

Closure modeling for the conditional Reynolds stresses in turbulent premixed combustion

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Abstract

Turbulence is significantly affected by combustion-induced dilatation in low Karlovitz number premixed flames. Conventional turbulence modeling approaches based on traditional unconditional averaging are limited in accurately capturing combustion heat release effects since they must capture both the direct influence of combustion heat release on turbulence and the flame dynamics. Solving momentum transport equations conditionally averaged with respect to a flame structure variable (progress variable for premixed combustion) could provide a superior framework for modeling combustion-affected turbulence since the flame dynamics are embedded into the flame structure variable conditioning. However, the conditional momentum equations contain numerous unclosed terms that evolve in both physical and phase spaces. Of the many unclosed terms, the conditional Reynolds stresses (conditional analog of the Reynolds stresses) represent the influence of turbulent transport on the conditional velocities. In this work, a new model consisting of two components for the conditional Reynolds stresses in turbulent pre-

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mixed flames is developed to capture heat release effects on turbulence. The first component is the conditional analog of the Boussinesq model that characterizes turbulent shear effects in physical space. The second component depends on the conditional velocity gradient not in physical space but in phase space and captures the anisotropy in the conditional Reynolds stresses driven by thermal expansion effects that vary within the flame structure. The model is validated a priori using DNS databases of turbulent premixed jet flames at low and high Karlovitz numbers. At low Karlovitz number, the phase space term enables the model to capture direct heat release effects on all conditional Reynolds stress components, specifically the correct anisotropy of the normal components and the sign of the shear component. At high Karlovitz number where heat release effects on turbulence are insignificant, turbulent shear effects are dominant, and the phase space term has a nearly negligible effect.

Keywords: Turbulent premixed combustion, Turbulence modeling, Conditional Reynolds stresses, Direct Numerical Simulation

1. Introduction

In conventional Reynolds-Averaged Navier-Stokes modeling (RANS) of turbulent combustion, unconditionally averaged momentum and scalar transport equations are solved. These equations include unclosed terms that require closure models. Of the many unclosed terms, the Reynolds stresses represent turbulent transport of the momentum, similar to the scalar fluxes in the scalar equations representing turbulent transport of the scalars. Closure of those turbulent transport terms has been commonly considered as a

turbulence modeling problem. Typically, the Reynolds stresses are modeled using the Boussinesq hypothesis, and the scalar fluxes are modeled using the gradient transport hypothesis, as in the case of non-reacting flows. This modeling approach implicitly assumes that turbulence is not significantly affected by combustion. However, many experimental and computational studies have shown that combustion heat release affects turbulence in turbulent premixed flames by introducing flow dilatation driven by thermal expansion in the flame, as reviewed by Sabelnikov and Lipatnikov [1].

Bilger [2] derived a scaling criterion for the conditions under which turbulence is dominated by the influence of the heat release, which, simply stated, occurs when the combustion-induced dilatation is faster than the turbulence-induced strain. MacArt et al. [3] recast this scaling argument in terms of the Karlovitz number in turbulent premixed flames. When a local Karlovitz number ($Ka \equiv \tau_L/\tau_\eta$, where τ_L is the laminar flame time scale and τ_η is the Kolmogorov time scale) is less than a critical Karlovitz number ($Ka_{cr} \equiv \rho_u/\rho_b - 1$, where ρ_u and ρ_b are the density of the unburned and burned gas, respectively), heat release effects on turbulence become significant. This Karlovitz number scaling has been confirmed with DNS [3, 4]. In the low Karlovitz number regime, both the Boussinesq hypothesis for the Reynolds stresses and the gradient transport hypothesis for the scalar fluxes are not valid [3–5]. Since the heat release effects occur at sub-Kolmogorov length scales in the low Karlovitz number regime, the same fundamental challenge exists for Large Eddy Simulation (LES), no matter how well resolved. Clearly, new modeling approaches are required that explicitly account for the influence of heat release on turbulence.

In the limit of zero Karlovitz number, that is, an infinitely thin flame, turbulence can be described with the Bray-Moss-Libby (BML) framework [6]. In the BML framework, only reactants and products are present, and the intermediate states of the reactant mixture are not considered. Knowing the velocity change across the flame due to thermal expansion, that is, the flame speed, explicit expressions can be written for any turbulence statistic. Veynante et al. [7] and MacArt et al. [3] have attempted to combine conventional turbulence models with BML theory for flames at finite Karlovitz number but with limited success, failing in particular to account for shear effects [3].

