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A PDF/PHOTON MONTE CARLO METHOD FOR RADIATIVE HEAT TRANSFER IN TURBULENT FLAMES

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ABSTRACT

Thermal radiation plays a dominant role in heat transfer for most combustion systems. Accurate predictions of radiative heat transfer are essential for the correct determination of flame temperature, flame structure, and pollutant emissions in combustion simulations. In turbulent flames, transported probability density function (PDF) methods provide a reliable treatment of nonlinear processes such as chemical reactions and radiative emission. Here a second statistical approach, a photon Monte Carlo (PMC) method, is employed to solve the radiative transfer equation (RTE). And a state-of-the-art model for spectral radiative properties, the full-spectrum k-distribution (FSK) method, is employed. The FSK method provides an efficient and accurate approach for spectral integration in radiation calculations. The resulting model is applied to simulate radiation and turbulence/radiation interactions in nonluminous turbulent nonpremixed jet flames. The initial results reported here emphasize sensitivities of computed results to variations in the physical and numerical models. Results with versus without radiation, results obtained using two different RTE solvers, and results with a gray-gas approximation versus a spectral FSK method are compared.

Keywords: Radiation Modeling, Turbulent Flames, PDF Method, Photon Monte Carlo Method, Full-Spectrum k-Distribution Method, Turbulence/Radiation Interactions

1 Introduction

Thermal radiation is a dominant mode of heat transfer in many combustion systems. In numerical simulation and modeling, accurate treatment of radiative heat transfer is essential to obtain the correct distributions of flame temperature and pollutant emissions: soot and NOx, in particular. Even the global properties of canonical steady one-dimensional laminar premixed flames (flame speeds and flammability limits) depend strongly on radiation heat transfer and on the spectral radiation properties of the participating gases ([6]). Yet, because of the physical and computational complexities associated with thermal radiation (integral nature of the radiative transfer equation - RTE, heat transfer rates varying as a high power of the temperature, large and irregular variations in radiation properties with wavenumber), radiation often has been ignored altogether or has been treated using simple models (e.g., an optically thin approximation) in combustion applications.

In turbulent flames, turbulence/radiation interactions (TRI) arise from the highly nonlinear coupling between temperature and composition fluctuations. The effects of TRI can be comparable to those of turbulence/chemistry interactions (TCI) in both luminous and nonluminous turbulent flames ([3, 5, 9]). Yet, TRI has received relatively little attention compared to TCI in the turbulent combustion community. Conventional Reynolds-averaged Navier-Stokes (RANS) modeling approaches are not well suited to dealing with TRI; statistical approaches such as probability density function (PDF) methods are more appropriate ([2, 8]). Recently, direct numerical simulation (DNS) has been used to explore TRI in an idealized premixed turbulent system ([16]).

Here progress towards a comprehensive model that accommodates detailed chemical kinetics and state-of-the-art modeling approaches for TCI (a PDF method), for the solution of the

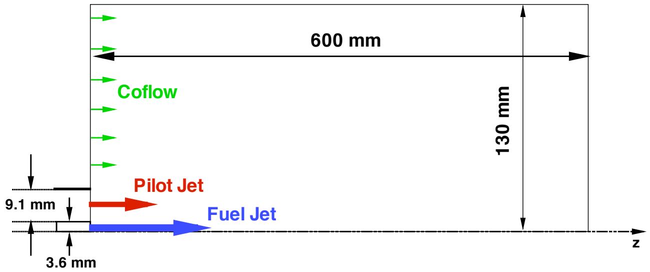

Figure 1. Sketch of computation domain.

RTE (a photon Monte Carlo - PMC - method), and for spectral radiation properties of participating gas-phase species (a full-spectrum k-distribution - FSK - method) is reported.

2 Flame Configuration

A piloted nonpremixed turbulent jet flame - the Sandia D flame ([1]) - is the subject of this study (Figure 1). Probably more modeling studies have been published for this flame than for any other turbulent flame configuration. While it generally had been accepted that an optically thin approximation should be valid for this flame (and for other nonsooting flames in this series), the importance of radiative absorption on NO ([4]) and the importance of spectral radiation properties ([2]) have been highlighted recently.

