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Computation of radiative transfer in combustion systems

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Abstract

Purpose – This paper seeks to review the literature on methods for solving the radiative transfer equation (RTE) and integrating the radiant energy quantities over the spectrum required to predict the flow, the flame and the thermal structures in chemically reacting and radiating combustion systems.

Design/methodology/approach – The focus is on methods that are fast and compatible with the numerical algorithms for solving the transport equations using the computational fluid dynamics techniques. In the methods discussed, the interaction of turbulence and radiation is ignored.

Findings – The overview is limited to four methods (differential approximation, discrete ordinates, discrete transfer, and finite volume) for predicting radiative transfer in multidimensional geometries that meet the desired requirements. Greater detail in the radiative transfer model is required to predict the local flame structure and transport quantities than the global (total) radiation heat transfer rate at the walls of the combustion chamber.

Research limitations/implications – The RTE solution methods and integration of radiant energy quantities over the spectrum are assessed for combustion systems containing only the infra-red radiating gases and gas particle mixtures. For strongly radiating (i.e. highly sooting) and turbulent flows the neglect of turbulence/radiation interaction may not be justified.

Practical implications – Methods of choice for solving the RTE and obtaining total radiant energy quantities for practical combustion devices are discussed.

Originality/value – The paper has identified relevant references that describe methods capable of accounting for radiative transfer to simulate processes arising in combustion systems.

Keywords Heat transfer, Combustion chambers

Paper type Literature review

Nomenclature

$\mathscr{F}$	= radiation flux vector, equation (3)
G	= irradiation, equation (12)
$\mathscr{G}$	= irradiance, equation (4)
g	= asymmetry factor
I	= intensity of radiation (radiance)
I_b	= Planck's function for blackbody radiation
$\mathbf{r}$	= position vector
$\mathbf{s}$	= direction vector
T	= temperature
x, y, z	= coordinates
$\tilde{\beta}$	= effective extinction coefficient, equation (7)
ε	= emissivity
κ	= absorption coefficient
σ	= scattering coefficient

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Ω	= solid angle	*Subscripts*	
$\Delta\Omega$	= solid angle increment	b	= refers to blackbody
ω	= single scattering albedo, $\sigma/(\kappa + \sigma)$	i	= refers to direction i
		m	= refers to direction
Φ	= scattering distribution function	λ	= refers to wavelength

1. Introduction

Thermal radiation plays an important role in thermal and combustion engineering. This is especially true for applications involving high-temperature chemically reacting flows where radiation can dominate the total energy transfer in the system. A combustion device is a concrete example where one typically needs to calculate the flame structure and heat transfer in the system in multiple dimensions systems. For such a purpose one must determine the radiation field and calculate the radiant flux divergence (i.e. radiation sources/sinks) in the thermal energy equation. The calculation of the radiant energy quantities is coupled to the transport equations for the momentum, energy and species concentration distributions (Khalil, 1982; Tsuji *et al.*, 2003; Baukal *et al.*, 2001). The current environmental and global warming concerns are driving technology to reduce combustion generated pollutant emissions (i.e. NO_x, SO_x, ozone, smog, etc.) and to increase energy efficiency. Increase in heat extraction from the flame, increase in heat transfer from the flame to the load, and decrease and/or complete elimination of greenhouse gas emissions to the atmosphere is a grand challenge for the twenty-first century. The goal of fossil fuel combustion research and development is to create combustion technology options that can mitigate adverse atmospheric climate changes, reduce pollutant emissions, and simultaneously increase fossil fuel utilization efficiencies.

Today's engineers/scientists are confronted with complex combustion phenomena that depend on interrelated processes of thermodynamics, chemical kinetics, fluid mechanics, heat and mass transfer, turbulence and radiative transfer. Computational fluid dynamics (CFD) tools are needed to help understand, design, optimize and operate high-temperature combustion devices where radiative transfer is an important mode of energy transport. Owing to the nature of the radiative transfer equation (RTE) such CFD computations are very time-consuming, because there is a need to integrate the radiation field (intensity) over all directions and the entire spectrum. Research efforts have been under way for the past several decades to make the computations more efficient and cost effective so that computational fluid dynamics tools could be used to perform design and optimization calculations.

During the last several decades considerable progress has been made in predicting radiative transfer in multidimensional "enclosures" containing absorbing, emitting and scattering media such as mixtures of gases and gases/polydisperse particles. Because the RTE is similar to the equations used for simulating neutron transport and flow of rarified gases, researchers have often adopted and assimilated the methods developed by scientists in these fields to solve radiation heat transfer problems encountered in thermal/combustion systems. These developments are summarized in graduate level textbooks on radiation heat transfer (Siegel and Howell, 2002; Modest, 2003) and in reviews (Viskanta and Mengüç 1987; Carvalho and Farias, 1998). The emphasis in this paper is on methodologies for predicting radiative transfer in multidimensional combustion systems that are compatible with CFD methods for solving the transport equations, recognizing the fact that the divergence of the radiative flux vector (i.e. radiant energy source/sink term) may account for the major computational effort.

When calculating radiation heat transfer in a combustion device, probably the first and most important decision one has to make is about the choice of the radiative transfer model, which is dictated by the specific application and the level of detail needed to analyze the problem. For example, the level of detail required to determine the local temperature and species concentration distributions in a flame is much greater than that required to calculate the local radiant heat flux on a load in a furnace or on the furnace wall. Next, one must decide if detailed spectral calculations of radiation transport is warranted or some approximate band model or gray treatment of radiative transfer will be adequate. One must also choose a numerical method for solving the RTE that is compatible with the technique employed for solving the transport equations. Finally, the model should also be accurate, robust and predict the desired radiant energy quantities in a computationally efficient manner.

A review is presented of the methods for predicting local radiative transfer in multi-dimensional combustion systems. Previous reviews (Viskanta and Mengüç 1987; Carvalho and Farias, 1998) are updated and both methods for solving the RTE and for integrating spectral results to obtain local radiative fluxes and flux divergences on the total (global) basis are examined. The advantages and disadvantages of the different methods are discussed, but the focus is on approaches which are practical for use with presently available computer resources. Where possible, the predictions are compared against benchmark results and relative CPU needs are discussed.

2. Conservation of radiant energy equations

The RTE is a mathematical statement of the conservation of spectral radiant energy applied to a solid angle $\mathrm{d}\Omega$ of radiatively participating (i.e. absorbing, emitting and scattering) medium propagating in a given direction $\mathbf{s}$. Radiation traversing along a path is attenuated by absorption and scattering and is enhanced by emission and by in-scattering from all other directions. The RTE for a moving medium has been given in its most general form (Mihalas and Klein, 1982). In the absence of turbulence/radiation interaction and the purposes of this discussion, it is adequate to focus on the following form of the time-independent, incoherent scattering RTE (Modest, 2003; Viskanta and Mengüç 1987) for radiative transfer calculations in engineering systems:

$$s \cdot \nabla I_\lambda(\mathbf{r}, \mathbf{s}) = -(\kappa_\lambda + \sigma_\lambda) I_\lambda(\mathbf{r}, \mathbf{s}) + \kappa_\lambda I_{\mathrm{b}\lambda}(\mathbf{r}) + \frac{\sigma_\lambda}{4\pi} \int_{\Omega'=4\pi} I_\lambda(\mathbf{r}, \mathbf{s}') \Phi_\lambda(\mathbf{s}' \rightarrow \mathbf{s}) \mathrm{d}\Omega' \quad (1)$$

where I_λ $(\mathbf{r},\mathbf{s})$ is the spectral intensity of radiation (radiance) at location $\mathbf{r}$ in direction $\mathbf{s}$. The scattering phase function $\Phi_\lambda(\mathbf{s}' \rightarrow \mathbf{s})\mathrm{d}\Omega'/4\pi$ represents the probability that radiation propagating in direction $\mathbf{s}'$ and confined in the solid angle $\mathrm{d}\Omega'$ is scattered into direction $\mathbf{s}$ confined to solid angle $\mathrm{d}\Omega$. The first term on the right hand side of equation (1) accounts for loss of radiant energy by attenuation (absorption plus scattering), the second for gain by emission and the last term gain of energy by in-scattering, the second for emission and the third for in-scattering.