Instead, for flames at finite Karlovitz number, MacArt et al. [8] have recently proposed a new turbulence modeling approach that aims to solve momentum transport equations conditionally averaged on a flame structure variable. Conditionally averaging of the thermochemical scalar equations forms the foundation of Conditional Moment Closure (CMC), which has been applied to both premixed and nonpremixed combustion, in the context of combustion modeling [9, 10]. The basic rationale of CMC is that the fluctuations of the scalars are highly correlated with the fluctuations of a flame structure variable. There are two main advantages to solving conditionally averaged momentum transport equations in the context of the turbulence modeling problem. First, since the flame dynamics (i.e., the local motion of the flame) are embedded into the flame conditioning, conditional velocities are only affected by the turbulence dynamics, including the direct heat release effects on turbulence (i.e., all heat release effects except for the flame dynamics), and not the flame dynamics. This claim is supported by the experimental work of Cheng et al. [11], using a lean ethylene-air turbulent premixed

v-flame, who showed that unconditional velocity fluctuations are much larger than conditional velocity fluctuations. This was attributed to intermittent contributions between the unburned reactants and burned products due to the flame motion in the unconditional case, which is a notion similar to the ideas of BML. Second, as the flame structure variable provides information about the local flame structure, modeling of the direct heat release effects on turbulence that vary in the flame is expected to be more easily achievable. As an additional note, beyond the turbulence modeling problem, the conditional velocity appears in the CMC equations for the thermochemical scalars for the combustion modeling problem. Typical approaches have replaced the conditional velocity with the unconditional velocity augmented with a gradient-diffusion term [9], so the conditional velocity could also directly aid the combustion modeling problem.

The primary challenge in this new turbulence modeling approach is in the development of closure models for various unclosed terms that appear in the conditionally averaged momentum equations. Of these unclosed terms, the conditional Reynolds stresses, which correspond to the conditional analog of the Reynolds stresses, represent the influence of turbulent transport on the conditional velocities. MacArt et al. [8] have analyzed the conditional velocity fluctuations from a Direct Numerical Simulation (DNS) of turbulent premixed jet flames at low and high Karlovitz numbers. The conditional velocity fluctuations were observed to vary in both physical and phase spaces at both Karlovitz numbers. The variation of the conditional velocity fluctuations in phase space is dominated by only turbulent shear effects at high Karlovitz number but not at low Karlovitz number. Therefore, a closure

model for the conditional Reynolds stresses must capture variation in both physical and phase spaces including the direct influence of heat release on turbulence.

In this work, a new model for the conditional Reynolds stresses in turbulent premixed flames is developed, which is the first step in a sequence of research needed to close all of the unclosed terms in the conditional momentum equation and then ultimately solve it. The performance of the new model is evaluated a priori using DNS databases [3] of turbulent premixed jet flames at both a low and high Karlovitz number, with respect to the critical Karlovitz number. As these DNS configurations have large-scale shear for generating turbulence, the model validation using this DNS configurations generally considers both heat release and large-scale shear effects on the conditional Reynolds stresses.

2. Formulation

2.1. Conditional Momentum Equation

For premixed flames, a progress variable Λ serves as a flame structure variable for conditioning. In this work, the normalized O_2 mass fraction will be used to define the progress variable. A quantity ψ conditionally averaged with respect to this progress variable will be denoted as $\bar{\psi}_\lambda$, where λ is the phase space analog of Λ , and density-weighted conditionally averaged quantities will be denoted by $\tilde{\psi}_\lambda$ or $\{\psi\}_\lambda$. In addition, unconditionally averaged quantities and density-weighted unconditionally averaged quantities will be denoted by $\bar{\psi}$ and $\tilde{\psi}$, respectively. The conditional momentum equation has been derived in MacArt et al. [8] by applying the joint PDF method [9] to

the momentum equation:

$$\begin{aligned}
& \frac{\partial \tilde{u}_{i\lambda}}{\partial t} + \tilde{u}_{j\lambda} \frac{\partial \tilde{u}_{i\lambda}}{\partial x_j} = -\frac{1}{\bar{\rho}\tilde{P}} \frac{\partial}{\partial x_j} \left[\bar{\rho}\tilde{P} (\widetilde{u_i u_{j\lambda}} - \tilde{u}_{i\lambda} \tilde{u}_{j\lambda}) \right] \\
& -\frac{1}{\bar{\rho}\tilde{P}} \left[\frac{\partial^2}{\partial x_j \partial \lambda} \left(\bar{\rho}\tilde{P} \left\{ u_i D_\Lambda \frac{\partial \Lambda}{\partial x_j} \right\}_\lambda \right) - \tilde{u}_{i\lambda} \frac{\partial^2}{\partial x_j \partial \lambda} \left(\bar{\rho}\tilde{P} \left\{ D_\Lambda \frac{\partial \Lambda}{\partial x_j} \right\}_\lambda \right) \right] \\
& -\frac{1}{\bar{\rho}_\lambda} \frac{\partial p}{\partial x_{i\lambda}} + \frac{1}{\bar{\rho}_\lambda} \frac{\partial \tau_{ij}}{\partial x_{j\lambda}} - \frac{1}{\bar{\rho}_\lambda} \bar{\dot{m}}_{\Lambda\lambda} \frac{\partial \tilde{u}_{i\lambda}}{\partial \lambda} - \frac{1}{\bar{\rho}\tilde{P}} \frac{\partial}{\partial \lambda} \left[\bar{P} (\overline{u_i \dot{m}_{\Lambda\lambda}} - \tilde{u}_{i\lambda} \bar{\dot{m}}_{\Lambda\lambda}) \right] \\
& -\frac{1}{\bar{\rho}\tilde{P}} \left[-\frac{\partial}{\partial \lambda} \left(\bar{\rho}\tilde{P} \left\{ D_\Lambda \frac{\partial u_i}{\partial x_j} \frac{\partial \Lambda}{\partial x_j} \right\}_\lambda \right) + \frac{1}{2} \frac{\partial^2}{\partial \lambda^2} (\overline{\rho u_i \chi_{\Lambda\lambda}} \bar{P}) - \frac{1}{2} \tilde{u}_{i\lambda} \frac{\partial^2}{\partial \lambda^2} (\overline{\rho \chi_{\Lambda\lambda}} \bar{P}) \right], \tag{1}
\end{aligned}$$

where u_i is the velocity, ρ is the density, $\tilde{P}$ is the density-weighted PDF of λ , $\bar{P}$ is the PDF of λ , D_Λ is the Λ diffusivity, p is the pressure, τ_{ij} is the viscous stress tensor, $\dot{m}_\Lambda$ is the Λ source term, and $\chi_\Lambda = 2D_\Lambda \nabla \Lambda \cdot \nabla \Lambda$ is the progress variable dissipation rate. In the first term on the right-hand side of Eq. 1, $\widetilde{u_i u_{j\lambda}} - \tilde{u}_{i\lambda} \tilde{u}_{j\lambda}$ corresponds to the conditional Reynolds stresses, which will subsequently be written as $\widetilde{u_i^* u_{j\lambda}^*}$, where $*$ denotes conditional fluctuations with respect to the density-weighted conditional mean. For further discussion of the budgets of this equation, see MacArt et al. [8].

2.2. Closure of the Conditional Reynolds Stresses

The most commonly used and well-established approach for closure of the density-weighted unconditional Reynolds stresses ($\widetilde{u_i'' u_j''} \equiv \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$) is the Boussinesq model:

$$\widetilde{u_i'' u_j''} - \frac{2}{3} \tilde{k} \delta_{ij} \approx -2\nu_t \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right), \tag{2}$$

where $\tilde{k} = \widetilde{u_k'' u_k''}/2$ is the turbulent kinetic energy (TKE), ν_t is the turbulent viscosity, and $\tilde{S}_{ij}$ is the mean strain rate tensor defined as

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \tag{3}$$

The Boussinesq model indicates that the deviatoric part of the unconditional Reynolds stresses is aligned with the strain rate tensor with a model coefficient depending on a turbulent velocity scale u' and length scale l .

One could initially propose that the conditional Reynolds stresses could be closed in direct analogy with the unconditional Reynolds stresses. This approach assumes that conditioning on a flame structure variable properly removes the flame dynamics (i.e., in the limit that the velocity fluctuations are due solely to flame dynamics, conditional fluctuations are zero), and the conditional Reynolds stresses only result from the turbulence dynamics without any further influence from combustion heat release. However, this naive assumption is likely not correct. Instead, this naive model is extended here by noting that the conditional Reynolds stresses evolve in both physical and phase spaces, so a model for the conditional Reynolds stresses should depend on both the velocity gradient in physical space and the velocity gradient in phase space. This argument results in a generalized Boussinesq model for the conditional Reynolds stresses:

$$\underbrace{\widetilde{u_i^* u_{j\lambda}^*} - \frac{2}{3} \tilde{k}_\lambda \delta_{ij}}_{\text{isotropic part}} \approx \underbrace{-2\nu_{t_\lambda} \left(\tilde{S}_{ij\lambda} - \frac{1}{3} \tilde{S}_{kk\lambda} \delta_{ij} \right)}_{\text{T1}} - \underbrace{2\phi_{t_\lambda} \left(\tilde{P}_{ij\lambda} - \frac{1}{3} \tilde{P}_{kk\lambda} \delta_{ij} \right)}_{\text{T2}}, \quad (4)$$

where $\tilde{k}_\lambda = \widetilde{u_k^* u_{k\lambda}^*}/2$ is the conditional TKE, ν_{t_λ} is the conditional turbulent viscosity in physical space, $\tilde{S}_{ij\lambda}$ is the conditional mean strain rate tensor defined as

$$\tilde{S}_{ij\lambda} = \frac{1}{2} \left(\frac{\partial \tilde{u}_{i\lambda}}{\partial x_j} + \frac{\partial \tilde{u}_{j\lambda}}{\partial x_i} \right), \quad (5)$$

