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Simulating turbulence–radiation interactions using a presumed probability density function method

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ABSTRACT

In turbulent combustion, the turbulent fluctuations of temperature and species concentrations have strong effects on chemical and radiative heat sources. Turbulence–chemistry interactions (TCI) and turbulence–radiation interactions (TRI) create a set of "closure" problems when the governing partial differential equations are averaged. The presumed probability distribution function (presumed-PDF) method assumes a form of probability distribution function to close the chemical source term. The emphasis of this work is developing a high-fidelity radiation model that works in tandem with combustion models that use the presumed-PDF method to close the turbulent source terms. A finite volume based photon Monte Carlo method with a line-by-line spectral model is applied with the presumed-PDFs of mixture fraction, scalar dissipation rate and enthalpy defect to account for TRI effects. An efficient wavenumber selection scheme is proposed for the line-by-line photon Monte Carlo method considering TRI. The model is validated with one-dimensional exact line-by-line solutions for different TRI treatments and with a coupled combustion simulation for an open jet flame.

1. Introduction

Many turbulent reacting flow simulations involve turbulence, chemistry and radiation; each of which ranks among the most challenging problems in the thermal sciences, and which interact in highly nonlinear ways. In turbulent combustion modeling, the transported probability density function (PDF) method solves the evolution of the one-point, one-time PDF for a set of variables that determines the local thermochemical and/or hydrodynamic state of a reacting system [1]. This method is fairly elaborate, and consequently, computationally expensive, especially when used in large eddy simulation (LES) and when the number of chemical species is large [2,3]. On the other hand, presumed-PDF methods give a form of PDF to close the chemical source term, which is computationally less expensive even if complex chemical mechanisms are considered. The purpose of this study is to develop a novel and more efficient high-fidelity radiation model including turbulence–radiation interactions (TRI) using a presumed-PDF method. The presumed-PDF method is commonly combined with a flamelet model to describe mean values of density and reactive scalars [4]. Due to the complexities encountered in reacting flow simulations, radiation is either neglected [5–10] or simulated with very simple radiation models [11–18]. Adding detailed treatment of radiation adds layers of complexities, making simulations computationally extremely expensive. However, radiation plays a major role in heat transfer at high temperatures as found in reacting flows, and radiation is affected by turbulence in much the same way as is convection [3]. In the present study, a radiation model is developed using a the presumed-PDF method to account for radiation and TRI in reacting flow simulations.

In traditional combustion simulations, radiation and turbulence are usually treated as uncoupled processes, using mean temperatures and concentrations to evaluate radiative intensities and properties [19]. To model radiative heat loss, the radiative transfer equation (RTE) has to be solved to calculate the radiative source term contained in the mean energy equation. The RTE is an integro-differential equation for radiative intensity in six independent variables (three spatial, two directional and one spectral). Consequently, the high dimensionality of the RTE prevents it from being solved exactly in general conditions [20]. In order to account for thermal radiation, many combustion simulations [18,21–24] have applied the optically-thin approximation (OT). In this approximation, emission is calculated and self-absorption is ignored. Thus, the RTE does not need to be solved. This method always overestimates radiative heat loss. More accurate radiative heat loss calculations may be carried out by transforming the RTE into a set of

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Nomenclature

$C_{\epsilon 1}$	k-ϵ model constant, –
C_χ	model constant, –
C_p	heat capacity at constant pressure, J/kg·K
C^*	non-dimensional radiative heat power, –
E	radiative emission, W/m^3
h	enthalpy, J/kg
I	spectral intensity, W/cm^2·sr·m^{-1}
k	turbulent kinetic energy, m^2/s^2
Le	Lewis number, –
L_{st}	stoichiometric flame length, m
P	pressure, bar
Pr	Prandtl number, –
q	heat flux, W/m^2
R_η	random number for wavenumber of emission, –
S_{rad}	total radiative heat power, W
$\dot{Q}_{em}$	total emission, kW
$\dot{Q}_{net}$	total net radiative heat loss, kW
Q_{rad}	radiative heat source, W/m^3
t	time, s
T	temperature, K
u_i	velocity components, m/s
w	numerical quadrature weight, –
x_i	spatial coordinate components, m
Y_k	mass fraction of species k, –
Z	mixture fraction, –