Integration of equation (1) over all directions ($\Omega = 4\pi$) results in:

$$\nabla \cdot \mathscr{F}_\lambda = \mathscr{E}_\lambda = \kappa_\lambda (4\pi I_{b,\lambda} - \mathscr{G}_\lambda) \quad (2)$$

where the radiation flux vector $\mathscr{F}_\lambda$ is defined as:

$$\mathscr{F}_\lambda(\mathbf{r}) = \int_{\Omega=4\pi} I_\lambda(\mathbf{r}, \mathbf{s}) \mathbf{s} \mathrm{d}\Omega \quad (3)$$

and the spectral irradiance $\mathscr{G}_\lambda$ is defined as:

$$\mathscr{G}_\lambda(\mathbf{r}) = \int_{\Omega=4\pi} I_\lambda(\mathbf{r}, \mathbf{s}) \mathrm{d}\Omega \tag{4}$$

The right-hand-side of equation (2) represents net (emission minus absorption) rate of loss or gain of radiant energy by the matter per unit volume in the spectral interval λ and $\lambda + \mathrm{d}\lambda$. The term $4\pi\kappa_\lambda I_{\mathrm{b}\lambda}(T)$ accounts for the local rate of emission, and $\kappa_\lambda \mathscr{G}_\lambda$ represents the local volumetric rate of absorption of radiation. The meaning of the terms can be further clarified when we note that the term $4\pi I_{\mathrm{b}\lambda}(T)$ is the product of the spectral radiant energy density of a black body at the local temperature times the local velocity of light c, while the spectral irradiance $\mathscr{G}_\lambda$ is related to the local radiant energy density of space defined by equation (4). Equation (2) is the conservation equation of spectral radiant energy. Note that the scattering terms have cancelled out. This just confirms the physical fact that scattered energy is not stored and should not appear in the equation. The right-hand side of equation (2) represents the net volumetric rate of loss/gain of radiant energy from an element of matter per unit volume in the wavelength interval λ and $\lambda + \mathrm{d}\lambda$.

Integration of equation (2) over the entire spectrum ($0 < \lambda < \infty$) results in the conservation equation of total (global) radiant energy:

$$\nabla \cdot \mathscr{F} = \int_0^\infty \kappa_\lambda [4\pi I_{\mathrm{b}\lambda}(T) - \mathscr{G}_\lambda] \mathrm{d}\lambda \tag{5}$$

Note that there is no convective term in equation (5) since radiation propagates independently of the local material velocity (Mihalas and Klein, 1982). The divergence of the radiation flux vector ($\nabla \cdot \mathscr{F}$) must be included in the thermal energy equation for calculating the velocity, temperature and species concentration fields in a moving medium (Khalil, 1982; Tsuji *et al.*, 2003; Baukal *et al.*, 2001; Siegel and Howell, 2002; Modest, 2003). It is the calculation of this source/sink term that presents major computational difficulties in predicting the flame structure and the performance of combustion systems.

Calculation of radiative transfer requires two types of models:

(1) models to account for directional nature of radiation; and

(2) models to describe the spectral nature of radiation.

Since, the directional and spectral models are not coupled or directly related, they can be discussed separately. Numerous approaches for both types of models have been proposed, and they will be divided into several groups for more logical and coherent discussion.

3. Solution methods

3.1 Overview of computational methods in radiative transfer

Integral formulations and exact solutions for multidimensional geometries have been reported in the literature (Dua and Cheng, 1975; Crosbie and Schenker, 1982; Crosbie and Farrell, 1984); but for most systems in which accounting of spectral effects is desired, exact integral solutions of RTE are not practical for engineering applications. Consequently, it is necessary to make simplifications before attempting to solve the RTE

and calculate the local radiant energy quantities. During the last four or so decades numerous methods have been developed and reviews are available (Modest, 2003; Viskanta and Mengüç 1987; Carvalho and Farias, 1998). This account is an update an earlier review (Viskanta and Mengüç 1987) that is specifically focused on radiative transfer in combustion systems that can handle multidimensional geometries.

The past approaches for calculating radiative transfer in multidimensional geometries can be grouped into four broad categories (Figure 1):

(1) directional averaging approximations;

(2) differential approximations (moment, modified moment, spherical harmonics, etc.);

(3) energy balance (zone, Monte Carlo, finite volume, finite element, boundary element, etc.) methods; and

(4) hybrid (discrete transfer, zone-Monte Carlo, ray tracing, etc.) methods.

The asymptotically thin and thick approximations are simple (Siegel and Howell, 2002; Modest, 2003), but unfortunately their range of validity are very limited; therefore, only the general optically selfabsorbing situations are considered here.

All of the directional averaging approximations involve some type of averaging of the radiance field with direction. The two-, four-, six-, and multi-flux methods (MFM) are probably the simplest to apply. They have been reviewed in some detail elsewhere (Viskanta and Mengüç 1987; Carvalho and Farias, 1998). The shortcomings of MFMs are primarily twofold. First, the accuracy of the predictions depend on the arbitrary choice of the solid angle subdivision over which the intensities are integrated to obtain the fluxes. Second, the fluxes for one direction are not coupled with those of another direction if the medium is not scattering. The MFMs have been popular three and four decades ago, and four- and six-flux approximations have been used to model axisymmetric and rectangular furnaces (Richter and Quack, 1973; Lowes *et al.*, 1973; Patankar and Spalding, 1973; Siddall and Selcuk, 1979). Since, they usually suffer from poor accuracy, use of the methods will not be considered further.

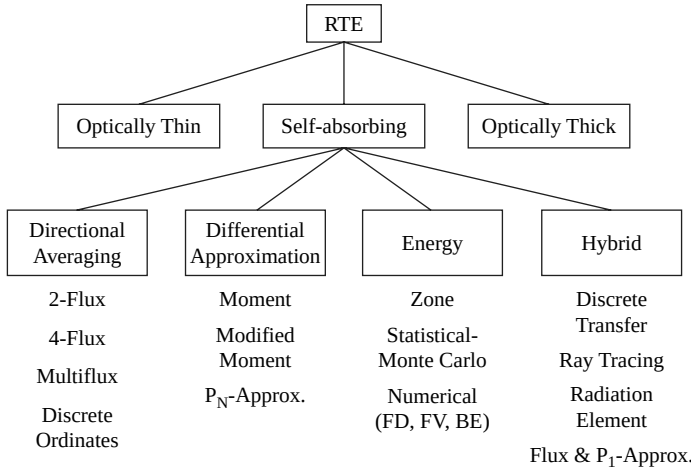


Figure 1.
Solution methods for the RTE

The first order differential approximations of the RTE (moment and spherical harmonics) are capable of treating radiatively participating media with scattering (Viskanta and Mengüç 1987). They yield radiative transfer predictions of reasonable accuracy and can be adopted for band calculations. The discrete ordinates method (DOM) for approximating the RTE and the finite volume method (FVM) for solving the RTE numerically are compatible with CFD methods for solving transport problems in combustion systems.

Energy balance methods such as the zone method (ZM) and its extensions as well as the boundary element method (BEM), which can be considered as a variant of the ZM, require exceedingly large storage for the local exchange factors if the methods are to be used to calculate the local quantities. The method is suitable for calculating heat fluxes or global heat transfer rates in a furnace if the temperatures and radiating species concentrations are known. The disadvantage of the ZM and BEM solvers is the difficulty of generating fine meshes in regions of large temperature and species concentration gradients (i.e. flame structure) as well as the difficulty in evaluating integrals whose integrands are singular. The statistical Monte Carlo method (MCM) is incompatible with CFD procedures for solving the transport equations (Baukal *et al.*, 2001; Viskanta and Mengüç 1987). Therefore, the ZM, BEM and MCM approaches are not discussed.

The discrete transfer method (DTM) is considered a hybrid method because it is derived from the combination of flux methods and the MCM for choosing the finite number of directions of the RTE (Carvalho and Farias, 1998). The method is well suited for CFD calculations. The disadvantages of the other hybrid methods are the same as those of the energy balance methods.

In summary, only the differential method based on the P_1-approximation, the DOM, the DTM, and the FVM are discussed. This is owing to the fact that these approaches are compatible with CFD procedures for solving the transport equations, can be adopted for complex multidimensional geometries, can be adopted for band calculations and do not demand excessive computer resources.