(i.e., the conditional velocity variations in physical space), ϕ_{t_λ} is the analog of ν_{t_λ} in phase space, and

$$\tilde{P}_{ij\lambda} = \frac{1}{2} \left(\frac{\partial \tilde{u}_{i\lambda}}{\partial \lambda} n_j + \frac{\partial \tilde{u}_{j\lambda}}{\partial \lambda} n_i \right), \quad n_i = \frac{\partial \tilde{\Lambda}}{\partial x_i} \left| \nabla \tilde{\Lambda} \right|^{-1}, \quad (6)$$

is the analogy of $\tilde{S}_{ij\lambda}$ in phase space (i.e., the conditional velocity variations in phase space), where the flame normal vector n_i provides directional information in the second-order tensor. ν_{t_λ} and ϕ_{t_λ} contain characteristic scales in physical space and phase space, respectively, which need to be specified for the closure of the model and represent the rate of turbulent transport in each space.

In Eq. (4), the left-hand side is the deviatoric part of the conditional Reynolds stresses, which characterizes the anisotropy of the conditional Reynolds stresses. The model consists of two terms: the term T1 is associated with turbulent shear effects in physical space while the term T2 is associated with the anisotropy driven by the thermal expansion effects in phase space. In term T1, ν_{t_λ} is modeled as

$$\nu_{t_\lambda} = C_\nu u' l = C_\nu \frac{\tilde{k}_\lambda^2}{\tilde{\epsilon}_\lambda}, \quad (7)$$

where C_ν is the model coefficient and $\tilde{\epsilon}_\lambda$ is the conditional TKE dissipation rate that appears in the conditional TKE transport equation [12]:

$$\tilde{\epsilon}_\lambda = \frac{1}{\bar{\rho}_\lambda} \overline{\tau_{mn} \frac{\partial u_m^*}{\partial x_n}}. \quad (8)$$

ν_{t_λ} is dimensionally a velocity scale times a physical length scale and is given in terms of $\tilde{k}_\lambda$ and $\tilde{\epsilon}_\lambda$. $\tilde{k}_\lambda$ and $\tilde{\epsilon}_\lambda$ are used instead of $\tilde{k}$ and $\tilde{\epsilon}$ as in the standard Boussinesq model, where $\tilde{\epsilon}$ is the unconditional TKE dissipation rate, because the underlying turbulence dynamics and the relevant characteristic scales

(specifically here, the TKE transport processes) are not represented by the unconditional quantities but rather by the conditional quantities. In term T2, ϕ_{t_λ} is likewise modeled as

$$\phi_{t_\lambda} = C_\phi u_F \Lambda_F, \quad (9)$$

where C_ϕ is the model coefficient, u_F is the characteristic velocity scale in phase space defined as

$$u_F = \frac{\overline{\dot{m}_{\Lambda\lambda}}/\bar{\rho}_\lambda}{\left|\nabla\tilde{\Lambda}\right|/\widetilde{\Lambda'^2}^{1/2}}, \quad (10)$$

and Λ_F is the characteristic progress variable scale defined using the progress variable fluctuations:

$$\Lambda_F = \widetilde{\Lambda'^2}^{1/2}. \quad (11)$$

For the quantity ν_{t_λ} , which is associated with gradients in physical space, the velocity and physical length scales are associated with turbulence scales; for the quantity ϕ_{t_λ} , which is associated with gradients in phase space, the velocity and phase “length” scales are associated with flame scales. Note that the sum of the isotropic part and term T1 will be referred to as the “conditional Boussinesq model” due to its physical and functional analogy to the Boussinesq model in Eq. (2), and the sum of the conditional Boussinesq model and term T2 will be referred to as the “conditional heat release model”.

The presented model formulation is based on dimensional analysis, the analogy between the unconditional and conditional quantities, and the analogy between physical and phase spaces. The physical implications of the presented model will be discussed using the DNS results in Section 4.