3 Physical and Numerical Models

3.1 Chemically Reacting Turbulent Flow

A consistent hybrid particle/finite-volume PDF method ([17]) is employed to compute this statistically stationary, axisymmetric flow. Mean velocity, mean pressure, mean mixture enthalpy, and turbulence transport quantities (here, a standard $k-\epsilon$ model) are computed using an unstructured finite-volume solver with second-order spatial accuracy; these are passed to the particle side of the calculation. On the particle side, the joint PDF of species mass fractions and mixture enthalpy fluctuations is computed using a Lagrangian Monte Carlo method. The mean mixture density field is computed based on particle properties, thereby capturing the influence of turbulent fluctuations in composition and temperature, and is passed back to the finite-volume side.

Here a nonuniform mesh of $2,552$ wedge-shaped elements is used with a nominal particle number density of 30 per element. A 16-species, 41-reaction methane-air mechanism is implemented using the CHEMKIN libraries ([7]).

3.2 The Radiative Transfer Equation

The radiation source term in the instantaneous energy equation can be expressed as the divergence of the radiative heat flux $\vec{q}_{rad}$,

$$\begin{aligned}\nabla\cdot\vec{q}_{rad} &= \int_0^\infty \kappa_\eta\Big(4\pi I_{b\eta} - \int_{4\pi} I_\eta d\Omega\Big)d\eta \\ &= 4\kappa_P\sigma T^4 - \int_0^\infty\int_{4\pi}\kappa_\eta I_\eta d\Omega d\eta\ , \end{aligned} \tag{1}$$

where

$$\kappa_P \equiv \frac{\int_0^\infty \kappa_\eta I_{b\eta}d\eta}{\int_0^\infty I_{b\eta}d\eta} = \frac{\pi}{\sigma T^4}\int_0^\infty \kappa_\eta I_{b\eta}d\eta \tag{2}$$

is the Planck-mean absorption coefficient and σ is the Stefan-Boltzmann constant. Here η denotes wavenumber, Ω is solid angle, κ_η is the spectral absorption coefficient, $I_{b\eta}$ is the Planck function (a known function of local temperature and wavenumber), and I_η is the spectral radiative intensity. Intensity is determined from the RTE ([10]):

$$\begin{aligned}\frac{dI_\eta}{ds} &= \hat{s}\cdot\nabla I_\eta \\ &= \kappa_\eta I_{b\eta} - \beta_\eta I_\eta + \frac{\sigma_{s\eta}}{4\pi}\int_{4\pi} I_\eta(\hat{s}_i)\Phi_\eta(\hat{s}_i,\hat{s})d\Omega_i\ . \end{aligned} \tag{3}$$

Here $\hat{s}$ and $\hat{s}_i$ denote unit direction vectors, $\sigma_{s\eta}$ is the spectral scattering coefficient, $\beta_\eta = \kappa_\eta + \sigma_{s\eta}$ is the spectral extinction coefficient, and $\Phi_\eta(\hat{s}_i,\hat{s})$ denotes the scattering phase function; the latter describes the probability that a ray from incident direction $\hat{s}_i$ is scattered into direction $\hat{s}$. The local value of I_η depends on nonlocal quantities, on direction ($\hat{s}$), and on wavenumber.

For Reynolds-averaged modeling of turbulent flows, one takes the mean of Eq. (1):

$$\begin{aligned}\langle\nabla\cdot\vec{q}_{rad}\rangle &= \int_0^\infty \Big(4\pi\langle\kappa_\eta I_{b\eta}\rangle - \int_{4\pi}\langle\kappa_\eta I_\eta\rangle d\Omega\Big)d\eta \\ &= 4\sigma\langle\kappa_P T^4\rangle - \int_0^\infty \langle\kappa_\eta G_\eta\rangle d\eta\ , \end{aligned} \tag{4}$$

where angled brackets denote mean quantities, and the direction-integrated incident radiation $G_\eta \equiv \int_{4\pi} I_\eta d\Omega$ has been introduced. Averaging of these highly nonlinear quantities introduces a closure problem that is akin to that encountered in averaging the highly nonlinear chemical source terms; this is the essence of TRI.

It is noteworthy that in a one-point PDF method, emission TRI ($\langle\kappa_\eta I_{b\eta}\rangle$ or $\langle\kappa_P T^4\rangle$) appears in closed form because κ_η is (in principle) a known function of composition, temperature, and pressure. In the initial calculations that are reported here, however, all mean radiation terms have been computed based on local mean values of composition and temperature, thereby ignoring TRI. PDF-based investigations of emission and absorption TRI have been reported by [9] and [8].