The most accurate modeling of radiative transfer for computation of local radiative flux vector and local volumetric radiant energy heat source/sink for laboratory or industrial combustion applications in 3D complex systems is the line-by-line (LBL) approach (Modest, 2003). Unfortunately, this approach requires too much computational time and storage, and so approximate models are needed, particularly for combustion applications involving the solution of coupled momentum, energy and species conservation equations. The less detailed models such as the statistical narrow band (SNB), the wide band (WB), the spectral line-based weighted-sum-of-gray-gases (SLW), the spectral group (SGM) and the weighted-sum-of-gray-gases (WSGG) models, and other approaches are briefly considered.

3.2 Differential (diffusion) approximation of RTE

Expression of the radiance in terms of spherical harmonics and associated Legendre poly-nominals results in a differential approximation of the RTE (Case and Zweifel, 1967). It is an elegant method that has a sound mathematical foundation. The method has been first introduced to solve radiative transfer problems in planetary atmospheres (Chandrasekhar, 1960) and then adopted for the solution of the Boltzmann equation for neutron transport (Davidson, 1958). The P_n-approximation is obtained from taking moments of the RTE. This yields a system of equations with the angular dependence

removed from each of them. The P_n-approximation results in a system of n^2-equations. For example, the P_1-approximation results in a single equation (diffusion approximation), while the P_3-approximation requires a solution of nine equations.

The P_3-approximation is rather cumbersome and does not yield improved results; therefore, only the P_1-approximation for the RTE is discussed here, with the details of the derivation omitted. The irradiance $\mathcal{G}$ is determined from the equation (Mengüç and Viskanta, 1985):

$$\nabla \cdot \left[\left(\frac{1}{3\tilde{\beta}} \right) \nabla \mathcal{G} \right] = -\kappa [4\pi I_b(T) - \mathcal{G}] \tag{6}$$

where $\mathcal{G}$ is the zeroth-order moment of intensity, and $\tilde{\beta}$ is the effective extinction coefficient:

$$\tilde{\beta} = \kappa + \sigma(1 - g) \tag{7}$$

with g being the asymmetry factor. In writing equation (6) the delta-Eddington approximation was employed for the scattering phase function (Mengüç and Viskanta, 1985). The subscript λ used to characterize spectral quantities has been omitted for the sake of simplicity but is implied. Other phase function approximations yield a similar equation.

The elliptic partial differential equation for the irradiance $\mathcal{G}$ (sometimes (Modest, 2003) called the Helmoltz equation) requires a single boundary condition everywhere on the "enclosure" wall. The Marshak boundary condition can be expressed as:

$$-\frac{2(2-\varepsilon)}{\varepsilon} \left(\frac{1}{3\tilde{\beta}} \right) \mathbf{n} \cdot \nabla \mathcal{G} + \mathcal{G} = 4\pi I_b(T_w) \tag{8}$$

where ε is the emissivity and T_w is the temperature of the chamber wall.

The first order spherical harmonics P_1-approximation is one of the most simple RTE models since it can be cast into a single second-order partial differential equation. In general, it does not yield accurate predictions of the radiative flux ($\sim$50 percent) for small optical dimensions. It is also possible to improve the accuracy of the approximation by obtaining the moments of radiation intensity in half or quarter spheres (Wilson and Sen, 1986). Since, the angular variation of moments is allowed for in this method, the anisotropy of the radiation field can be modeled more accurately than by the P_1-approximation. An improvement of the P_1-approximation can be obtained by defining moments not in the entire solid angle range but within predetermined solid angle divisions (Iyer and Mengüç 1989; Carlson and Lathrop, 1968). In this approach, the number of resulting moment equations is proportional to the number of solid angle divisions used.

3.3 Discrete ordinates method

The DOM is also in a way a MFM, but is considered separately because of its importance. The method does not require any assumptions concerning the directional dependence of the intensity. It was originally suggested by Chandrasekhar (1960) for astrophysical applications, and detailed derivation of the relevant model equations were discussed in application to neutron transport (Davidson, 1958; Carlson and Lathrop, 1968; Lewis and Miller, 1984) problems. The method has been applied to solve

radiation heat transfer problems (Viskanta and Mengüç 1987; Carvalho and Farias, 1998), including those arising in combustion systems. Currently, there are two types of RTE used in DOM. One is the conventional approach which approximates the RTE by a system of first-order ordinary differential equations (Carlson and Lathrop, 1968), and the other is the even parity formulation (EPF-DOM) which is a second-order partial differential equation (Cheong and Song, 1995). The approximation is obtained by discretizing the entire solid angle ($\Omega = 4\pi$) using a finite number of ordinate directions and corresponding weight factors. The RTE is written for each ordinate, and the integral terms are replaced by a quadrature summed over each ordinate.

A simpler but more accurate version of this method obtained later using Gaussian or Lobatto quadrature is called the S_n-approximation (Lewis and Miller, 1984). The approximation was obtained by dividing the spherical space into N equal solid angles or $N(N+2)$ angular subdomains, where N is determined by the order of quadrature scheme used. For axisymmetric systems the number of angular subdivisions required is reduced by a factor to be uniform within each of these angular domains whose extent is determined by the weights of the quadrature scheme employed. The S_n approximation denotes the discrete ordinates in that there are N discrete values of direction cosines (ξ_n, η_n, μ_n), which always satisfy the identity $\xi_n^2 + \eta_n^2 + \mu_n^2 = 1$.

As a concrete example, the RTE for a 3D enclosure in Cartesian ordinates is written for each quadrature point n as:

$$\xi_m \frac{\partial I_m}{\partial x} + \eta_m \frac{\partial I_m}{\partial y} + \mu_m \frac{\partial I_m}{\partial z} = -(\kappa + \sigma) I_m + \kappa I_b(T) + \frac{\sigma}{4\pi} \sum_{m'=1}^{N} w_{m'} \Phi(m', m) I_{m'} \quad (9)$$

where μ_m, η_m *and* ξ_m represent direction cosines for the discrete angular direction $\mathbf{s}_m$; $w_{m'}$ is the angular (Gaussian) weights associated with the $\mathbf{s}_{m'}$ direction, and the summation is over the total number of discrete angular directions, N, used in the approximation. Appropriate boundary conditions need to be imposed to complete the mathematical statement of the problem. If a surface bounding the medium, say, at $x = 0$ emits and reflects radiation diffusely, then the boundary condition for equation (9) is given by:

$$I_m = \varepsilon I_b + \left(\frac{\rho}{\pi}\right) \sum_{m'=1}^{M} w_{m'} |\mu_m| I_{m'}; \quad \mu_m > 0 \quad (10)$$

where ε is the emissivity and ρ the reflectivity of the surface. Similar expressions can be written for the other five surfaces in the 3D enclosure.

A comprehensive state of the art review of numerical methods for solving the DOM approximation equations has been prepared (Balsara, 2001). A large number of numerical schemes for solving the DOM equations has been critically reviewed and their advantages and disadvantages discussed. Methods for increasing the rate of convergence such as total variation diminishing, transport synthetic approximation, mesh rebalance, second order accurate schemes, etc. are discussed. Balsara (2001) has concluded that the first-order schemes (Jesse *et al.*, 1998; Howell *et al.*, 1999) may be unsuitable for general-purpose use. They converge fast but are extremely diffusive. The second-order accurate discretizations that have been tried (Fiveland, 1988; van Leer, 1974) have poor convergence characteristics.

Finite-differencing of equation (9) over a control volume has been carried out using a second-order CLAM discretization method (van Leer, 1974; Jesse and Fiveland, 1997). The scheme is significantly more accurate and robust than the STEP scheme and is free of spurious oscillations and negative intensities. The intensity at the downstream cell faces are calculated according to the CLAM scheme (Khosla and Rubin, 1974) using the intensities computed at the previous iteration for downstream grid nodes and at the current iteration for upstream nodes. The STEP scheme (Jesse and Fiveland, 1997) is recovered if the deferred correction term is set to zero. The solution algorithm and calculation of fluxes and flux divergence follows standard practice (Jesse and Fiveland, 1997).

