modeling effort quite challenging. Among the different gas property models, the LBL method makes computations time intensive and it is therefore mainly used to obtain benchmark results. Global models are very popular for their simplicity and acceptable accuracy. However, a compromise between the two can be found in spectral band models and their different variations which have found extensive use by the researchers.

The radiative and optical properties of entrained particles (like soot or ash) play an important role during combustion. These properties are usually found using the Mie theory which, however, is not valid for particle aggregates. Hence other theories such as the Rayleigh–Debye–Gans theory are employed to describe the radiative properties of particulate aggregates.

Various types of solution methods are used to solve the integro-differential RTE. It is not possible to develop a single solution method that is equally applicable for different systems. Therefore, several solution methods (with varying degrees of approximation) have been developed and can be applied according to the nature of the physical system, characteristic of the medium, the degree of accuracy required, and the availability of computer facilities.

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