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Zone conditional analysis of a freely propagating one-dimensional turbulent premixed flame

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Abstract

The zone conditional conservation equations are derived and validated against the DNS data of a freely propagating one-dimensional turbulent premixed flame. Conditional flow velocities are calculated by the conditional continuity and momentum equations, and a modeled transport equation for the Reynolds average reaction progress variable. An asymptotic formula for turbulent burning velocity is obtained with the effects of a finite Damköhler number accounted for as an additional factor. It is shown that flame generated turbulence is primarily due to correlations between fluctuating gas velocities and fluctuating unit normal vector on a flame surface. More investigation is required to validate general predictive capability of the derived conditional conservation equations and the relationships modeled for closure.

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Keywords: Zone conditional averaging; Premixed turbulent combustion; Turbulent burning velocity; Flame generated turbulence

1. Introduction

The Bray–Moss–Libby formulation for premixed turbulent combustion is based on Favre averaging in terms of the mixture properties of burned and unburned gas. Although Favre averaging produces the same form of equations as in a non-reacting flow, they involve additional complexities such as countergradient diffusion due to large disparity between burned and unburned gas properties. In our previous work [\[1,2\]](#page--1-0) the conditional conservation equations for mass, momentum, and enthalpy were derived by zone conditional averaging with flame surface averages modeled for closure. Similar efforts by a few investigators [\[3,4\]](#page--1-0) were not applicable to flames with intense heat release and a large density ratio. Zone conditional averaging is suitable for high Damköhler number flames, in which two distinct zones, unburned and fully burned gas, are separated by infinitesimally thin stretched flamelets. In the present work, conditional flow velocities and pressures, flame propagation characteristics, and flame generated turbulence are calculated from conditional conservation equations of mass, momentum, and turbulent kinetic energy by a CFD solution procedure. The results are compared with the DNS data [\[5\]](#page--1-0) of a one-dimensional freely propagating flame, which does not involve uncertainties due to an externally imposed pressure gradient and multidimensional effects in an impinging jet [\[1,2\]](#page--1-0).

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2. Mathematical procedures

2.1. Zone conditional averaging

Instantaneous reaction field is divided into three distinct zones; unburned ($\rho = \rho_{\rm u}$), burned $(\rho = \rho_b)$, and reaction zone $(\rho_b < \rho < \rho_u)$. The Heaviside function is defined as

$$
H_{c^*}(\mathbf{x}, t, c) = H(c - c^*) = \begin{cases} 1 & \text{if } c(\mathbf{x}, t) \geq c^*, \\ 0 & \text{otherwise}, \end{cases}
$$
(1)

where c^* is usually set equal to 0.5. The reaction zone becomes infinitesimally thin with negligible probability of $0 \leq c \leq 1$ in the limit of a high Damköhler number. For any quantity, Φ , it holds that

$$
\langle H_{c^*} \Phi \rangle = \bar{c} \langle \Phi \rangle_b,\tag{2}
$$

$$
\langle (1 - H_{c^*})\Phi \rangle = (1 - \bar{c}) \langle \Phi \rangle_u,\tag{3}
$$

where $\langle \Phi \rangle$ and $\langle \Phi \rangle$ are the conditional averages in burned and unburned gas. Define that

$$
\Phi_i = \langle \Phi \rangle_i + \Phi'_i,\tag{4}
$$

where the subscript i can be any of u , b , su or sb . The notations, sb and su, represent the conditional average quantities in burned and unburned gas adjacent to the thin reaction zone as shown in Fig. 1. The two averages, $\langle \Phi \rangle$ _u and $\langle \Phi \rangle$ _{su} (or $\langle \Phi \rangle$ _b and $\langle \Phi \rangle_{sb}$, may not necessarily be equal to each other. When integrated over volume, the former represents a volumetric average while the latter represents a surface average on the unburned (or burned) side of flame surfaces. The conditional surface averages are defined as:

$$
\langle \Phi \rangle_{\rm su} = \lim_{\delta_f \to 0} \langle \Phi \mid c = 0 + \varepsilon \rangle,\tag{5}
$$

$$
\langle \Phi \rangle_{\rm sb} = \lim_{\delta_{\rm f} \to 0} \langle \Phi \mid c = 1 - \varepsilon \rangle,\tag{6}
$$

where δ_f is the reaction zone thickness defined as $0 + \varepsilon \leqslant c \leqslant 1 - \varepsilon$ for a small positive number, ε .