DOM has received considerable development and application for gray (Fiveland, 1988; Jesse and Fiveland, 1997; Fiveland, 1984) and non-gray (Fiveland and Jamaludin, 1991; Park *et al.*, 1999; Coelho, 2002; Joseph *et al.*, 2003) media confined in multidimensional enclosures. For example, in a recent study (Harmandr and Selçuk, 2004) DOM has been used to solve the RTE and predict radiative heat transfer in a cylindrical enclosure containing an absorbing-emitting medium. Three upwind and two downwind differencing schemes were implemented and tested for predictive accuracy. The method was applied to two test problems:

(1) cylindrical enclosures with black and gray walls; and

(2) a gas turbine combustor simulator.

Comparisons of the results show that accurate predictions of incident radiant heat fluxes can be made with the method of lines. In a recent computational study (Joseph *et al.*, 2003), the standard DOM has been extended to unstructured meshes in order to facilitate coupling with a CFD code for complex geometries. The computer program has been especially written for unstructured grids using tetrahedral cells, and the results are compared with those obtained with an accurate ray-tracing method.

The even parity DOM was originally applied for the solution of neutron transport problems, and the formulation was first adopted by Song and Park (1992) for radiative transfer. They transformed the RTE into a set of second-order parabolic partial differential equations. Later Cheong and Song (1996) developed and critically assessed various solution schemes and recommended the exponential scheme with cubic interpolation method. Fiveland and Jessee (1995) compared the even parity results with other solutions for different cases and found that the accuracy of the EPF-DOM predictions degraded as the optical dimension and the wall emissivity were increased. Koch *et al.* (1996) applied the parabolic formulation of DOM to treatment of complex geometries and found ray effects to be present in even parity DOM and directional biasing still existed. The findings of Koo *et al.* (1997) were somewhat disappointing. The conventional DOM yielded more accurate results than EPF-DOM for most of the optical dimensions, the number of grids and the ordinates tested.

The DOMs are better than the intuitive MFMs which usually cannot couple angular divisions adequately. In general, the approximation yields acceptable results with increasing number of directions considered. However, if there are strong local sinks and/or sources (i.e. flame), then the ray effects would begin to affect the accuracy of the results (Iyer and Mengüç 1989). Even with the increasing order of the approximation, the ray effects show an oscillatory behavior in the boundary fluxes. The conventional primitive variable DOM approximation solutions compare better with the exact

solutions than the EPF-DOM, and the control volume-based finite element approaches are recommended since they can be applied to complex geometries. In a recent comprehensive study Koch and Becker (2004) evaluated the presently available quadrature schemes for the DOM. The error analysis showed that among the schemes examined, the highest accuracy was obtained with the LC-11 (Chebyshev type) quadrature which requires 96 discrete ordinates. This scheme is rarely used but should be considered for high accuracy (benchmark) predictions of radiative transfer.

Very recently a domain decomposition paradigm has been applied to solve the DOM-based RTE on parallel computers (Krishnamoorthy *et al.*, 2005). Mathematical libraries developed by others are used to solve the matrices that result during the procedure. Numerical experiments have been performed to compare the performances of different techniques and preconditioners for solving the matrix systems. Time taken to solve the differential form of the RTE using 1 and 125 processors are compared, and numerical experiments helped to identify regions of the solution procedure that consumed the most computational time.

3.4 Discrete transfer method

The DTM is based on the solution of the RTE along specified directions (Lockwood and Shah, 1981). The method is derived from the combination of flux methods and the MCM is well adopted for CFD calculations. Instead of choosing the direction of the originating intensities (i.e. due to emission, reflection or scattering), they suggested a deterministic approach. The physical domain is subdivided into isothermal control volumes and surface elements having constant radiation properties. The RTE is integrated analytically and is solved iteratively along an arbitrary chosen direction (path). The ray is traced along its way until the first boundary is encountered. The intensity at its starting point, say, at a boundary, is assumed and is determined at every point in each direction until the intersection of the ray with the boundary. Solution of the RTE gives the value of the local intensity for any ray in the chosen direction. Integration of the intensity over the solid angles by means of quadratures results in the radiative flux. Calculation of the radiation sources/sinks in volume cells is accomplished by a control volume approach having each ray and determining the net gain/loss of radiant energy from a given cell.

Along a given direction and in the absence of scattering the RTE can be integrated at any point P (denoted by n) to yield:

$$I_{n+1}^{+} = I_{n}^{-} e^{-\kappa \Delta s} + I_{\mathrm{b}}(T)(1 - e^{-\kappa \Delta s}) \tag{11}$$

where Δs is the distance traversed by the radiation beam within the control volume and the superscripts $+$ and $-$ denote the intensity leaving and entering the control volume, respectively.

The irradiation (incident radiant heat flux) on a boundary surface is calculated as:

$$G = \int_{ns'<0} I\,(s') \left| ns' \right| d\Omega' \approx \sum_{k}^{N_k} I_k \cos\theta_k \,\Delta\, \Omega_k' \tag{12}$$

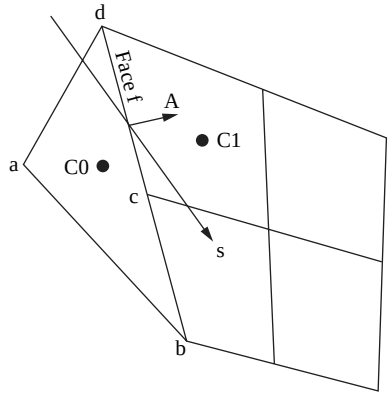
where θ_k is the angle between the incident radiation along the k-th direction and the normal to the boundary, and $\Delta\Omega_k'$ is discrete solid angle increment associated with direction k. The index k extends over all the directions resulting from the angular discretizations of the hemisphere around the point of interest on the wall.

The DTM is simple, relatively easy to apply and has been coupled to the energy equation to compute the performance of gas turbine combustor, combustion chamber of glass melting furnaces, pulverized coal-fired furnaces and other combustion systems (Viskanta and Mengüç 1987; Carvalho and Farias, 1998). The method has some advantages and some restrictions. Among the advantages is its flexibility that allows its use for complicated geometries. Its accuracy can be controlled through the variation of the number of rays without increasing too greatly the storage requirements. The most serious restriction of the method is the difficulty to anisotropic scattering problems. Very good results have been reported for isotropic scattering (Coelho *et al.*, 1993). Its non-conservative nature is disadvantageous when coupling radiative transfer calculations based on the method to CFD codes where the energy equation is solved using a finite volume or finite element method that is conservative. The reason for this behavior has been examined, and a conservative formulation has been proposed and evaluated (Coelho and Carvalho, 1997).

3.5 Finite volume method

The FVM has many similarities with DOM. The magnitude of the radiance is also assumed constant in each discrete direction, and the RTE is solved for a set of discrete directions which span the solid angle of 4π sterradian. Chui and Raithby (Raithby and Chui, 1990; Chui and Raithby, 1993) have developed a finite volume scheme for solving the RTE by imposing energy conservation principles over discrete solid angles. The original scheme has been extended to non-orthogonal body-fitted meshes (Chui and Raithby, 1993). A similar approach was employed by Chai *et al.* (1994) and Chai and Moder (1996) who developed a cell-based FVM using structured body-fitted meshes. Unlike the node-based schemes of earlier investigators, a cell-centered formulation based on arbitrary polyhedral control volume has been developed for arbitrary geometries (Baek *et al.*, 1998; Kim *et al.*, 2001; Murthy and Mathur, 1998).

The main ideas behind the discretization of the RTE using unstructured meshes (Murthy and Mathur, 1998) are summarized below. The spatial domain is discretized into convex polyhydral control volumes (Figure 2). The angular space at any spatial location is discretized into discrete non-overlapping control angles Ω_i, the centroids of



Source: Murthy and Mathur (1998)

Figure 2.
Control volume for the finite element method

which are denoted by the directions vector $\mathbf{s}_i$. The polar and azimuthal angles are θ_i and ϕ_I, respectively, are measured with respect to the Cartesian coordinate system. Each octant is descretized into $N_\theta \times N_\phi$ solid angles, and the angular discretization is uniform. However, the subtended solid angles are not equal and vary with θ. Control volume extents are given by $\Delta\theta$ and $\Delta\phi$.

