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Detailed numerical simulation of thermal radiation influence in Sandia flame D

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Abstract

In order to investigate the influence of thermal radiation in turbulent combustion processes, Sandia flame D is numerically simulated, with multiple-time scale (MTS) k–ε turbulence model for turbulence, the combination of probability density function (PDF) transportation method, Lagrangian flamelet model (LFM) and the detailed chemical reaction mechanism GRI 3.0 (consisting of 53 species and 325 elemental reactions) for combustion and finite volume/correlated-k (FV/CK) method for radiation heat transfer. To account for turbulence's influence on radiation, the effects of turbulence–radiation interactions (TRI) are investigated in radiation calculations and it is recommended that for detailed numerical simulation TRI should be considered. Numerical results with and without radiation influence being taken into accounted are compared with experimental data. Different from reports by other researchers, our simulation results show that although the magnitude of thermal radiation is relatively small, its influence on combustion process is significant. It is suggested that turbulence and chemical reactions may magnify the influence of thermal radiation.

Keywords: Sandia flame D; PDF; LFM; FVM; Correlated-k; TRI

1. Introduction

A lot of efforts have been devoted to numerical simulation of flames and commercial combustion systems, in many cases of which thermal radiation may be an important heat transfer mode. However, to simulate thermal radiation in combustion processes accurately, there are several fundamental difficulties to overcome. First, the treatment of turbulent reacting flows itself is a challenging task [1,2]. Secondly, a solver of radiative transfer equation (RTE) which can be easily incorporated into CFD code is required. Thirdly, the radiative properties of real (non-gray) gases need to be determined. Finally, accurate prediction of influences of turbulence–radiation interaction (TRI) is necessary.

Although PDF transportation methods [3] significant advantage of exact treatment of chemical reactions is well known, the pure PDF method is rather computation expensive, especially when a detailed chemical mechanism such as GRI 3.0 [4] is implemented. In the present paper, a much more economical combustion submodel, namely the Lagrangian flamelet model [5] is used together with PDF transportation equation of mixture fraction to simulate the combustion process.

Up to date, there are many explored RTE solvers [6]. Among all these solvers, both DOM and FVM can be easily incorporated into CFD codes and FVM is the choice of the present work. Along with FVM, the correlated-k distribution (CK) method, which assumes absorption coefficient as the basic radiative property, is used to calculate the absorption coefficients of the radiative medium. The parameters for CK model are provided by EM2C [7].

The effect of turbulence–radiation interactions (TRI) has long been known. To the authors' best knowledge,

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Nomenclature

$c_{p\alpha}$	specific heat capacity of species α
c_p	specific heat capacity of the mixture
d	diameter of fuel jet nozzle for Sandia flame D
$\tilde{f}$	PDF of mixture fraction
g	cumulative distribution function of absorption coefficient
I_η	spectral radiative intensity
$I_{b\eta}$	spectral Plank function
J_i	molecular diffusive flux of mixture fraction
k	turbulent kinetic energy, $=k_p + k_t$
k_p	turbulent kinetic energy of large eddies in production range
k_t	turbulent kinetic energy of fine-scale eddies in dissipation range
k	absorption coefficient
k_η	spectral absorption coefficient
k_i^*	parameters of the correlated k-distribution model
L, M	total number of discrete polar and azimuthal angle
N_b	total number of molecular gas bands
N_Q	total number of quadrature points in each gas band
Q	partial function of an isolated absorbing molecule
S_α	reaction rate
S_R	rate of radiative heat loss per unit volume
T	temperature
t	time
W_H, W_C	atomic weight of the element H and O
x, r	cylindrical coordinates
X_s	molar partial pressure of s species
Y_α	mass fraction of species α
Y_H, Y_C	mass fraction of element H and O

Greek symbols

$\alpha_{m+1/2}$, $\alpha_{m-1/2}$	coefficients for angular-distribution term
ε_p	energy transfer rate from production range to dissipation range
ε, ε_t	dissipation rate of turbulent kinetic energy
μ_t	turbulent eddy-viscosity
ξ	mixture fraction
χ	scalar dissipation rate
ρ	density
$\bar{\rho}$	mixture density
Ω	solid angle
ξ^{lm}	direction-cosines of the axial direction
μ^{lm}	radial tangential direction
η^{lm}	tangential direction
$\Delta\eta$	wavenumber interval
ω_i	ith quadrature weight in the correlated k-distribution method
θ	polar angle measured from $\hat{e}_z$
ϕ	azimuthal (planar) angle measured from $\hat{e}_x$

Superscripts

1, 2	inlet of fuel and oxidant
l, m	angular direction

Subscripts

b	black-body
η	wavenumber
i	values at ith quadrature points
k	kth narrow band
st	stoichiometric condition

Mazumder and Modest are the first ones to present the idea of treating turbulence–radiation interactions by PDF/MC method [8]. Li and Modest [9], with the aid of FLUENT, investigated TRI in gaseous flames. In both works, a simplified reaction mechanism is chosen for the chemical reaction rate and P_1 is used to solve the RTE. In the present work, TRI is fully taken into accounted when doing radiation calculations and its influence on thermal radiation is briefly discussed as well.

Sandia flame D is selected here as the simulation case for the reason that organizers of the international workshop on computation of turbulent non-premixed flames (TNF) have recommended to consider radiation effects in the simulation of Flame D, especially when NO levels are to be predicted [10]. And there are some related research reports [11–13], which can be used as comparisons for our own research. The main purpose of this paper is to investigate the influence of thermal radiation on combustion calculations.

2. Mathematical modeling

For Sandia flame D, turbulent transportations along the axis are much larger than those of the radial direction, which justifies the flow being formulated into the boundary layer form. The flow can be described by parabolized Navier–Stokes (PNS) equation, which, in cylindrical coordinate system, can be written as

$$\frac{\partial(r\bar{\rho}\tilde{u})}{\partial x} + \frac{\partial(r\bar{\rho}\tilde{v})}{\partial r} = 0 \tag{1}$$

$$\bar{\rho}\tilde{u}\frac{\partial\tilde{u}}{\partial x} + \bar{\rho}\tilde{v}\frac{\partial\tilde{u}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_t\frac{\partial\tilde{u}}{\partial r} + (\rho_\infty - \bar{\rho})g\right) \tag{2}$$

2.1. Turbulence model

A multiple-time scale (MTS) k–ε turbulence model [14] is used for the turbulence calculation. The concept of the