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Effect of an inlet temperature disturbance on the propagation of methane–air premixed flames in small tubes

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ABSTRACT

A flame stabilized in a tube is affected by the temperature disturbance and velocity profile at the inlet boundary. Thus, a multi-dimensional analysis is necessary near the flame. The deviation between one-dimensional and two-dimensional analyses near the flame was investigated quantitatively. The temperature profile in the radial direction was varied to investigate its effects on the propagation of methane–air premixed flames in small tubes. A numerical experiment with Navier–Stokes equations, an energy equation and species equations was conducted coupled with a single-step global-reaction model. Three different temperature profiles were examined for slip and no-slip wall boundary conditions. The effect of temperature profiles on the flame propagation velocity and flame shapes was not negligible depending on the magnitude of the temperature deviation and the tube diameter. This study evaluated a critical length scale of a computational domain or a thermal entrance length of a premixed flame over which the inlet temperature disturbance does not affect the flame characteristics.

1. Introduction

In the development of a small combustion device to be used as an energy source [1–5], heat regeneration using thermal conduction has been an important issue to overcome flame quenching in a small combustion space. As the simplest model of the premixed flame in a combustion space, a premixed flame in a channel or in a tube has been investigated experimentally [6,7]. Premixed flame propagation in a stream tube has been also studied as a fundamental issue in combustion. Two representative approaches concerned with this issue are one-dimensional (hereafter 1-D) analytical studies and two-dimensional (hereafter 2-D) numerical studies. However, the 2-D numerical results, even with fixed flow fields, differed greatly relative to the 1-D analytical results [8–10]. Moreover, this deviation between the 1-D and 2-D analyses becomes more significant when the flow redirection by the flame is considered either in terms of matched jump conditions [11–13] or by finite reaction rates [14–20]. Concerned with the conduction through the tube, previous studies investigated flame propagation in conductive narrow tubes with 1-D analyses [5,7,21–23] and 2-D computations [24–27]. However, many studies of the 2-D computations on the subject of tube conduction were not free from the developments of the temperature and velocity near the inlet boundary. This implies that there are a number of solutions depending on the tube length, even for a fixed specific tube. Thus, a unique solution for a stationary flame corresponding to a sufficiently long tube has yet to be clarified.

Here, an idea is suggested to decouple the problem of a flame in an infinitely long conductive tube into two separate regimes of 1-D and 2-D. Within a conductive tube, the wall temperature varies significantly near the flame. Hence, the temperature and velocity profiles of the gas mixture will vary depending on the wall temperature in both the radial and axial directions. A flame is thus affected by multi-dimensional phenomena, including the temperature disturbance and the flow redirection near the flame. Consequently, this becomes a 2-D or multi-dimensional problem. In contrast, temperature deviation in a sufficiently far upstream field may diffuse before it approaches the flame surface; only the mean temperature will then affect the flame propagation. This becomes a 1-D heat transfer problem that is consequently less difficult to estimate.

It then becomes possible to define the critical length scale or the thermal entrance length of a premixed flame below which a finite temperature disturbance in the radial direction affects the flame characteristics and thus where a multi-dimensional approach is necessary. The largest critical length scale will then correspond to that of an adiabatic condition. By choosing the critical length scale corresponding to an adiabatic condition, the computational results are decoupled from the wall properties. A sufficient computational domain is then guaranteed for all boundary condition cases.

In this study, therefore, the computational domain is limited to the gas phase, and the outermost boundary in the radial direction

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is imposed as an adiabatic condition. Two cases of velocity profiles of slip and no-slip conditions on the wall are imposed. Additionally, three cases of temperature profiles are imposed as inlet thermal conditions. Through a comparison of the propagation velocities and the flame shapes for these six compositing cases, the following issues are investigated. (1) Dependency of the propagation velocity on the mean temperature for slip and no-slip conditions, (2) effect of the inlet temperature disturbance on the flame propagation in slip and no-slip conditions, and (3) the critical length scale below which the temperature disturbance affects the flame propagation.

2. Numerical method

2.1. Equations

The governing equations of continuity, momentum, energy, and five species were solved simultaneously.

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{1}$$

Momentum equation:

$$\frac{\partial}{\partial t}(\rho u_i) + \nabla \cdot (\rho \mathbf{u} u_i) = \nabla \cdot (\mu \nabla u_i) - \frac{\partial P}{\partial x_i}. \tag{2}$$

Energy equation:

$$\frac{\partial}{\partial t}(\rho h) + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot \left(\frac{k}{c_p} \nabla h\right) - \sum_i^5 h_i^0 \omega_i M_i. \quad (\omega_i = \gamma_i \omega_{CH_4}, i = 1,\ 2,\ \ldots,\ 5) \tag{3}$$

Species equation:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i) = \nabla \cdot (\rho \mathscr{D}_i \nabla Y_i) + \omega_i M_i. \tag{4}$$

Here, ρ is the density, t the time, $\mathbf{u}$ the velocity vector, u_i the velocity composition, μ the viscosity, P the pressure, x_i the displacement coordinate, h the enthalpy, k the thermal conductivity, and c_p is the constant pressure heat capacity. For a particular species i, h_i^0 is the enthalpy of formation, ω_i the reaction rate, M_i the molar weight, γ_i the stoichiometric ratio, Y_i the mass fraction, and $\mathscr{D}_i$ is the mass diffusivity.