For each discrete direction i the RTE, equation (1), is integrated over the control volume CO (Figure 2) and the solid angle $\Delta\Omega_i$ to yield:

$$\sum_f J_f I_{if} = [-(\kappa + \sigma) I_{io} + S_i] \Delta\Omega_i \Delta V_o \tag{13}$$

where I_{if} is the spectral (e.g. subscript λ is omitted) intensity associated with the direction i at the face f of the control volume, and S_i is the source function at the cell center in the direction i and is given by:

$$S_i = \kappa \mathrm{I}_{b,o} + \frac{\sigma}{4\pi} \sum_j I_{jo} \gamma_{ij} \tag{14}$$

where:

$$\gamma_{ij} = \frac{1}{\Delta\Omega_i} \int_{\Delta\Omega_i} \int_{\Delta\Omega_j} \Phi(s_i, s_j) \mathrm{d}\Omega'_j \mathrm{d}\Omega'_i. \tag{15}$$

The geometric factor J_f for directions with no control angle overhang is written as:

$$J_f = \left(\frac{A}{|A|}\right) \cdot \int_{\Delta\theta} \int_{\Delta\phi} s \sin\theta \mathrm{d}\theta \mathrm{d}\phi, \tag{16}$$

where $\mathbf{A}$ is the area vector. For body-fitted and unstructured meshes the discretization of equation (13) is complicated by the possibility of control-volume overhangs. Computational details are given by Murthy and Mathur (1998), including the discretization of I_{if}.

The FVM procedure for solving the RTE has been demonstrated for several example problems using both explicit and implicit solution procedures. The detailed analyses are given in the original papers (Raithby and Chui, 1990; Chui and Raithby, 1993) and are not repeated here for the sake of space limitations. For unstructured meshes an algebraic multigrid procedure has been proposed (Murthy and Mathur, 1998), and for accelerating the convergence a coupled multigrid method has been used in the literature (Mathur and Murthy, 1999). Numerous examples of radiative transfer in irregular geometries are given by Murthy and Mathur (2001). The FVM method for calculating radiative transfer has been used in the fire dynamics simulator (Floyd *et al.*, 2001) and more recently to the study of radiative transfer in an industrial combustor of wood carbonization fumes (Abbassi *et al.*, 2005).

4. Modeling of spectral nature of radiative transfer

Prediction of radiative transfer in combustion systems requires modeling of the radiation characteristics of combustion products: gases (CO_2, H_2O, CO, NO_2, CH_4, etc.), particles (soot, liquid fuel droplets, pulverized coal, char, fly-ash, dust, etc.) and their mixtures. It is beyond the scope of this account to review the models and experimental data base for these characteristics. Reference is made to recent reviews on gaseous

radiation (Taine and Soufiani, 1999) and to the literature on radiation characteristics of particles (Siegel and Howell, 2002; Modest, 2003).

4.1 Integration over spectrum

Use of the global (total) gas and gas + particle emittance as well as mean-beam-length concepts may be adequate for radiant heat transfer but not for temperature and flame structure calculations in flames and combustion chambers. In the order of decreasing detail the models are: LBL, narrow band (NB) and WB (Taine and Soufiani, 1999). The LBL models are the most accurate approaches for calculation radiative transfer when based on precise spectroscopic data bases (Modest, 2003) such as HITRAN or HITEMP. They yield accurate results, but are computationally too expensive for engineering application of radiative transfer in combustion systems since the entire spectrum consists of millions of single lines. In combustion applications global (integrated over spectrum) radiative transfer calculations in 3D geometries, which of necessity are based on spatial, directional and spectral discretizations, require the use of approximate models.

For an absorbing and emitting but nonscattering gaseous medium the spectral radiance in the direction $\mathbf{s}$ and at the location $\mathbf{r}$ can be obtained from the integration of the RTE, equation (1), in terms of the spectral transmittance of the inhomogeneous column between $\mathbf{s}'$ and $\mathbf{s}$ (Viskanta and Mengüç 1987; Taine and Soufiani, 1999). Once the spectral radiance has been calculated, the radiant flux vector and the radiant flux divergence (i.e. source/sink term) in the governing thermal energy equation is obtained by double integration over the solid angles and the bands.

Narrow and WB models cannot be applied to multidimensional radiative transfer problems which require solution of the differential RTE, where the knowledge of the spectral absorption coefficient or its average over a spectral interval is required. The NB model gives the spectral transmittance over a NB, and the WB model yields the WB absorptance. These models can be used only with the integral representation of the RTE. Unfortunately, these approaches are prohibitively expensive for practical applications (Coelho, 2002). For this reason it is necessary to turn to more efficient methods to solve the RTE based on the differential formulation.

The total emittance and absorptance concepts (Siegel and Howell, 2002; Modest, 2003) are useful for zero or one-dimensional radiative transfer analyses or for zonal predictions of global radiant energy quantities. In addition, the emittance/absorptance concepts cannot be readily adopted to combustion systems containing mixtures of radiatively participating gases and absorbing and scattering particles. For multidimensional radiative transfer calculation absorption and scattering coefficients as well as single scattering albedo are needed. Mean absorption/emission coefficients for use in the radiant energy equation have been suggested some time ago (Viskanta, 1964), and the concept of equivalent absorption and emission coefficients for gray radiant heat transfer analysis have been recently reintroduced and applied (Liu *et al.*, 2005). Unfortunately, the mean absorption coefficients calculated from total emittances/absorptances depend on temperature, pathlength, pressure and ratio of CO_2 and H_2O partial pressures. A detailed assessment of the effective absorption coefficients calculated from different total emittance correlations has been reported (Lallemant *et al.*, 1996), but only in the optically thin and thick limiting cases can the mean absorption coefficients be defined uniquely and treated as properties (i.e. functions of composition, pressure and temperature).

4.2 WSGG model and its enhancements

It is clear from recent publications (Coelho, 2002; Taine and Soufiani, 1999; Rivière *et al.*, 1994) that the WSGG model (Lallemant *et al.*, 1996; Hottel and Sarofim, 1967) and its enhancements such as the spectral group model (SGM) (Song, 1993), the SLW model (Denison and Webb, 1993), the correlated *k*-distribution (CK) (Rivière *et al.*, 1994) as well as their extensions to include scattering by particles (Tang and Brewster, 1994; Marin and Buckius, 1996), are compatible with RTE solvers such as DOM and DTM, and represent the best compromise for multi-dimensional combustion system geometrics. The CK method has been found to be very accurate (Coelho, 2002; Taine and Soufiani, 1999; Rivière *et al.*, 1994), but it is time consuming for engineering calculations of radiative transfer in practical combustion devices. Coelho (2002) has recommended the SLW method as a best compromise in terms of accuracy and computer resources. It yields accurate results without large computational effort (Coelho, 2002; Ströhle and Coelho, 2002). The CK method and its extensions (CKFD, absorption distribution function (ADF), ADF fictitious gas (ADFFG)) are computationally too costly for practical combustions systems where large temperature and radiating species concentration gradients are present (Taine and Soufiani, 1999; Pierrot *et al.*, 1999a, b). Therefore, only the WSGG, SLW and CK models are briefly discussed here in conjunction with the DOM for solving the RTE.

In spite of the fact that the WSGG, SLW and CK models have been extended to IR gas mixtures and gas-particle mixtures (Tang and Brewster, 1994; Marin and Buckius, 1996; Pierrot *et al.*, 1999), the discussion to follow is restricted to analysis of radiative transfer in gases only. When these or similar methods are used, the RTE for the *j*-th "gray gas" component of the radiating gas mixture in the 3D Cartesian coordinates is expressed as (Denison and Webb, 1993; Modest, 1991):

$$\xi\frac{\partial I_j}{\partial x}+\eta\frac{\partial I_j}{\partial y}+\mu\frac{\partial I_j}{\partial z}=\kappa_j\left[a_jI_{\mathrm{b}}(T)-I_j\right] \tag{17}$$

The gray absorption coefficients κ_j and the weighting functions of temperature $a_j(T)$ in the WSGG (Lallemant *et al.*, 1996), SLW (Denison and Webb, 1993) and CK (Taine and Soufiani, 1999; Rivière *et al.*, 1994) models are calculated from the correlations given in the corresponding models. The total radiation intensity integrated over the spectrum is simply:

$$I=\sum_{j=1}^{N}I_j$$

The radiant energy equation (5), is approximated:

$$-\nabla\cdot\mathscr{F}\simeq\sum_{j=1}^{N}\kappa_j\left[\int_{\Omega=4\pi}\mathrm{I}_j\mathrm{d}\Omega-4\pi a_jI_{\mathrm{b}}(T)\right] \tag{18}$$

and the radiant heat flux components are evaluated as:

$$\mathscr{F}_i(r)=\sum_{j=1}^{N}\int_{\Omega=4\pi}I_js_i\mathrm{d}\Omega \tag{19}$$

where s_i is the direction cosines for the x, y and z directions. Reference is made to literature (Coelho, 2002; Liu *et al.*, 1998) for model implementation details.

