On Characterization of Turbulence in Premixed Flames

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1 Introduction

The problem of premixed turbulent combustion modeling may be divided into two equally important parts: modeling of the effects of turbulence on flame propagation and modeling of the effects of the heat release in the flame on the turbulence. For instance, expressions for the turbulent burning velocity $U_t = U_t(u'/S_L, L/\delta_L)$ or the mean mass rate $\bar{w} = \bar{w}(\tilde{c}, \sigma, u'/S_L, L/\delta_L)$ of product creation as functions of the Favre-averaged combustion progress variable $\tilde{c}$, the density ratio $\sigma \equiv \rho_u/\rho_b$, the laminar flame speed S_L and thickness δ_L, and such turbulence characteristics as rms velocity u' and integral length scale L result from studying the former subproblem, with the progress obtained in this field being reviewed elsewhere [1]. The latter subproblem involves particularly an evaluation of the Reynolds stresses $\overline{\rho u_i'' u_j''}$, turbulent kinetic energy $\tilde{k}$, and dissipation rate $\tilde{\varepsilon}$ in a flame. Here, ρ is the gas density, u_i is the i-th component of the flow velocity vector, indexes u and b designate the unburned and burned mixture, respectively, overbars denote Reynolds averaging with $q' \equiv q - \bar{q}$ for a quantity q, and $\tilde{q} \equiv \overline{\rho q}/\bar{q}$ is the Favre averaged value of q with $q'' \equiv q - \tilde{q}$.

Modeling of the effects of the heat release on turbulence is not reduced solely to the evaluation of $\overline{\rho u_i'' u_j''}$, $\tilde{k}$, $\tilde{\varepsilon}$, etc. Even if submodels which perfectly predict both $\bar{w}(\tilde{c}, \sigma, u'/S_L, L/\delta_L)$ and $\overline{\rho u_i'' u_j''}$ in flames were available, the problem of premixed turbulent combustion modeling would not be solved. The point is that all available consistent physical models of the effects of turbulence on premixed combustion consider u' to be the turbulence characteristic, whereas $\overline{\rho u_i'' u_j''}$ in a flame is affected not only by the turbulence but also by the velocity jump across an instantaneous flame front (flamelet), which typically is much thinner than the mean flame thickness δ_t. For instance, if the probability γ of finding intermediate (between unburned and burned) states of the mixture is much less than unity everywhere within a turbulent flame, the well-known BML approach yields the following expression [2]

$$\overline{\rho u_i'' u_j''} = \underbrace{\bar{\rho}(1-\tilde{c})(\overline{u_i' u_j'})_u + \bar{\rho}\tilde{c}(\overline{u_i' u_j'})_b}_{A} + \underbrace{\bar{\rho}\tilde{c}(1-\tilde{c})\,(\bar{u}_{i,b} - \bar{u}_{i,u})\,(\bar{u}_{j,b} - \bar{u}_{j,u})}_{B}, \tag{1}$$

where term B is controlled by the velocity jump. Thus, to evaluate $\bar{w}(\tilde{c}, \sigma, u'/S_L, L/\delta_L)$, one has to determine the turbulence characteristics u' and L based on computed fields of $\overline{\rho u_i'' u_j''}$ (or $\tilde{k}$) and $\tilde{\varepsilon}$ by taking into account that the latter quantities characterize not only the turbulence but also the unburned/burned intermittency due to flamelet motion.

A common way of resolving this problem consists of using conditionally averaged quantities like $(\overline{u_i' u_j'})_u$ and $(\overline{u_i' u_j'})_b$ to characterize the turbulence in the unburned and burned mixture, respectively. Such conditioned second moments were determined in many experimental and DNS studies of premixed

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turbulent combustion. Bray et al. [2] proposed certain hypotheses that allowed ones to evaluate the conditioned second moments using Eq. 1 and the computed field of $\overline{\rho u_i'' u_j''}$.

The main goal of the present work is to show that the conditioned Reynolds stresses $(\overline{u_i' u_j'})_u$ and $(\overline{u_i' u_j'})_b$ are controlled not only by turbulence but also by flamelet motion (i.e., combustion) and, hence, the use of them as the turbulence characteristics is not justified in a general case.

To show this, a very simple model problem is considered in the next section followed by a discussion of a more general case in the subsequent section.