3. Direct Numerical Simulations

The presented model for the conditional Reynolds stresses is validated a priori using DNS databases [3] of spatially-evolving turbulent premixed planar jet flames at a low (Case K1) and high (Case K2) Karlovitz number. In the DNS configuration for both cases, a turbulent central jet at $T_0 = 300$ K is composed of a nitrogen-diluted (20% by volume) stoichiometric H_2 -air reactant mixture, and laminar coflow jets at $T_c = 2047.5$ K, separated by walls from the central jet at the inlet, are composed of equilibrium products of the reactant mixture. The nitrogen dilution in the reactants prevents flashback. The pressure is 1 atm. In the domain, x , y , and z denote the streamwise, cross-stream, and spanwise directions, respectively. The spanwise direction is statistically homogeneous. The streamwise location $x/H_0 = 3$ has been considered in this work for analysis, where H_0 is the central jet height. At $x/H_0 = 3$, the effects of the walls at the inlet can be avoided, but there still remains some unburned reactants for both cases [3]. Furthermore, the cross-stream direction is preferentially aligned with the flame normal vector. DNS of fully-developed turbulent channel flow is used to initialize the inflow of the turbulent central jet, and the bulk Reynolds number based on the central jet velocity U_0 and height H_0 is $Re_0 = 5,000$ for both cases. For the coflow jet velocity U_c and height H_c , the ratios of $U_0/U_c = 3.88$ and $H_0/H_c = 1.43$ are maintained for both cases. The laminar flame thickness δ_L , the laminar flame speed s_L , and the critical Karlovitz number are $\delta_L = 0.435$ mm, $s_L = 1.195$ m/s, and $Ka_{cr} = 6.7$ for both cases, respectively. The Karlovitz number through the flame is less than Ka_{cr} for K1 (3.7 at $x/H_0 = 3$) and greater than Ka_{cr} for K2 (54.0 at $x/H_0 = 3$). Simulation parameters are

Table 1: Parameters for the DNS databases [3]

Case	K1	K2
U_0 (m/s)	23.4	93.4
H_0 (mm)	4.32	1.08
Re_0	5,000	5,000
Ka_{cr}	6.7	6.7
$Ka_{\tilde{\Lambda}=0.5}$	3.7	54.0
Domain	$12H_0 \times 24H_0 \times 3H_0$	$24H_0 \times 16H_0 \times 3H_0$
Grid points	$768 \times 586 \times 256$	$1536 \times 576 \times 256$

summarized in Table 1.

A low Mach, semi-implicit, iterative, and finite difference code with a structured grid has been used for solving the governing equations for the mass, momentum, species mass fraction, and temperature equations with the ideal gas equation of state [13, 14]. A detailed kinetic model for H_2 combustion by Davis et al. [15] has been used. Constant non-unity Lewis numbers have been used for each species for molecular transport [16]. To obtain conditional statistics, the phase space λ for Λ has been discretized with 50 bins. Results were insensitive to increasing the number of bins. Conditional averaging has been performed over the homogeneous spanwise direction and in time and for 47.9 (Case K1) and 29.7 (Case K2) centerline integral times. More details on the simulations can be found in Refs. [3, 12].

4. Results and Discussion

The components of the density-weighted conditional Reynolds stresses are shown in Fig. 1 for Case K1 and in Fig. 2 for Case K2. The results from the DNS are compared with the conditional Boussinesq model and the conditional heat release model at several y -locations in physical space in