As it is known that even a single-step reaction model can effectively serve to investigate the flame interaction concerned with external perturbations in the flow and heat transfer [28], the reaction rate of methane was evaluated using the irreversible single-step global-reaction model, as follows:

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2, \tag{5}$$

$$\omega_{CH_4} = 2.3 \times 10^{13} \exp(-T_a/T)[CH_4]^{0.2}[O_2]^{1.3}. \tag{6}$$

In these equations, the dimension of the reaction rate ω_{CH_4} and the densities of the species were gmol $cm^{-3}s^{-1}$ and gmol cm^{-3}, respectively. This reaction model fundamentally follows the study of Westbrook and Dryer [29], and the activation temperature T_a was 24,358 K. As the pre-exponential constant depends on the method of evaluating mixture properties, it was re-adjusted to match the burning velocity at a stoichiometric condition to 40 cm/s. Gas properties for the corresponding mixture composition were evaluated using the CHEMKIN-II [30] and TRANFIT [31] packages.

According to a previous study [20], the grid scale around the reaction zone should be smaller than 25 μm to guarantee less than 0.1% error in the propagation velocity of a wrinkled flame. To investigate a moving premixed flame more efficiently, an adaptive grid system was applied starting from 100 to 12.5 μm. These adaptive grid points were continuously generated or eliminated during the computation depending on the flame position and shapes. Discussion in greater detail is available in the previous study [20].

2.2. Boundary conditions

The ordinary quenching diameter of methane–air stoichiometric mixtures is approximately 2.5 mm [32]. The computational quenching scale corresponding to a stationary flame in a cold wall was 2.47 mm in the aforementioned previous study [20]. As the present study originated from a practical issue regarding the development of a small combustor to overcome the ordinary quenching scale, a stream tube with a diameter of 2 mm (radius $R = 1$ mm) was chosen as a representative configuration.

Two cases of velocity profiles with the same total mass flow rate of $\rho_m U_m \pi R^2$ were examined in this study, where ρ_m and U_m are the gas density and mean velocity at the mean temperature, respectively. The first is a uniform velocity profile with the slip condition (UV) presented as Eq. (7a), and the second is a parabolic velocity profile with a no-slip condition (PV) presented as Eq. (7b).

$$u_x(r) = U_m, \quad \text{(for UV)}, \tag{7a}$$

$$u_x(r) = 2U_m\left\{1 - (r/R)^2\right\}, \quad \text{(for PV)}. \tag{7b}$$

It is notable that the mean velocity U_m at the inlet boundary was suitably adjusted to obtain a stationary flame. When the flame does not move during hundreds of computational time steps, that mean velocity was chosen as the propagation velocity. Additionally, to investigate the effect of the temperature disturbance at the inlet boundary conditions, different temperature profiles were examined. In this study, the range of the mean temperature T_m was 300–400 K. In a comparison of the temperature profiles, the averaged mean temperatures at the inlet boundary were kept equal to each other. To simplify the inlet boundary condition, c_p at the inlet boundary was assumed to be constant because its deviation within the temperature range was approximately 1%. The total sensible enthalpy at the inlet boundary can then be expressed coupled with velocity profile depending on the temperature and radius $u_x(T, r)$; it should be equal to the value corresponding to the uniform temperature and slip condition (UV). This can be expressed as follows:

$$2\pi c_p \int_0^R \rho(T) u_x(T, r)\{T(r) - T_0\} r dr = \rho_m U_m c_p (T_m - T_0)\pi R^2. \tag{8}$$

As the density of the premixed gas varies depending on the gas temperature, the velocity profiles are also affected by the temperature profile. To clarify the definition of the inlet boundary condition, it was assumed that the local mass flow rate is kept constant without depending on the temperature; i.e., $\rho(T)u_x(T, r) = \rho_m u_{x,T_m}(r)$; here, $u_{x,T_m}(r)$ is the axial velocity with a constant mean temperature. This assumption is widely used in an analytical approach. Eq. (8) then becomes

$$2\pi \rho_m c_p \int_0^R u_{x,T_m}(r)\{T(r) - T_0\} r dr = \rho_m U_m c_p (T_m - T_0)\pi R^2, \tag{9}$$

or

$$\int_0^R u_{x,T_m}(r)\{T(r) - T_0\} r dr = U_m (T_m - T_0) R^2/2. \tag{10}$$

There could be infinite number of temperature profiles that satisfy Eq. (10). In this study, three representative temperature profiles were adopted, as shown in Fig. 1; a uniform temperature profile (hereafter UT, Fig. 1a), a negative temperature profile (NT, Fig. 1b), and a positive temperature profile (PT, Fig. 1c). In the case of the NT and PT, the temperature gradient in the radial direction is negative and positive, respectively. The mean temperature is defined as $T_m = (T_H + T_0)/2$, where T_0 is the reference temperature of 300 K and T_H is the highest temperature. Temperature deviation is defined