2 A simple problem

Let us consider a planar, one-dimensional, infinitely thin, self-propagating interface between reactants and products, which oscillates in a planar one-dimensional flow

$$u(t) = S_L + U \sin(\omega t) \tag{2}$$

in the case of ρ =const. Since the density is constant, such a hypothetical flame does not affect the flow and, hence, the rms velocity $\overline{u'^2} = \overline{(u - S_L)^2} = u^2/2$ is the same in the oncoming flow and within the flame. However, $(\overline{u'^2})_u \neq (\overline{u'^2})_b \neq \overline{u'^2}$. Indeed, in any point $-U/\omega \leq x \leq U/\omega$ within the flame, the unburned mixture is observed from $t_f = \arccos(-\omega x/U)/\omega$ till $T - t_f$ during a single period $T = 2\pi/\omega$ of the oscillations (the interface is located in $x = -U/\omega$ at $t = 0$). Accordingly, for any quantity q,

$$\bar{q}_u = \frac{1}{T - 2t_f} \int_{t_f}^{T-t_f} q dt, \qquad \bar{q}_b = \frac{1}{2t_f} \left(\int_0^{t_f} q dt + \int_{T-t_f}^{T} q dt \right). \tag{3}$$

Using these equations one easily can show that $\bar{u}_u = \bar{u}_b = S_L$,

$$(\overline{u'^2})_u = \frac{U^2}{2} \left[1 - \frac{\sin(2 \arccos(\omega x/U))}{2 \arccos(\omega x/U)} \right], \qquad (\overline{u'^2})_b = \frac{U^2}{2} \left[1 + \frac{\sin(2 \arccos(\omega x/U))}{2\pi - 2 \arccos(\omega x/U)} \right]. \tag{4}$$

For instance, if $x = U/(\omega\sqrt{2})$, then $\arccos(\omega x/U) = \pi/4$ and Eq. 4 yields

$$\frac{(\overline{u'^2})_u}{(\overline{u'^2})_b} = \frac{1 - 2/\pi}{1 + 2/(3\pi)} \approx 0.3. \tag{5}$$

If $x = -U/(\omega\sqrt{2})$, then $(\overline{u'^2})_u/(\overline{u'^2})_b \approx 3.3$. Thus, the conditionally averaged rms velocities may substantially vary across the flame considered, whereas the real rms velocity is spatially uniform and equal to $U^2/2$ everywhere within the flame in the constant density case analyzed here.

This simple particular example clearly shows that the conditioned Reynolds stresses $(\overline{u_i' u_j'})_u$ and $(\overline{u_i' u_j'})_b$ characterize not only the turbulence but also the unburned/burned intermittency.

3 Premixed turbulent combustion in the flamelet regime

The above example deals with a deterministic flow field. Let us consider a more realistic case of premixed turbulent combustion in the flamelet regime, with the probability γ of finding the flamelet being assumed to be much less than unity everywhere within the flame. By invoking the BML approach [2] to study this problem, one can express conditioned velocities and Reynolds stresses through the following Favre-averaged second, $\overline{\rho u_i'' u_j''}$ and $\overline{\rho u_i'' c''}$, and third, $\overline{\rho u_i'' u_j'' c''}$, moments. For instance,

$$\bar{u}_{i,b} = \tilde{u}_i + \frac{\overline{\rho u_i'' c''}}{\bar{\rho} \tilde{c}} \tag{6}$$

and

$$\bar{\rho}\tilde{c}(\overline{u_i'u_j'})_b = \tilde{c}\overline{\rho u_i''u_j''} + \overline{\rho u_i''u_j''c''} - \frac{\overline{\rho u_i''c''}\cdot\overline{\rho u_j''c''}}{\bar{\rho}\tilde{c}}. \quad (7)$$

Due to space limitation, only equations conditioned to the burned mixture are reported here.

By manipulating with the balance equations for $\overline{\rho u_i''u_j''}$, $\overline{\rho u_i''c''}$, and $\overline{\rho u_i''u_j''c''}$ and the instantaneous mass, impulse, and progress variable balance equations, the following conditioned equations

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}) + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{c}\bar{u}_{k,b}) = \gamma\overline{\left(\rho\frac{\mathrm{D}c}{\mathrm{D}t}\right)_f}, \quad (8)$$

where the right hand side is approximately equal to the mean mass rate $\bar{w}$ of product creation,

