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Comparison of accuracy and computational expense of radiation models in simulation of non-premixed turbulent jet flames

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ABSTRACT

The accuracy and computational expense of various radiation models in the simulation of turbulent jet flames are compared. Both nonluminous and luminous methane–air nonpremixed turbulent jet flames are simulated using a comprehensive combustion solver. The combustion solver consists of a finite-volume/probability density function-based flow–chemistry solver interfaced with a high-accuracy spectral radiation solver. Flame simulations were performed using various *k*-distribution-based spectral models and radiative transfer equation (RTE) solvers, such as *P-1*, *P-3*, finite volume/discrete ordinates method (FVM/DOM), and line-by-line (LBL) accurate Photon Monte Carlo (PMC) methods, with and without consideration of turbulence–radiation interaction (TRI). Various spectral models and RTE solvers are observed to have strong effects on peak flame temperature, total radiant heat source and NO emission. The *P-1* method is found to be the computationally least expensive RTE solver and the FVM the most expensive for any spectral model. For optically thinner flames all radiation models yield excellent accuracy. For optically thicker flames the *P-3* and the FVM with advanced *k*-distribution methods predict radiation more accurately than the *P-1* method with any spectral model when compared to the benchmark LBL PMC. The LBL PMC yields exact results with sufficient number of samples and is found to be less expensive than the FVM (for all spectral models) and the *P-3* (for some spectral models) in statistically stationary combustion simulations. TRI is found to drop the peak temperature by close to 150 K for a luminous flame (optically thicker) and 25–100 K for a nonluminous flame (optically thinner).

1. Introduction

Thermal radiation plays an important role in multi-phase (gas + particulate phase) turbulent combustion systems. Until recently it was not possible to make high-accuracy predictions of radiative heat transfer rates in high-temperature combustion applications. The reasons for this deficiency are: (i) lack of high accuracy and efficient radiative transfer equation (RTE) solvers and (ii) lack of versatile, robust and computationally efficient models to predict radiation from nongray multi-phase media.

Because of the difficulties associated with radiation calculations, it has been common practice in turbulent flame simulations to invoke the optically-thin approximation, and/or to assume the medium to be gray, for both luminous [1] and nonluminous [2] flames. The optically-thin radiation model can result in substantial error due to its neglect of self-absorption, as has been shown by both numerical and experimental studies [3]. The gray medium assumption can also result in large errors as was shown by Li and Modest [4] and Wang et al. [5,6]. Nongray radiation modeling has begun to draw attention in combustion simulations [6,5]. Nongray radiation calculations in participating media can be most accurately performed using the line-by-line (LBL) approach, which, in order to resolve the spectrum, requires in excess of one million spectral solutions of the RTE, making such radiation calculations prohibitive. Models for nongray radiative properties include the weighted sum of gray gases (WSGG) [7], the spectral line-based weighted sum of gray gases (SLW) [8], and the full spectrum *k*-distribution (FSK) method [9]. The FSK method is an exact method for a homogeneous or correlated medium using a continuous *k*-distribution over the entire spectrum. Several advancements to the *k*-distribution method have been

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proposed to address the shortcomings of the basic FSK scheme in strongly inhomogeneous media based on the multi-scale (MS) [10] and the multi-group (MG) approaches [11], which may be summarized as: (1) the hybrid multi-scale multi-group FSK (MSMGFSK) method [12] for inhomogeneous gas mixtures, (2) the MSFSK method [13] for mixing of nongray soot with gas mixtures with/without gray wall emission, and (3) the narrow band-based hybrid MSMGFSK method [14] for inhomogeneous nongray gas–soot mixtures with/without wall emission. Recently, a portable spectral module has been developed by Pal et al. incorporating the LBL and all of the *k*-distribution methods with corresponding *k*-distribution databases to facilitate spectral radiation calculations [15].

Common methods for the solution of the RTE in turbulent combustion simulations are: (1) the spherical harmonics method (SHM), (2) the finite volume/discrete ordinates method (FVM/DOM), and (3) the photon Monte Carlo (PMC) method [16]. While the first two are deterministic in nature, the third is a statistical method. Statistical methods like the PMC can solve the most complicated problems with relative ease, but they are always subject to statistical error and require great computational power. Both the SHM and the FVM/DOM approximate the directional variation of the radiative intensity. However, the underlying approaches to represent the directional dependence of radiative intensity for SHM and FVM/DOM are quite different. The FVM/DOM employs a discrete representation of the directional variation with integrals over total solid angle 4π while the SHM captures the directional distribution of intensity by expressing it into a series of spherical harmonics. The FVM/DOM method is relatively simple to implement, but has several drawbacks, such as the fact that an iterative solution is required in the presence of scattering media or reflecting surfaces. In addition, its convergence is known to slow down for optically thick media where the directional discretization is required to be as fine as the spatial discretization to avoid the ray effects. The *P-1* method has so far been the most popular RTE solver within the SHM framework because of its simplicity, fairly good accuracy and its low requirement of computational time [4–6]. However, its accuracy is questionable in the presence of directionally inhomogeneous intensity distributions [16]. To achieve better accuracy, a number of higher-order *P-N*-approximations have been formulated [16]. Recently, Modest and Yang formulated a generic methodology that decomposes the RTE into $N(N+1)/2$ coupled second-order elliptic partial differential equations (PDE) for a given odd order *N*, allowing for variable properties and arbitrary three-dimensional geometries, including a set of generic boundary conditions [17].