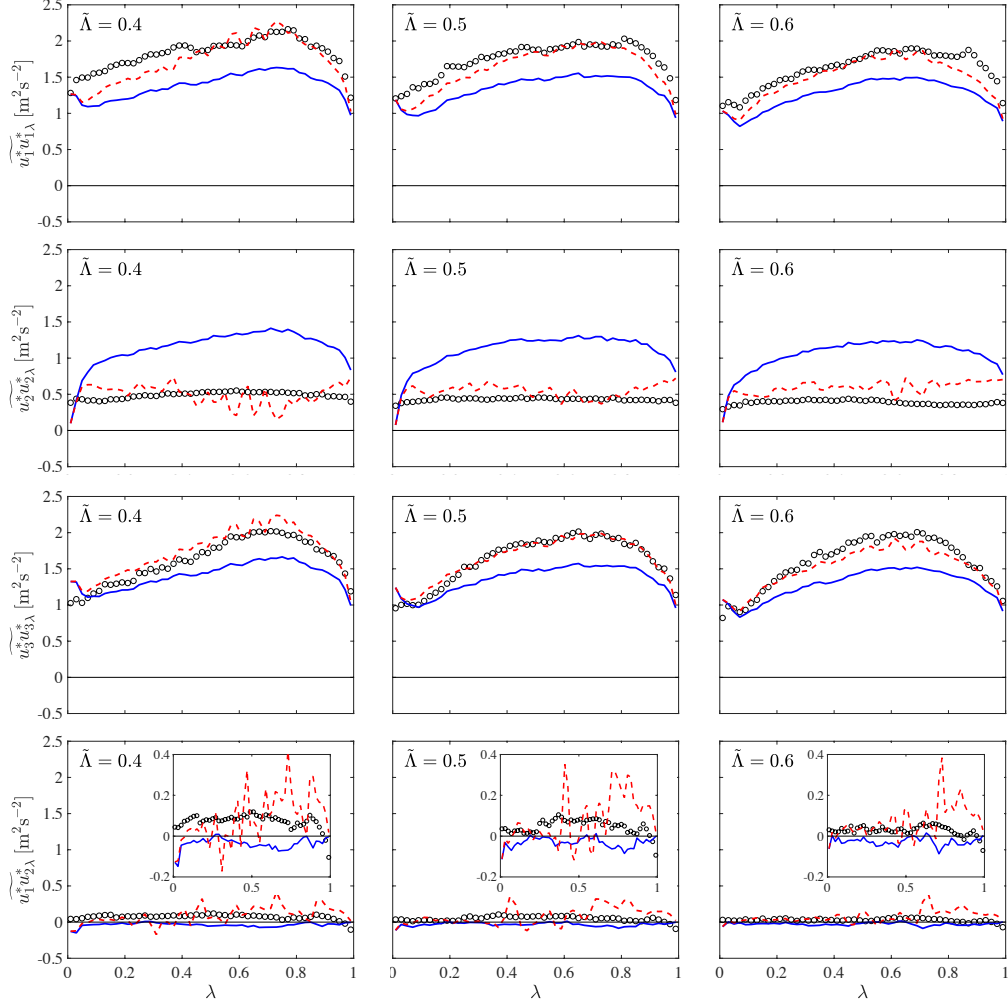


Figure 1: Density-weighted conditional Reynolds stresses plotted against λ from DNS ($\circ$), the conditional Boussinesq model (—), and the conditional heat release model (---) at $x/H_0 = 3$ at three different cross-stream locations (corresponding to $\tilde{\Lambda} = 0.4, 0.5$, and 0.6 , left to right, respectively) for Case K1. The three normal components of the conditional Reynolds stresses (streamwise, cross-stream, and spanwise) and the shear component are shown from top to bottom. The insets show magnified plots of the shear component.

terms of the the mean progress variable. The model coefficient C_ν in Eq. (7) was chosen to be 0.18 by matching the shear component $\widetilde{u_1^* u_{2\lambda}^*}$ from the DNS and from the conditional Boussinesq model at $\tilde{\Lambda} = 0.5$ in Case K2. The

