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Direct numerical simulation of the turbulent premixed flame propagation with radiation effects

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ABSTRACT

This paper investigates the effects of turbulence on radiative heat transfer in premixed flame propagation using a combination of direct numerical simulation (DNS) and the discrete ordinates method (DOM). The DNS code has been validated and established in previous research, and the newly written DOM code is validated by solving a sample radiative heat transfer problem. The DOM code is explicitly combined with the DNS code using the 3rd-order Runge–Kutta scheme. In the numerical experiments, an initially flat laminar premixed flame interacts with imposed turbulent fluctuations and evolves over time. A remarkable increase in the temperature self-correlation factor $< T^4 > / < T>^4$ is observed in the middle of the reaction. Higher u' conditions induced faster and more intensive flame wrinkle evolution. However, flow turbulence reduces the radiative heat loss in planar premixed flame due to the flame curvature effects.
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1. Introduction

Premixed flame propagation and its interactions with turbulent flows involve complex and various types of physical phenomena. Due to their complexities, direct numerical simulations (DNSs) are frequently used for understanding premixed flame dynamics and flame–turbulence interactions [1]. With minimal use of numerical models and approximations, direct simulation of the full differential equations yields more accurate results than any other numerical approach. Asymptotic analysis is another accurate method to investigate premixed flame behavior [2]. However, asymptotic analysis cannot be applied to the highly fluctuating nonlinear behavior of a premixed flame. In contrast, DNSs can be used to investigate the nonlinear range of the flame in addition to the linear range [3,4].

Depending on the situation, radiative heat transfer plays an important role in flame dynamics. Radiative heat addition and loss influences the local flame temperature and flame speed. Turbulence and radiation interactions (TRIs) in reactive flows have long been studied due to their importance and complexities [5]. Coelho demonstrated that turbulent fluctuations can result in a 50% increase in computed radiative heat loss depending on the flame configuration [6]. Thus, radiative heat transfer should be carefully considered to accurately predict flame behavior. Because numerical errors in radiative heat transfer in turbulent flows result from averaging processes of the scalar data fluctuation, the radiative transfer equation should be solved using instantaneous scalar data without averaging to achieve a more accurate prediction of the radiation. To accomplish this, DNS should be employed in the study of TRIs. However, DNS has rarely been used to study TRIs [5]. Wu et al. were the first to present an investigation of TRIs in a premixed flame using DNS for the reactive flow simulation and the photon Monte Carlo method for radiative heat transfer [5,7]. In their results, the effects of TRIs were successfully quantified by accurate DNS and the photon Monte Carlo method. However, the photon Monte Carlo method required approximately ten times the CPU time of the simple-chemistry DNS code and was thus difficult to apply to more practical problems. Therefore, an accurate yet computationally inexpensive numerical code is necessary for the study of premixed flame dynamics with radiation effects.

The discrete ordinates method (DOM) [8] is one of the most widely used radiation models, as represents a good compromise between solution accuracy and computational requirements in many practical applications.

In the present study, DNS and the DOM are combined for the accurate yet relatively inexpensive calculation of a turbulent premixed flame with radiation effects. Formulations and numerical methods for the analysis are introduced. The accuracy of the DOM code is verified by solving a sample radiative heat transfer problem. The effects of flow turbulence on the radiative heat transfer in the premixed flame are explored with the validated code. The

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Nomenclature

c_0	speed of sound
D	mass diffusivity
k	wave number
k_i	wave number of the most energetic eddies
L_{ref}	reference acoustic length scale
L_{11}	longitudinal integral length scale
L_i	wavelength of the most energetic eddies
Le	Lewis number (=α/D)
Pr	Prandtl number
Q	heat release
R	gas constant
Re_a	acoustic Reynolds number $(= \frac{\rho_0 c_0 L_{ref}}{\mu_0})$
Sc	Schmidt number
S_L	Laminar flame speed
T	temperature
Y	mass fraction

Greek symbols

α	thermal diffusivity (=ν/Pr)
β	Zeldovich number (=$\frac{E_a}{RT_f^2}(T_f - T_0)$)
γ	ratio of specific heats (=C_p/C_v)
δ_{th}	thermal flame thickness $= \frac{T_f - T_0}{(dT/dx)\|_{T=(T_f+T_0)/2}}$
ε	emissivity
κ	absorption coefficient
λ_T	thermal conductivity
Λ	pre-exponential factor
θ	nondimensional temperature $= \frac{T-T_0}{T_f-T_0}$
μ	molecular viscosity
ν	kinematic viscosity (= $\frac{\mu}{\rho}$)
σ	heat release parameter (= $\frac{T_f - T_0}{T_f}$)
σ_s	scattering coefficient
$\dot{\omega}_R$	reaction rate
ω_z	vorticity
ω_0	scattering albedo (= $\frac{\sigma_s}{\kappa+\sigma_s}$)
Φ	scattering phase function
Ω	solid angle

Subscript

0	upstream reactants
2	downstream products
b	black body
f	flame
P	product
R	reactant
r	radiation
w	wall

Superscript

+	normalized by reference parameters shown in Table 1

computation speed, including for the radiative heat transfer analysis, is also discussed.