Several approaches are available to solve the RTE ([10]). Here two methods are used and compared: a spherical harmonics (P1) approximation; and a photon Monte Carlo (PMC) method. The P1 method is relatively straightforward to implement, yet is robust and has been found to be satisfactory in many combustion applications. However, its suitability for turbulent jet flame configurations with localized, near-opaque soot regions has been found to be limited [15]. One objective of the present study is to investigate the performance of the P1 approximation in nonluminous flames. The implementation of a P1 method in a RANS-based CFD code using both gray (Planck-mean) and nongray (FSK) radiation properties has been described in detail in [15].

To assess the P1 approximation, a more accurate RTE solver (PMC) has been implemented. PMC involves tracing the trajectories of a large number of representative photon bundles from their points of emission to their points of absorption using statistical sampling techniques ([10, 16]). While subject to statistical errors and relatively high computational costs, PMC methods involve no intrinsic approximations to the RTE and can provide highly accurate results for arbitrarily complex geometric configurations and physical situations. Here as a first step, PMC calculations have been performed for a gray medium with radiative properties based on local mean values of composition and temperature.

3.3 Radiation Properties

Two radiatively participating species have been considered: H_2O and CO_2. Contributions from CO and CH_4 have been neglected. The spectral absorption coefficients (κ_η) of H_2O and CO_2 are determined from the HITEMP ([12]) and CDSD ([13]) spectral databases, respectively. The full-spectrum k-distribution (FSK) method is employed for nongray radiation calculations, i.e., the spectral integrations shown in Eqs. (1) and (4). The FSK method reorders the irregularly varying absorption coefficients into monotonically increasing k-distributions so that 10 or fewer RTE evaluations are required ([10]), by contrast to the millions of RTE evaluations that would be required for a line-by-line calculation of comparable accuracy.

To assess the importance of accounting for nongray radiation properties, computations also have been performed using a gray-medium approximation. In that case, the effective Planck-mean absorption coefficients have been determined from local full-spectrum k-distributions ([15]) to ensure a fair comparison.

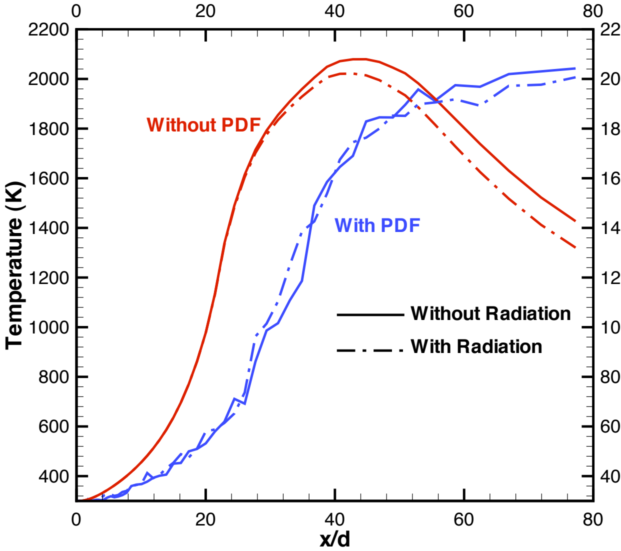

Figure 2. TCI and radiation effects on computed centerline mean temperature profiles.

4 Results and Discussion

To establish the relative importance of various physical phenomena in the flame, computed mean temperature profiles and other quantities are compared with systematic variations in the physical models.

4.1 Turbulence/Chemistry Interactions

The effect of TCI is shown in Figure 2. There centerline mean temperatures are compared with and without the PDF method; the latter correspond to a presumed joint-delta-function PDF at the local mean values of composition and enthalpy. Without consideration of TCI, the temperature peaks further upstream and at a higher value (by about 40 K) compared to the case with TCI. Consideration of turbulent fluctuations about the local mean slows the mean reaction rate.

4.2 Thermal Radiation

Also shown in Figure 2 is the effect of radiation on the computed mean flame temperature. Here the P1-gray radiation model has been used. Accounting for radiation reduces the peak mean axial temperature by about 50 K both with and without TCI. The radiation effect is more prominent downstream in the flame.