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{c}\bar{u}_{i,b}) + \frac{\partial}{\partial x_k}(\bar{\rho}\tilde{c}\bar{u}_{i,b}\bar{u}_{k,b}) + \frac{\partial}{\partial x_k}\left[\bar{\rho}\tilde{c}(\overline{u_i'u_k'})_b\right] + \bar{c}\overline{\left(\frac{\partial p}{\partial x_i}\right)_b} - \bar{c}\overline{\left(\frac{\partial \tau_{i,k}}{\partial x_k}\right)_b} = \gamma\overline{\left[\rho\frac{\mathrm{D}}{\mathrm{D}t}(u_i c)\right]_f}, \quad (9)$$

and

$$\frac{\partial}{\partial t}\left[\bar{\rho}\tilde{c}(\overline{u_i'u_j'})_b)\right] + \frac{\partial}{\partial x_k}\left[\bar{\rho}\bar{u}_{k,b}\tilde{c}(\overline{u_i'u_j'})_b\right] + \frac{\partial}{\partial x_k}\left[\bar{\rho}\tilde{c}(\overline{u_i'u_j'u_k'})_b\right] + \bar{\rho}\tilde{c}(\overline{u_j'u_k'})_b\frac{\partial \bar{u}_{i,b}}{\partial x_k} + \bar{\rho}\tilde{c}(\overline{u_i'u_k'})_b\frac{\partial \bar{u}_{j,b}}{\partial x_k} \quad (10)$$

$$-\bar{c}\overline{\left(u_j'\frac{\partial \tau_{i,k}}{\partial x_k}\right)_b} - \bar{c}\overline{\left(u_i'\frac{\partial \tau_{j,k}}{\partial x_k}\right)_b} + \bar{c}\overline{\left(u_j'\frac{\partial p}{\partial x_i}\right)_b} + \bar{c}\overline{\left(u_i'\frac{\partial p}{\partial x_j}\right)_b}$$

$$= \gamma\overline{\left[\rho\frac{\mathrm{D}}{\mathrm{D}t}(u_i u_j c)\right]_f} - \gamma\bar{u}_{j,b}\overline{\left[\rho\frac{\mathrm{D}}{\mathrm{D}t}(u_i c)\right]_f} - \gamma\bar{u}_{i,b}\overline{\left[\rho\frac{\mathrm{D}}{\mathrm{D}t}(u_j c)\right]_f} + \gamma\bar{u}_{i,b}\bar{u}_{j,b}\overline{\left(\rho\frac{\mathrm{D}c}{\mathrm{D}t}\right)_f}$$

can be derived starting from Eqs. 6 and 7 without invoking any assumptions with the exception of the well-known BML decomposition [2]

$$\bar{q} = (1-\bar{c})q_u + \bar{c}q_b, \qquad \tilde{q} = (1-\tilde{c})q_u + \tilde{c}q_b, \qquad \overline{\frac{\partial q}{\partial x_i}} = (1-\bar{c})\overline{\left(\frac{\partial q}{\partial x_i}\right)_u} + \bar{c}\overline{\left(\frac{\partial q}{\partial x_i}\right)_b} + \gamma\overline{\left(\frac{\partial q}{\partial x_i}\right)_f}, \quad (11)$$

with the last term being kept in the last expression, because the gradient of q may be large inside flamelets. Balance equations conditioned to the unburned mixture look similar to Eqs. 8-10, with $\tilde{c}$ being replaced by $1-\tilde{c}$. Here, q is any flow characteristic, p is the pressure, $\tau_{i,j}$ is the viscous stress tensor, the summation convention applies for repeated index k, and

$$\frac{\mathrm{D}}{\mathrm{D}t} \equiv \frac{\partial}{\partial t} + u_k\frac{\partial}{\partial x_k}. \quad (12)$$

If $\gamma \equiv 0$ and $\bar{c} \equiv 1$ (no flamelets), Eqs. 8-10 reduce to the standard Reynolds-averaged balance equations. However, if $\gamma > 0$, the right hand sides of Eqs. 8-10 contain terms, which are absent in the Reynolds-averaged equations, these terms being controlled by flamelet structure and flamelet motion, i.e., by combustion. Thus, Eqs. 8-10 show that the conditioned Reynolds stresses are not the characteristics of turbulence, but they are also affected by chemical reactions even in the constant density case.