2. Formulation

The conservation equations for mass, momentum, energy, and species are solved to investigate the flame behavior. The governing equations in the compressible formulation are written as follows:

$$\frac{\partial \rho^+}{\partial t^+} + \frac{\partial}{\partial x_i^+}(\rho^+ u_i^+) = 0 \tag{1}$$

$$\frac{\partial}{\partial t^+}(\rho^+ u_i^+) + \frac{\partial}{\partial x_j^+}\left(u_j^+ \rho^+ u_i^+\right) = -\frac{\partial P^+}{\partial x_i^+} + \frac{1}{Re_a}\frac{\partial \tau_{ij}^+}{\partial x_j^+} \tag{2}$$

$$\frac{\partial e^+}{\partial t^+} + \frac{\partial}{\partial x_j^+}\left[(e^+ + P^+)u_j^+\right] = \frac{1}{Re_a}\frac{\partial}{\partial x_j^+}\left(u_i^+ \tau_{ij}^+\right) + \frac{1}{Re_a Pr} \times \frac{\partial}{\partial x_j^+}\left(\mu^+ \frac{\partial T^+}{\partial x_i^+}\right) + Q_R^+ \dot{\omega}_R^+ - \nabla \cdot q_r \tag{3}$$

$$\frac{\partial}{\partial t^+}(\rho^+ Y_i^+) + \frac{\partial}{\partial x_j^+}\left(u_j^+ \rho^+ Y_i^+\right) = \frac{1}{Re_a Sc}\frac{\partial}{\partial x_j^+}\left(\mu^+ \frac{\partial Y_i^+}{\partial x_j^+}\right) - \dot{\omega}_R^+ \tag{4}$$

where superscript "+" denotes a dimensionless variable based on the acoustic length and time scales. The reference parameters for nondimensionalization are listed in Table 1.

The divergence of the radiative heat flux term in the energy Eq. (3) acts as the radiative heat loss. With the gray gas assumption, this divergence can be expressed as

$$\nabla \cdot q_r = \kappa \cdot \left(4\pi I_b - \int_{4\pi} I(\vec{r}, \vec{s})d\Omega\right) \tag{5}$$

The reaction term in Eqs. (3) and (4) is modeled by a single species and single-step irreversible reaction (R → P), for which the heat release and the reaction rate are given by

$$Q_R^+ = \frac{1}{Y_{R,0}} c_0^2 (T_f^+ - T_0^+) = \frac{1}{Y_{R,0}} c_0^2 \left(\frac{\sigma}{1-\sigma}\right)\left(\frac{1}{\gamma - 1}\right) \tag{6}$$

$$\dot{\omega}_R^+ = \Lambda^+ \rho^+ Y_R^+ \exp\left(-\frac{\beta(1-\theta)}{1-\sigma(1-\theta)}\right) \tag{7}$$

where $\beta = \frac{E_a}{RT_f^2}(T_f - T_0)$ is the Zeldovich number and $\sigma = \frac{T_f - T_0}{T_f}$ is the heat release parameter.

With the gray gas assumption, the radiative intensity I can be obtained from the radiative transfer equation (RTE):

$$\frac{1}{\kappa + \sigma_s}\frac{dI(\vec{r},\vec{s})}{ds} = -I(\vec{r},\vec{s}) + (1-\omega_0)I_b(\vec{r}) + \frac{\omega_0}{4\pi}\int_{\Omega'=4\pi} I(\vec{r},\vec{s})\Phi(\vec{s}' \to \vec{s})d\Omega \tag{8}$$

3. Numerical method

3.1. Direct numerical simulation

The 2-D system of Eqs. (1)–(4) is discretized by a sixth-order explicit finite difference scheme [9] and is integrated by the

Table 1
Reference parameters for nondimensionalization.

Variables	Symbol	Reference scale
Velocity	u_i	c_0
Length	x_i	L_{ref}
Time	t	L_{ref}/c_0
Energy	E	c_0^2
Density	ρ	ρ_0
Pressure	P	$\rho_0 c_0^2$
Mass gas constant	R	$c_{p,0}$
Mass fraction	Y_i	$Y_{i,0}$
Viscosity	μ	μ_0
Mass diffusivity	D_i	$c_0 L$
Thermal conductivity	λ_T	$\mu_0 c_{p,0}$
Frequency factor	Λ	c_0/L_{ref}
Temperature	T	$T_{ref} = (\gamma - 1)T_0$

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