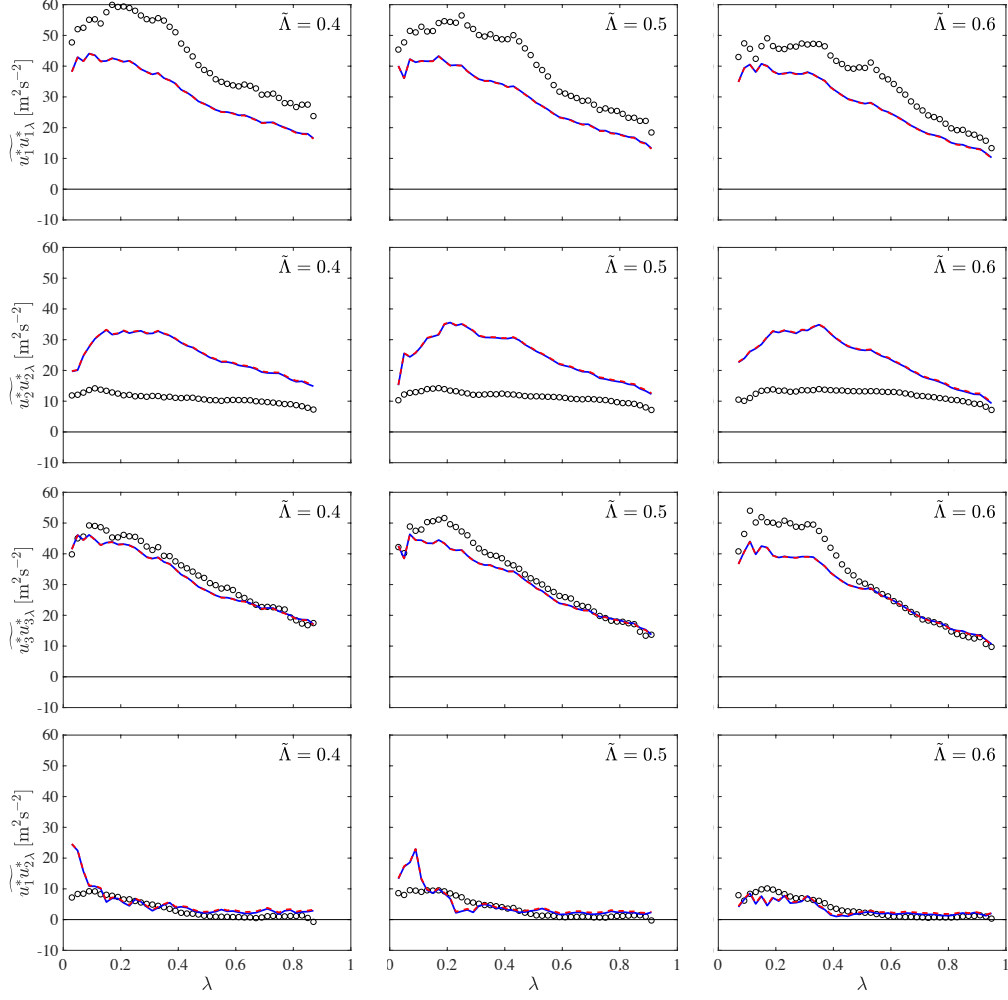


Figure 2: Density-weighted conditional Reynolds stresses plotted against λ from DNS ($\circ$), the conditional Boussinesq model (—), and the conditional heat release model (---) at $x/H_0 = 3$ at three different cross-stream locations (corresponding to $\tilde{\Lambda} = 0.4, 0.5$, and 0.6 , left to right, respectively) for Case K2. The three normal components of the conditional Reynolds stresses (streamwise, cross-stream, and spanwise) and the shear component are shown from top to bottom.

model coefficient C_ϕ in Eq. (9) was chosen to be 0.07 by matching the cross-stream normal component $\widetilde{u_2^* u_{2\lambda}^*}$ from the DNS and from the heat release model at $\tilde{\Lambda} = 0.5$ in Case K1. Both figures show the conditional statistics

only where $\tilde{P}(\lambda) > 0.005$.

For Case K1, the conditional Boussinesq model underpredicts both the streamwise component $\widetilde{u_1^* u_{1\lambda}^*}$ and the spanwise component $\widetilde{u_3^* u_{3\lambda}^*}$ and overpredicts the cross-stream component $\widetilde{u_2^* u_{2\lambda}^*}$ of the normal conditional Reynolds stresses. The extent of the misprediction by the conditional Boussinesq model is largest for $\widetilde{u_2^* u_{2\lambda}^*}$ among the normal components. In addition, $\widetilde{u_1^* u_{2\lambda}^*}$ predicted by the conditional Boussinesq model is negative, while $\widetilde{u_1^* u_{2\lambda}^*}$ from the DNS is generally positive. Overall, the conventional Boussinesq type model alone cannot predict the correct magnitude and sign of the conditional Reynolds stresses, which would be further manifested as an incorrect turbulent production of conditional TKE.

On the other hand, the conditional heat release model captures nearly all of the components with respect to the sign and magnitude. Correction of the conditional Boussinesq model by the term T2 is most important in $\widetilde{u_2^* u_{2\lambda}^*}$ and $\widetilde{u_1^* u_{2\lambda}^*}$, both of which include the cross-stream velocity component. As the cross-stream direction is aligned with the flame-normal vector, the cross-stream conditional velocity component $\tilde{u}_{2\lambda}$ is directly affected by the combustion heat release such that $\tilde{u}_{2\lambda}$ mostly increases in phase space [8] due to thermal expansion effects. Therefore, the accuracy and significance of the term T2 in the predictions of $\widetilde{u_2^* u_{2\lambda}^*}$ and $\widetilde{u_1^* u_{2\lambda}^*}$ indicate that the heat release model can account for the heat release effects on the conditional Reynolds stresses. Compared to the normal components, $\widetilde{u_1^* u_{2\lambda}^*}$ and its model predictions are significantly smaller. This is consistent with the experimental work of Cheng et al. [11], who showed that the joint PDF of the conditional streamwise and cross-stream velocities is nearly symmetric around their con-

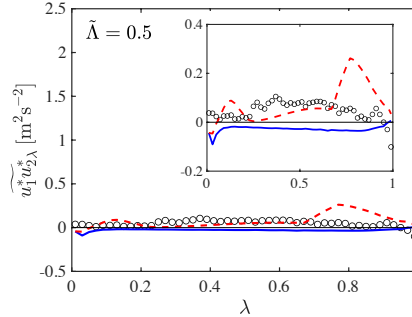


Figure 3: Shear component of density-weighted conditional Reynolds stresses plotted against λ from DNS ($\circ$), the conditional Boussinesq model (—), and the conditional heat release model (- - -) at $x/H_0 = 3$ and $\tilde{\Lambda} = 0.5$ for Case K1. The models are recomputed using total-variation regularization. The inset show the magnified plot.

ditional means, resulting in small conditional Reynolds shear stress. As a note, due to the sparsity of data, the model results for the shear component in Fig. 1 are quite noisy due to utilizing a finite difference to compute gradients in phase space. As shown in Fig. 3, the derivative in phase space for the conditional Reynolds stress models was recomputed using regularization [17], resulting in significant reduction in noise and further supporting the previous discussion.