Equations 8-10 offer an opportunity to separate modeling different physical mechanisms from one another. For instance, if (i) the Kolmogorov length scale $\eta = (\nu_u^3/\tilde{\varepsilon})^{1/4}$ is much larger than δ_L and (ii) the Kolmogorov time scale $\tau_\eta = (\nu_u/\tilde{\varepsilon})^{1/2}$ is much larger than the chemical time scale $\tau_c = \delta_L/S_L$, then, (i) variations in the tangential flow velocity across flamelets are negligible i.e., $\overline{[\mathrm{D}/\mathrm{D}t(\mathbf{u}_t c)]_f} = \bar{\mathbf{u}}_{t,f}\overline{(\mathrm{D}c/\mathrm{D}t)_f}$, and (ii) flamelets retain the structure of the unperturbed laminar flame, i.e., $\overline{[\mathrm{D}/\mathrm{D}t(u_n^q c)]_f} = \rho_u(\sigma S_L)^q/\tau_c$ for any power exponent q. Here, ν_u is the kinematic viscosity of the unburned mixture, $u_n = n_k u_k$ and $\mathbf{u}_t = \mathbf{u} - \mathbf{n}(\mathbf{un})$ are components of the flow velocity vector, normal and tangential, respectively, to the flamelet surface, $\bar{\mathbf{u}}_{t,f}$ is the tangential velocity conditionally averaged on the flamelet surface, $\mathbf{n}$ is the unity normal to the surface, and n_i is the i-th component of this vector.

Accordingly, since $\gamma\rho_u/\tau_c = \gamma\overline{(\mathrm{D}c/\mathrm{D}t)}_f \approx \bar{w}$,

$$\overline{\rho\left[\frac{\mathrm{D}}{\mathrm{D}t}(u_i c)\right]}_f = \left\{\sigma S_L + \bar{u}_{i,f} - \overline{[(u_k n_k) n_i]_f}\right\}\bar{w} = \underbrace{\left\{S_L + \bar{u}_{i,f} - \overline{[(u_k n_k) n_i]_f}\right\}\bar{w}}_{I} + \underbrace{(\sigma - 1) S_L \bar{w}}_{II} \tag{13}$$

and

$$\overline{\left[\rho\frac{\mathrm{D}}{\mathrm{D}t}(u_i u_j c)\right]}_f = \underbrace{\left\{S_L^2 + S_L\left[\bar{u}_{i,f} + \bar{u}_{j,f} - \overline{[(u_k n_k) n_i]_f} - \overline{[(u_k n_k) n_j]_f}\right]\right.}_{III} \tag{14}$$

$$\underbrace{\left. + \bar{u}_{i,f}\bar{u}_{j,f} - \bar{u}_{i,f}\overline{[(u_k n_k) n_j]_f} - \bar{u}_{j,f}\overline{[(u_k n_k) n_i]_f} + \overline{[(u_k n_k)^2 n_i n_j]_f}\right\}\bar{w}}_{III}$$

$$+ \underbrace{\left\{(\sigma^2 - 1) S_L^2 + (\sigma - 1) S_L\left[\bar{u}_{i,f} + \bar{u}_{j,f} - \overline{[(u_k n_k) n_i]_f} - \overline{[(u_k n_k) n_j]_f}\right]\right\}}_{IV}.$$

Terms I and III in Eqs. 13 and 14, respectively, model the differences between the unconditioned and conditioned quantities due to flamelet motion and structure, whereas terms II and IV are controlled by the velocity jump across flamelets due to the heat release. Thus, not only term B in Eq. 1 but also term A are affected by the velocity jump. Moreover, both terms A and B are also affected by chemical reactions even in the constant density case, whereas the reactions do not modify the real turbulence if ρ =const. Therefore, to close $\bar{w}(\tilde{c}, \sigma, u'/S_L, L/\delta_L)$, the two above effects should be eliminated when evaluating u' based on computed fields of $(\overline{u_i' u_j'})_u$ and $(\overline{u_i' u_j'})_b$, or, alternatively, the effect of the velocity jump on the Favre-averaged Reynolds stresses should be eliminated when evaluating u' based on computed field of $\overline{\rho u_i'' u_j''}$. From this prospective, the use of conditioned Reynolds stresses makes the problem of characterizing turbulence in premixed flames more difficult, rather than resolves it.

However, the use of Eqs. 8-10 supplemented with Eq. 1 may substantially facilitate modeling the effects of the heat release on the Favre-averaged Reynolds stresses, because these equations evade a very difficult problem [3] of closing correlations between velocity and pressure gradient in the conventional balance equations for $\overline{\rho u_i'' u_j''}$. Equations 13 and 14 further simplify modeling the effects discussed.

4 Conclusions

In premixed flames, conditioned Reynolds stresses should not be considered to be the turbulence characteristic, because they are also affected by flamelet motion even in the constant density case.

Mass, impulse, and Reynolds stresses balance equations conditioned to the burned mixture have been reported in a form that offers an opportunity to separate modeling of turbulence itself, the effects of chemical reactions on $(\overline{u_i' u_j'})_b$, and the effects of the heat release on the turbulence.

References

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