Greek symbols

α	beta distribution parameter, –
β	beta distribution parameter, –
χ	scalar dissipation rate, s^{-1}
ϵ	turbulent dissipation rate, m^2/s^3
η	wavenumber, cm^{-1}
γ	beta distribution parameter, –
Γ	gamma function, –
κ_η	absorption coefficient, cm^{-1}
κ_P	Planck-mean absorption coefficient, cm^{-1}
μ_t	turbulent viscosity, kg/m·s
μ_{eff}	effective turbulent viscosity, kg/m·s
ϕ	gas state variable, –
$\dot{\omega}$	gas species production rates, kg/m^3·s
ρ	density, kg/m^3
σ	log-normal distribution parameter, –

Abbreviations

DNS	direct numerical simulation
DOM	discrete ordinates method
LBL	line-by-line
LES	large eddy simulation
OT	optically thin approximation
OTFA	optically thin fluctuation assumption
PDF	probability density function
PMC	photon Monte Carlo
RANS	Reynolds-averaged Navier-Stokes
RTE	radiative transfer equation
TCI	turbulence–chemistry interaction
TRI	turbulence–radiation interaction

simultaneous partial differential equations, such as the discrete ordinates method (DOM) or the spherical harmonics method (or PN method) [20]. The DOM is very popular in combustion solvers because of its ease of implementation and extension to high orders, and is commonly used for industrial combustor simulations with radiative heat transfer but is usually implemented with simple spectral models, mainly because of the large computational cost of the method [20,25]. On the other hand, the lowest order spherical harmonics method, the P1 method, is relatively easy to implement and has reasonable computational efficiency. However, the P1 method is usually only accurate in media with near-isotropic radiative intensity, and is extremely difficult to be extended to high orders due to the complicated mathematics involved. Recently, the PN method was extended to the order up to P7 for general 3-D and 2-D axisymmetric radiative heat transfer simulations [26–29]. It is evident [19,20,30,31] that among RTE solution methods, no single one can be regarded as the best for all problems. On the other hand, the photon Monte Carlo (PMC) method solves the RTE in a stochastic manner, which directly mimics the physical processes by releasing representative energy bundles (rays) into random directions, which are traced until they are absorbed at certain points in the medium or escape from the domain. This allows the accurate treatment of almost all the complications in radiative heat transfer modeling, such as nongray spectral properties, inhomogeneous media and irregular geometries, with relative ease. Early PMC studies were often applied with simplified spectral models for radiatively participating species, such as the gray-gas model [32,33], statistical narrow-band model [34,35], exponential wide-band model [36,37] and full-spectrum k-distribution (FSK) model [38]. The line-by-line (LBL) spectral model resolves all individual spectral lines, and is the most accurate spectral model. In PMC calculations, the LBL outperforms the FSK model in many aspects, as discussed in [39]; and thus is incorporated together with PMC (PMC–LBL) in the present study.

Experimental and numerical studies [40–48] have shown that turbulent fluctuations can significantly enhance radiative heat loss from turbulent flames. Accurate radiation modeling in turbulent combustion has to take TRI effects into account. However, full consideration of turbulence–radiation interactions is a rather difficult challenge [49] for traditional RTE solvers. Most works have applied the optically thin fluctuation assumption (OTFA) [50] to simplify the analysis, and it was found that this assumption is valid over the vast majority of situations in small-scale, lower-sooting flames. Mazumder and Modest [51] studied TRI with the OTFA in nonluminous flames using a velocity-composition joint PDF method. Thermal radiation was calculated using the P1–approximation with a wide band spectral model. Giordano and Lentini [52] applied the OTFA with a discrete transfer RTE solver and fitted Planck-mean absorption coefficients to study combustion–radiation–turbulence interaction in nonpremixed flames. Li and Modest [53,54] used a composition PDF method to study TRI in turbulent diffusion jet flames by applying the OTFA; radiation is solved with the P1–approximation and a full-spectrum correlated-k model. Snegirev [33] took TRI into account for a turbulent sooting flame by a Taylor expansion for emission around the mean temperature and neglecting higher order terms, and the OTFA was applied. Habibi et al. [55] investigated TRI effects in nonpremixed piloted turbulent laboratory-scale flames using DOM with the Weighted Sum of Gray Gases (WSGG) spectral model. They formulated five different TRI terms and also compared results with a simple optically thin model. Individual TRI contributions were isolated and quantified, and the OTFA was applied in all the cases. Poitou et al. [56]