The CK method and its extensions are very accurate for radiative transfer calculations in gas mixtures (Taine and Soufiani, 1999; Pierrot *et al.*, 1999a, b), but the methods are too costly for calculations of radiative transfer in practical combustion systems where large temperature and radiating species concentration gradients are present. New developments are needed to speed up the calculations and apply the CK and related models to compute the structure of individual flames.

The ADF model and the ADFFG formulation, the correlated-*k*-fictitious gas, and the multi-scale-full-spectrum-correlated-k models are extensions of the CK model. Different implementations of these models for mixtures of absorbing gases have been discussed in detail by Taine and Soufiani (1999) and the available data bases (Rivière *et al.*, 1994; Soufiani and Taine, 1997) can be used to carry out the calculations.

5. Assessment of solution methods

5.1 Comparison of RTE solution methods

A number of investigators have published comparisons of performance of different monochromatic or gray radiative transfer models using test cases or experimental data (Viskanta and Mengüç 1987; Carvalho and Farias, 1998; Coelho, 2002; Liu *et al.*, 1998; Rivière *et al.*, 1994; Soufiani and Taine, 1997; Liu, 1999; Coelho *et al.*, 1995; Helbig *et al.*, 2001; Versteeg *et al.*, 2001). A comparison of different methods for predicting radiative transfer in 2D rectangular (Viskanta and Mengüç 1987; Carvalho and Farias, 1998; Coelho *et al.*, 1995) and axisymmetric (Viskanta and Mengüç 1987; Carvalho and Farias, 1998) as well as 3D rectangular (Carvalho and Farias, 1998; Versteeg *et al.*, 2001) enclosures has been reported, and the discussions will not be repeated. Suffice it to state that it is difficult to generalize the findings as the results depend on the choice of the radiation property model for the participating medium, the radiation characteristics of the walls and the geometry considered. Emphasis here is on recent comparisons as earlier results were obtained using cruder grids, owing to limited availability of computational resources. Focus is on approaches which are likely to find application for analyzing combustion systems.

The accuracy of the P_1-approximation, along with the δ-Eddington approximation for the scattering phase function, was assessed for radiative transfer in a gray absorbing, emitting and scattering medium confined in a two-dimensional square enclosure (Liu *et al.*, 1992). Two examples were considered:

(1) the bottom wall has a unit blackbody emitted flux, $E_{bw} = \pi I_b(T_w) = 1.0$, with the other three walls as well as the medium are kept cold; and

(2) the boundaries are all cold and the medium has a blackbody emitted flux of unity.

The radiative fluxes predicted by the P_1-approximation are in good agreement with the numerically exact results of Kim and Lee (1990) (Figure 3). The approximation is not accurate in the corner regions and in pure and highly forward scattering media. Furthermore, the results reveal that effects of scattering on radiation transfer can be neglected if the medium has a highly forward scattering phase function.

Extensive radiative transfer predictions based on DOM, DTM and DFM results for 2D rectangular and 3D axisymmetric and rectangular furnaces have been made by Coelho *et al.*(1995). In all cases the enclosures contained an absorbing and emitting gray medium. The focus was on the assessment of different methods for solving the RTE.

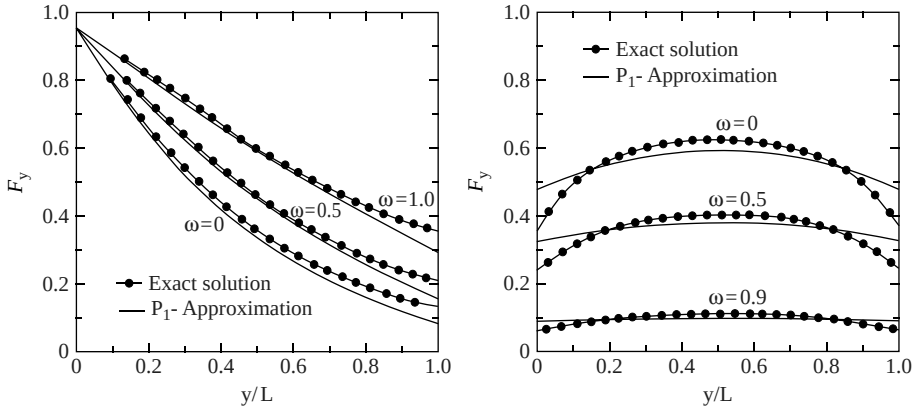


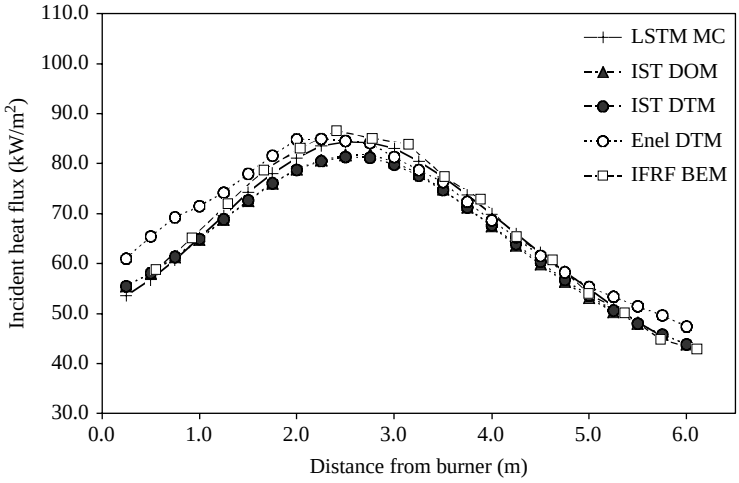
Figure 3.
Comparison of P_1-approximation and exact solution for radiation transfer in a square, diffuse enclosure filled with an absorbing, emitting and scattering medium

Notes: ϵ = 1.0, L = 1.0 m, g = 0.67 and $\tilde{\beta}$ = 1.0 m^{-1}. Imposed wall emission (left panel) and imposed medium temperature (right panel) (from [80])

Radiative transfer results obtained with DOM, DTM and FVM for a 2D diffuse enclosure have been compared with exact solutions. Similar comparisons have been made for a 3D rectangular enclosure, but with the results based on the ZM rather than exact solution. The mesh used for DTM was rather crude and only 32 rays per wall node were employed. The results obtained using DOM, DTM and ZM were also compared with the test data for the International Flame Research Foundation (IFRF) furnace (M3 trials).

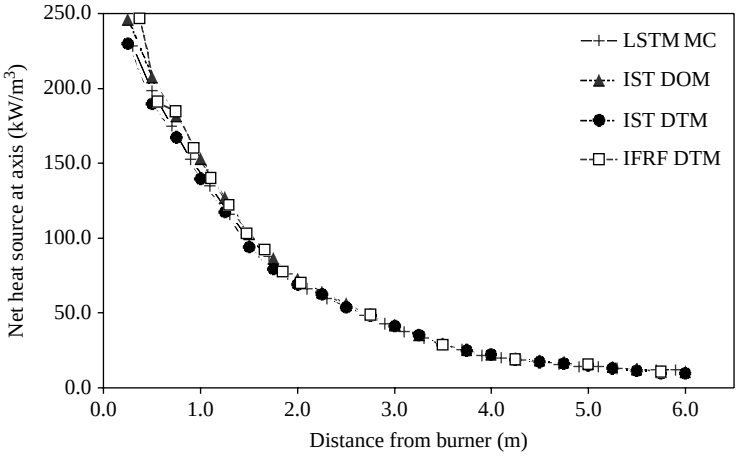
Recently, a cooperative program has been undertaken by a group of four complementary research teams to compare various radiative transfer methods for a set of four benchmark test cases (Helbig *et al.*, 2001). Case 1 involved a cylindrical 1 m diameter and 3 m long furnace, and Case 4 was for a 2 × 2 m cross-section and 6.25 m long furnace. The combustion products were modeled as a gray, non-scattering medium having a constant absorption coefficient $\kappa = 0.1\,m^{-1}$. The primary purpose of the exercise was to compare the radiative transfer methods and not to simulate the performance of the two IFRF test furnaces.