Fig. 1. Illustration of an instantaneous reaction field around a flamelet surface.

The conditional surface averages, $\langle \Phi \rangle_{\text{su}}$ and $\langle \Phi \rangle_{\text{sb}}$, become independent of c^* or ε in the limiting condition that δ_f goes to zero. Conditional density fluctuation is ignored as negligible with constant $\rho_{\rm b}$ and $\rho_{\rm u}$. Since variable density and chemical reaction are confined to the thin reaction zone, all reaction terms can be represented as simple interfacial transfer in terms of surface average quantities and mean reaction rate.

2.2. Conditional conservation equations for mass and momentum

The instantaneous local balance equations are:

$$
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,\tag{7}
$$

$$
\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p - \nabla \cdot \mathbf{\tau},\tag{8}
$$

where τ is the shear stress tensor due to molecular viscosity. Conditionally averaged conservation equations may be derived by averaging the instantaneous mass and momentum equations multiplied by H_{c^*} for burned zone and by $1 - H_{c^*}$ for unburned zone [\[1\].](#page--1-0) The conditional continuity and momentum equations in burned and unburned gas are given as:

$$
\frac{\partial}{\partial t} (\bar{c}\rho_{b}) + \nabla \cdot (\bar{c}\rho_{b} \langle \mathbf{v} \rangle_{b}) = \rho_{b} S_{\mathrm{L}b} \Sigma_{\mathrm{f}},\tag{9}
$$
\n
$$
\frac{\partial}{\partial t} [(1 - \bar{c})\rho_{\mathrm{u}}] + \nabla \cdot [(1 - \bar{c})\rho_{\mathrm{u}} \langle \mathbf{v} \rangle_{\mathrm{u}}] = -\rho_{\mathrm{u}} S_{\mathrm{L}u} \Sigma_{\mathrm{f}},\tag{10}
$$

$$
\frac{\partial}{\partial t} (\bar{c}\rho_{b}\langle \mathbf{v} \rangle_{b}) + \nabla \cdot (\bar{c}\rho_{b}\langle \mathbf{v} \rangle_{b}\langle \mathbf{v} \rangle_{b})
$$
\n
$$
= -\nabla (\bar{c}\langle \rho \rangle_{b}) - \nabla \cdot (\bar{c}\rho_{b}\langle \mathbf{v}'_{b}\mathbf{v}'_{b}\rangle)
$$

$$
+\rho_{b}S_{Lb}\langle \mathbf{v}\rangle_{sb}\Sigma_{f}-\langle p\mathbf{n}\rangle_{sb}\Sigma_{f},\tag{11}
$$

$$
\frac{\partial}{\partial t} \left[(1 - \bar{c}) \rho_{\rm u} \langle \mathbf{v} \rangle_{\rm u} \right] + \nabla \cdot \left[(1 - \bar{c}) \rho_{\rm u} \langle \mathbf{v} \rangle_{\rm u} \langle \mathbf{v} \rangle_{\rm u} \right] \n= -\nabla \left[(1 - \bar{c}) \langle p \rangle_{\rm u} \right] - \nabla \cdot \left[(1 - \bar{c}) \rho_{\rm u} \langle \mathbf{v}^{\prime}_{\rm u} \mathbf{v}^{\prime}_{\rm u} \rangle \right] \n- \rho_{\rm u} S_{\rm Lu} \langle \mathbf{v} \rangle_{\rm su} \Sigma_{\rm f} + \langle p \mathbf{n} \rangle_{\rm su} \Sigma_{\rm f},
$$
\n(12)

where the shear stress on a flame surface is ignored in comparison with the terms due to pressure difference and interfacial momentum flux. The laminar flame speed, S_{Lu} , is the displacement speed of a flame surface relative to adjacent unburned gas, i.e., $\mathbf{v}_s = \mathbf{v}_{su} + \mathbf{n}S_{Lu}$, where \mathbf{v}_s is the velocity of an iso- c flame surface. The laminar flame speed, S_{Lb} , is the displacement speed relative to adjacent burned gas, i.e., $\mathbf{v}_s = \mathbf{v}_{sb} + \mathbf{n}S_{Lb}$. Note that $\rho_b S_{\text{Lb}} = \rho_u S_{\text{Lu}}$. The interfacial transfer terms in Eqs. (9) – (12) all involve flame surface density and should add up to zero to guarantee overall conservation as follows:

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