4.3 RTE Solution Method

Figure 3 illustrates sensitivity to the RTE solver, in the absence of TCI. The computed centerline mean temperature pro-

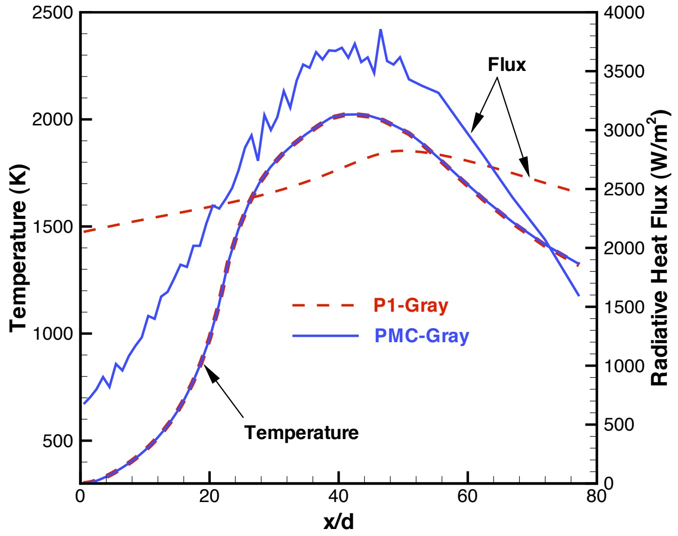

Figure 3. Effect of RTE solution method on mean temperature and radiant heat flux profiles.

files and global radiant fractions are relatively insensitive to the choice of RTE solver; computed global radiant fractions for P1 and PMC are about 7.8% and 7.5%, respectively. However, the computed radiant heat flux profiles at the outer periphery of the computational domain differ dramatically. The PMC heat flux profile follows more closely the axial mean temperature profile, and is far more plausible. This is consistent with an earlier modeling study for a highly luminous sooting jet flame ([15]). There P1 was found to give a satisfactory global radiant fraction, but an unrealistic spatial distribution of radiant heat flux compared to experimental measurements.

4.4 Nongray-Gas Effects

Figure 4 shows the effect of spectral radiation properties. There radial mean temperature profiles at three axial locations are plotted. The differences in mean temperature resulting from consideration of nongray radiation properties are small upstream, and become larger (although still modest) further downstream. Here the maximum computed mean temperature differences are about 20 K. While these differences in mean temperature appear to be small, the difference in global radiant fraction is significant: the computed global radiant fraction drops from approximately 7.8% for the gray case to approximately 5.1% for the nongray case. Further investigation is underway to sort out these differences.

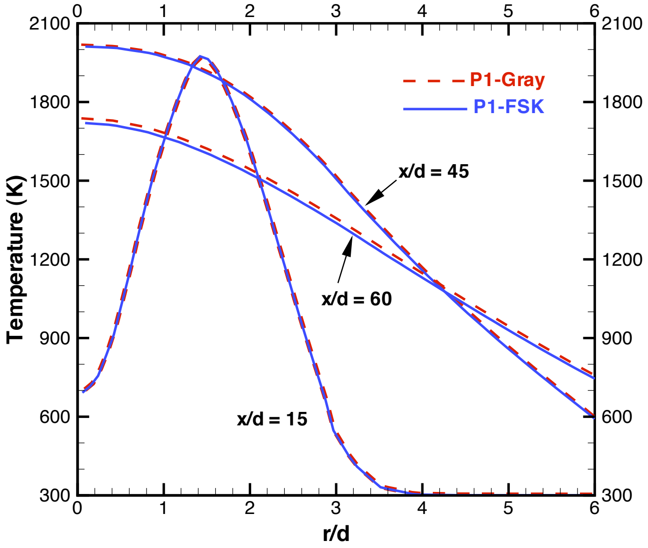

Figure 4. Nongray radiation effect on radial temperature.

5 Conclusion

The preliminary results reported here suggest that the effect of thermal radiation on mean temperature is comparable to that of turbulence/chemistry interactions; the influence of radiation is stronger further downstream in the flame. Gray radiation models yield higher total radiative heat loss compared to nongray models. And while differences between the P1- and PMC-computed mean temperature profiles are small, P1 yields a qualitatively incorrect heat flux profile.

Detailed quantitative comparisons between model results and experimental measurements are underway for the Sandia D flame, and other nonluminous flames in that series. Next steps include coupling PDF and PMC at the particle level (rather than through mean quantities) to explicitly capture and study TRI effects, implementing larger chemical mechanisms including NOx (using storage/retrieval-based chemistry acceleration strategies; [11, 14]), and consideration of sooting flames.

Acknowledgments

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