Numerical results for Case 4 were obtained using measured wall and in-furnace temperatures as well as imposed wall emissivities. The results were obtained using MCM, DOM, DTM and BEM. The DTM results were obtained by two research groups at the Instituto Superior Technico, Lisbon, Portugal and at the ENEL Produzione-Research (ENEL), Pisa, Italy. The number of control volumes used were different, but the radiation heat flux results obtained using four computing systems and different radiation transfer models are in close agreement (Figures 4 and 5) and are within an error margin generally below 5 percent. The reason for the good agreement is that in the test cases examined the temperatures in the furnaces were smooth enough to avoid the occurrence of ray effects in the low-order DOM and DTM methods. Of course, the calculations were non-interactive, – the temperatures were assumed and not calculated from the appropriate energy equations for the gas volume and surface elements. Also, a direct comparison of computer time needed to perform the calculations cannot be assessed because of four different computer systems employed. From the results reported, the execution times for the computations were as follows:



Source: Helbig *et al*. (2001) (left panel)

Figure 4.
Incident heat flux for test Case 4



Source: Helbig *et al*. (2001) (right panel)

Figure 5.
Net volumetric radiant energy loss/gain at axis for test Case 4

MCM (with 512 processors) 277 s, DTM 56 min, BEM 6 min, DOM between 1.75 min and 38 s depending on the S_n-approximation employed. In the MCM ray tracing took more than 99 percent of the time. Additional camparisons of incident radiant heat fluxes at a furnace wall have been reported for the same furnace but different cases and good agreement has been found between the BEM (Węcel and Bialecki, 2006; Bialecki and Węcel, 2004) and the benchmark (Helbig *et al.*, 2001) results.

A comparison of radiative transfer predictions with experimental data obtained in the M2 trials at the IFRF Furnace 1 have been reported (Jamaluddin and Smith, 1988; Mbiock and Weber, 2000). For example, Mbiock and Weber (2000) have carried out calculations for a rectangular 2 × 2 m in cross-section and 6.25 m long furnace. Natural gas and propane were the fuels and no-swirl and swirl burners were used.

Gas temperatures and combustion product distributions were prescribed, and an absorbing-emitting medium having a mean absorption coefficient filled the enclosure. The radiative transfer problem was formulated and the numerical solutions were obtained using a BEM. The mean (gray) absorption coefficients were varied parametrically in the calculations. The case of $\kappa = 0\,\mathrm{m}^{-1}$, of course, corresponds to completely transparent combustion products. The results reported suggest that the arbitrary choice of the mean absorption coefficient having a value of $0.05\,\mathrm{m}^{-1}$ for the combustion products may be a reasonable compromise value to yield good agreement between data and predictions for a non-sooty natural gas flame (Flame 30). This good agreement between calculations and data, however, may be fortuitous as there is no sound physical basis for determining (choosing) a spectrum-averaged mean absorption coefficient. Other results reported for non-swirl and swirl flames indicate that the value of the mean absorption coefficient should be higher ($\kappa = 0.1$ or $0.15\,\mathrm{m}^{-1}$) (Mbiock and Weber, 2000). This suggests that the non-interactive simulations of the combustion system using measured in-furnace and wall temperature distributions as well as the medium and surface radiation characteristics is neither complete nor sufficiently critical for validating the radiative transfer model.

5.2 Comparison of global computational results

In the early 1990s a group of investigators undertook a task of comparing several methods for obtaining solutions of a specified radiative transfer problem (Tong and Skocypec, 1992). To assess the capability of solving non-gray, anisotropically scattering radiative transfer problems in a planar and 3D geometries were solved using 12 different computer programs. Times required for execution were not compared. The conclusion was that there was considerable uncertainty (i.e. by a factor of 2 or 3) in predicting both the radiation heat flux and the heat source, depending on the computer program used for the 3D geometry.

Benchmark solutions and comparison of non-gray radiative transfer calculations in 3D parallelepiped (Coelho, 2002; Liu *et al.*, 1998; Liu, 1999; Kim *et al.*, 2001; Liu and Smallwood, 2004; Ströhle *et al.*, 2003) and cylindrical (Park and Kim, 2002) enclosures have been reported. For example, a comparison of predictions using the gray and WSGG approximations for the radiation characteristics in two model enclosures and real multidimensional, natural gas-fired research furnace of semi-industrial scale has been made (Liu *et al.*, 1998). The effective absorption coefficient in the gray gas model was estimated from the total gas emittance of the system or found by optimizing the gray gas results against a benchmark solution. The model equations in both cases were solved using DOM. When the temperature distribution is specified and the RTE is then solved, the radiant wall heat fluxes predicted are in serious error compared to the WSGG model. In the full simulation of the gas-fired furnace the WSGG model predicted more accurately the heat fluxes and temperature distributions than the gray gas model (Liu *et al.*, 1998).

In a comprehensive study DOM and DTM have been applied to simulate radiative transfer in a 3D ($2 \times 2 \times 4$ m) gas-fired furnace with prescribed temperature radiating species composition (Coelho, 2002). The WSGG, the SLW, SNB, and the correlated k-distribution (CK) methods for integrating over the spectrum were employed and the results were compared (Figure 6). The results for the SLW model overlap those based on the CK method, and are, therefore, not shown in the figure for the sake of clarity. The critical assessment showed that for a single iteration DOM is faster than DTM. The CK method is the most accurate of the three models compared, but it is too

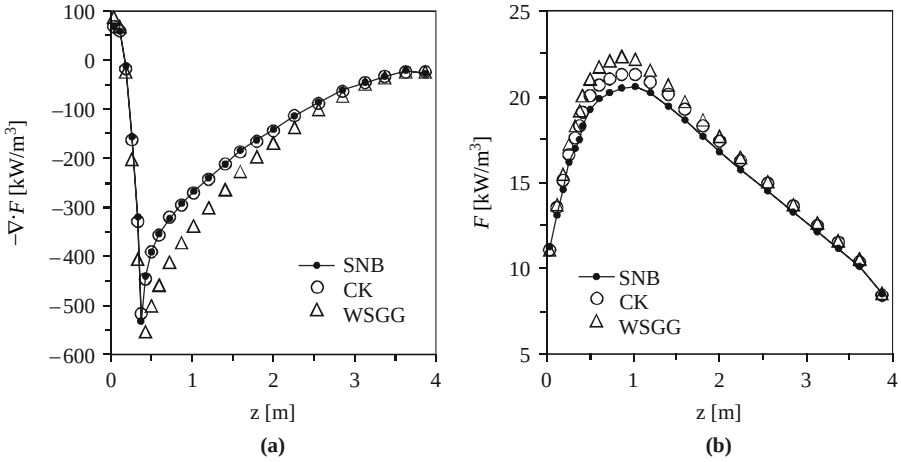


Figure 6.
Comparison of net volumetric radiant energy loss/gain rates along center line z (1 m, 2 m) (a) and of heat fluxes incident along center line z (2 m, 1 m) (b)

Source: Coelho (2002)

time-consuming for engineering applications. The SLW model is the best compromise regarding accuracy and numerical efficiency (Coelho, 2002). The methods considered may yield results of acceptable accuracy for global radiant heat transfer calculations in furnaces, but the current methodologies need to be enhanced for flame structure and practical combustion system performance calculations.

Benchmark solutions of radiative transfer in a gas-soot particle mixture contained in axisymmetric enclosures have been reported (Coelho *et al.*, 2003a, b). The SNB model is used for gases, and the soot absorption coefficient is modeled on the spectral basis. The ray tracing, Monte Carlo and discrete ordinates methods are employed to calculate radiative transfer for three model enclosures containing a mixture of H_2O-CO_2-N_2-soot at atmospheric pressure. The authors conclude that DOM combined with correlated CK-method yields less accurate, but more economical, solutions than the former two (ray tracing and Monte Carlo) approaches, which are adequate for most practical problems.