Traditional turbulent combustion calculations treat radiation and turbulence as uncoupled processes using mean temperatures and concentrations to evaluate radiative properties and intensities [18]. Turbulence–radiation interaction (TRI) has been largely ignored to date due to its extreme complexity, even though its importance has been widely recognized [18]. Modest and coworkers [19] were the first to accurately model turbulent radiative emission within the context of the stochastic probability density function (PDF) method [20]. Typically the absorption coefficient–intensity correlation, i.e., "absorption TRI" was closed by invoking the optically thin fluctuation assumption (OTFA) [21]. Recently, a new approach, based on the photon Monte Carlo method for media represented by particle fields, has been developed by Wang and Modest [22], which evaluates absorption TRI exactly. Modest, Haworth and coworkers [18] used the composition PDF/Monte Carlo method to study radiative heat transfer in reactive flows.

The objective of this paper is to compare the effects of various spectral models for nongray multi-phase media, RTE solvers, and turbulence–radiation interactions in simulations of nonluminous and luminous methane–air turbulent jet flames. To the authors' knowledge, such detailed comparative study of radiation modeling in turbulent combustion simulation is absent from the literature. A high-accuracy hybrid flow–chemistry solver (finite volume flow solver + stochastic PDF chemistry solver) is interfaced with a spectral radiation solver, which is capable of performing combustion calculations for a three-dimensional unstructured mesh. The radiation module comprises four RTE solvers: *P-1*, *P-3* and FVM solvers implemented using the data structures of the finite-volume flow solver, and a stochastic PMC solver. The finite-volume-based radiation solvers are interfaced with a *k*-distribution-based spectral module and the stochastic PMC solver with a LBL module. The effects of various spectral models, RTE solvers and the consideration of TRI on flame radiant heat source, temperature, and NO emissions are discussed.

2. Numerical and physical models

2.1. Turbulent flow field

In this study a high-fidelity open source-code flow calculation software OpenFOAM [23] is employed as a finite-volume (FV) solver for Favre-averaged flow equations on an unstructured mesh. The equations include conservation of mass, momentum and enthalpy. A standard two equation k–ε model is employed as a turbulence model [24]. An iteratively implicit, segregated solution procedure solves the coupled system of governing PDEs for collocated cell-centered variables. Here statistically steady-state solutions are reached by time marching.

2.2. Composition PDF method

In composition PDF methods physical scalars, including temperature and species concentrations, are treated as independent random variables. The joint PDF is a function of spatial location, time and composition space. Once the joint PDF is obtained at a certain position $\underline{x}$ and time instant t, the mean value for any function, Q, of these scalars can be evaluated exactly as

$$\langle Q(\underline{x},t)\rangle = \int_{-\infty}^{\infty} Q(\underline{x},t) f(\underline{\psi};\underline{x},t)\,\mathrm{d}\underline{\psi} \tag{1}$$

where $\underline{\phi}(\underline{x},t)$ is the vector of physical scalars, $\underline{\psi}$ is the corresponding random variable vector, Q is a function of $\underline{\phi}$ only and f is the joint PDF, which represents the probability density of a compound event $\underline{\phi}=\underline{\psi}$. In practice the mass density PDF, $\mathcal{F}(\underline{\psi};\underline{\mathbf{x}},t)=\langle\rho(\underline{\mathbf{x}},t)\rangle f(\underline{\psi};\underline{\mathbf{x}},t)$, is more convenient and frequently used and its transport equation can be derived based on the conservation of scalars as [18]

$$\begin{aligned}\frac{\partial\mathcal{F}}{\partial t}+\frac{\partial}{\partial x_i}[\widetilde{u}_i\mathcal{F}]+\frac{\partial}{\partial\psi_\alpha}[S_{\alpha,\mathrm{reac}}(\underline{\psi})\mathcal{F}] = &-\frac{\partial}{\partial x_i}\left[\left\langle u_i''\mid\underline{\psi}\right\rangle\mathcal{F}\right]\\ &+\frac{\partial}{\partial\psi_\alpha}\left[\left\langle\frac{1}{\rho}\frac{\partial J_i^\alpha}{\partial x_i}\mid\underline{\psi}\right\rangle\mathcal{F}\right]\\ &-\frac{\partial}{\partial\psi_s}[\langle S_{\mathrm{rad}}|\underline{\psi}\rangle)\mathcal{F}]\end{aligned} \tag{2}$$

where i and α are summation indices in physical space and composition space, respectively, and $\langle A|B\rangle$ is the conditional mean of event A, given that event B occurs. Variables with tildes and double primes are Favre means of the variables and fluctuations about them. u is the velocity vector, J is the flux due to molecular diffusion and S source term due to chemical reaction and radiation. Terms appearing on the left-hand side of Eq. (2) can be accounted for exactly. The first two terms are the rate of change and the advection of the PDF in the Favre-averaged mean flow. The third term is the transport of the PDF in composition space due to