Results for a 3D model problem obtained using DOM (S_4-approximation), P_1-approximation and a modified P_1-approximation have been compared (Park *et al.*, 1999). The calculations were performed on a band basis by dividing the spectrum into a finite number of bands. Solutions were found for each band and then were summed to obtain the total contribution. The results obtained for radiation heat flux and temperature were of comparable accuracy (using S_4-method as benchmark), but the DOM required the greatest amount of CPU time for all single scattering albedoes and the modified differential approximation the least.

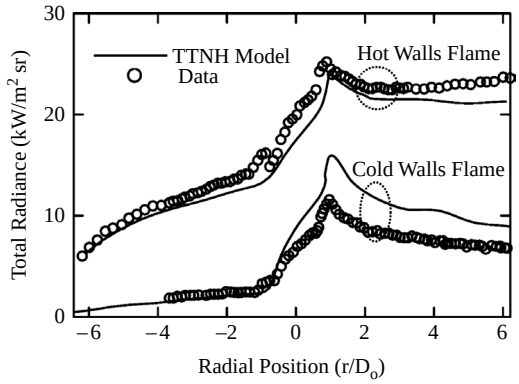
Recently, the reciprocal and forward Monte Carlo methods, based on the reciprocity principle, have been developed to examine the feasibility of the methods to predict radiative transfer in real gases using 3D calculational grids (Tessé *et al.*, 2002). The radiation characteristics of actual gas mixtures are treated in a correlated manner by the CK model. The results are compared with recently published reference calculations and demonstrate the feasibility of obtaining reliable radiative transfer predictions in situations where the temperature and gas concentration distributions are relatively smooth functions of position.

A comprehensive assessment of the total transmittance nonhomogeneous (TTNH) (Grosshandler, 1980), exponential wide band (EWB) and WSGG models for the calculations of the total radiance has been carried out by Lallemant *et al.* (1996). The radiances calculated by different versions of these models have been compared against narrow angle radiometer traverse data on flames enclosed by cold and hot walls. A comparison between the measured total radiance and the predictions using the TTNH model (Lallemant *et al.*, 1996) is shown in Figure 7 for two flames. The homogeneous transmittance was calculated using Modak's (1979) model. The total radiance predictions based on the TTNH model are in better agreement with the measured values for the hot walls than the cold walls flame. For the latter flame, the TTNH model overestimates the peak radiance by about 25 percent. As a consequence, of this overshoot, the calculated radiances in the external recirculation zone ($r/D_o \geq 1$) remain higher than the measured values. Lallemant *et al.* (1996) conclude that the main reason for the discrepancies between predictions and measurements are due to inaccurate treatment of the temperature gradients, and this identifies the total transmittance as the source of the discrepancy.

The total radiances have been predicted for hot and cold wall flames using the SG model in combination with the several versions of the WSGG, and CK models for the radiation characteristics of H_2O-CO_2. The detailed results are given by Lallemant *et al.* (1996). A comparison of calculated and measured total radiances is shown in Figure 8. The predictions using the WSGG models of Smith *et al.*, Taylor and Foster, and Truelove underpredict the measured data for the hot walls flame, but usually overpredict the data for the cold walls flame (not shown). Therefore, the good agreement between the model predictions and the measured data may be considered as coincidental. Reference is made to Lallemant *et al.* (1996) for the detailed discussion of the results and explanation of the discrepancies. Included in the discussion is the comparison of predictions based on the EWB, SLW and CK models with the measured total radiance data.

6. Concluding summary remarks

Before deciding on which method to use for solving the RTE and how to carry out the integrations over the spectrum for predicting radiative transfer in



Source: Lallemant *et al*. (1996) (left panel)

Figure 7.
Comparison between total radiance measurements and predictions based on the TTNH model in hot and cold walls flames at $x/D_o = 22/87\,\text{mm} = 0.31$

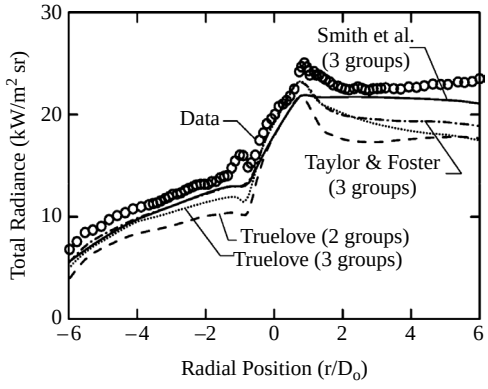
a combustion system, the researcher/designer must determine the level of detail required for the calculations:

- total heat flux to load/walls in a combustion chamber;
- temperature and species distributions in the combustion chamber; and
- local flame structure.

The level of resolution and detail in radiative transfer predictions required to calculate the flame structure is much greater and more critical than is required to calculate the global radiant heat flux, radiant heat transfer rate or radiation efficiency of a combustion system. Additional factors to consider include the available radiation property database and the time needed to perform the calculations. One must also keep in mind that these calculations may comprise an input to only a single term in the energy equation, but all transport equations need to be solved to predict the structure of chemically reacting and radiating flows. Finally, before selecting a method for predicting radiative transfer the user must keep in mind the application and purpose of the calculations. Are the calculations preliminary in nature to identify the trends for optimizing the performance of a combustion system or are detailed results required to address a specific issue?

It is clear from the results reported up to date that the choice of the model for the radiation characteristics of combustion products and integration over the spectrum is more critical for accurate prediction of radiative transfer than the choice of the method for solving the spectral (or gray) RTE. Several methods (DOM, DTM and FVM) developed capture the correct solution if sufficiently fine node network and directional resolution is used. The radiation characteristics of the combustion products, however, depend on local conditions of temperature, radiating species concentrations, partial pressure, etc. and use of a mean or effective absorption coefficient for the calculations is not likely to yield accurate radiative transfer predictions.

Presently it is generally accepted that the LBL, SNB and EWB are not suitable for flame structure calculations using CFD methods. The first two models are not suitable because they require excessive computational resources and the last one because of its complexity in the mathematical formulation of radiative transfer. There is a need for



Source: Lallemant *et al*. (1996) (right panel)

Figure 8.
Comparison between total radiance measurements in a hot flame and predictions based on SGM together with four H_2O-CO_2 SGGW models at $x/D_o = 0.31$, with x being the distance along axis of the furnace and $D_o = 87$ mm is the diameter of the combustion air duct

theory to replace (simplify) spectral radiative transfer calculations by some type of "gray" or "semi-gray" calculations. Reductions of the spectrum (in the range of 1-20 μm) from about 400 intervals to less than, say, 40 for CFD calculations would be a step in the right direction. The empirical WSGG model does not possess the accuracy or the generality of the EWB band or of the SNB models. The generality of the EWB, along with the relatively modest computational requirements, makes the procedure attractive for calculating the total emittance of gas mixtures or for incorporation in CFD codes for flame calculations. The concept of total gas emissivity, however, is not suitable for calculating either the mean absorption coefficient or the flame structure, say, in combustion devices where either the temperature and/or gas composition very greatly over a small distance.

The least detailed model is required for predicting local, global radiation heat flux at the walls of the combustion chamber (i.e. furnace walls) or load. The WSGG, SLW, and CK and similar models are adequate. Other more detailed methods available appear to be too time consuming for radiative transfer predictions in practical combustion systems at the present time. The methods considered may yield results of acceptable accuracy for global radiant heat transfer calculations in furnaces, but the current methodologies need to be enhanced for flame structure and practical combustion device performance calculations.

Much greater detail and nodal resolution is required to predict radiative transfer and flame structure in small laboratory or individual flames. The CK-model is the most accurate of the methods evaluated up to now for use in multidimensional combustion systems; however, new developments are needed for treating band and particle radiation, and integration over the spectrum for accurate calculation of radiation in flames and in practical combustion systems.

In the modeling considered the turbulence/radiation interaction has been ignored. That may not be justified for highly turbulent luminous flames. Recently, some investigators have shown (Li and Modest, 2003; Tessé *et al.*, 2004) (and references cited therein) that radiant energy quantities may differ significantly from those predictions based on the mean temperature and concentration fields because of their strong nonlinear dependence on these fields. Radiant energy losses from flames are increased when turbulence/radiation interactions are accounted for. This suggests that the effect would have to be considered in the future when calculating radiative transfer in highly turbulent combusting and radiating flows.

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