At low Karlovitz number, thermal expansion effects are strong, so the cross-stream velocity is highly correlated with the progress variable. This results in $\widetilde{u_2^* u_{2\lambda}^*}$ being smaller than $\widetilde{u_1^* u_{1\lambda}^*}$ and $\widetilde{u_3^* u_{3\lambda}^*}$, which are not strongly affected by thermal expansion effects. However, due to the relative lack of turbulent shear effects at this condition and the uniformity of the conditional velocity, which is influenced largely by thermal expansion effects, the term T1 becomes negligible, and the conditional Boussinesq model predicts essentially isotropic conditional Reynolds stresses. This discrepancy between the isotropic prediction and the conditional Reynolds normal stresses (i.e., the

anisotropy in the conditional Reynolds normal stresses) is driven by the thermal expansion effects and is correctly captured by term T2 by considering velocity variations in phase space. In other words, the term T2 corrects the conditional Boussinesq model by subtracting out the flame dynamics effects that are removed with conditioning.

For Case K2, differences between the conditional Boussinesq model and the conditional heat release model (i.e., the term T2) are negligible, as expected, indicating that the effects of the flame on the conditional Reynolds stresses are insignificant at high Karlovitz number. In addition, the variations of the conditional Reynolds stresses in physical space (at a fixed λ) for Case K2 are mostly larger than those for Case K1. Both models are well capturing the shear component and qualitatively correct for the normal components, only slightly underpredicting the degree of anisotropy of the normal components. Specifically, $\widetilde{u_1^* u_{1\lambda}^*}$ and $\widetilde{u_3^* u_{3\lambda}^*}$ are slightly underpredicted and $\widetilde{u_2^* u_{2\lambda}^*}$ is overpredicted at all $\tilde{\Lambda}$ locations. MacArt et al. [3] observed similar trends in the predictions of the unconditional Reynolds stresses from the Boussinesq model. Given that the term T2 is negligible and the relative magnitude of the term T1 compared to the isotropic part is larger in Case K2 than in Case K1, the mispredictions of the normal components by the conditional Boussinesq model are not due to neglecting the heat release effects. Instead, these mispredictions are intrinsic to such a linear k - ϵ -type model in the RANS context, which cannot fully account for higher-order and nonlinear processes generating turbulence anisotropy [18].

5. Conclusions

A new model for the conditional Reynolds stresses in the conditional momentum equation has been developed to consider heat release effects on turbulence. The deviatoric part of the conditional Reynolds stresses is modeled with two terms, one related to turbulent shear effects in physical space and the other related to the anisotropy driven by thermal expansion effects in phase space. The model performance has been evaluated a priori using DNS databases of turbulent premixed jet flames at low and high Karlovitz numbers. The phase space term enables the model to capture the direct heat release effects on all of the conditional Reynolds stress components at low Karlovitz number and is negligible at high Karlovitz number. The turbulent shear effects are only dominant at high Karlovitz number.

This work provides closure for one of the terms in the conditional momentum equation (Eq. 1). In future work, additional closure models would be required for the remaining unclosed terms, notably the conditional pressure gradient, in addition to models for the conditional turbulent kinetic energy and conditional dissipation for evaluating the conditional turbulent viscosity.

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References

- [1] V. A. Sabelnikov, A. N. Lipatnikov, Recent advances in understanding of thermal expansion effects in premixed turbulent flames, *Annu. Rev. Fluid Mech.* 49 (2017) 91–117.
- [2] R. W. Bilger, Some aspects of scalar dissipation, *Flow, Turbul. Combust.* 72 (2004) 93–114.
- [3] J. F. MacArt, T. Grenga, M. E. Mueller, Effects of combustion heat release on velocity and scalar statistics in turbulent premixed jet flames at low and high Karlovitz numbers, *Combust. Flame* 191 (2018) 468–485.
- [4] J. Lee, J. F. MacArt, M. E. Mueller, Heat release effects on the Reynolds stress budgets in turbulent premixed jet flames at low and high Karlovitz numbers, *Combust. Flame* 216 (2020) 1–8.
- [5] R. K. Cheng, T. T. Ng, Velocity statistics in premixed turbulent flames, *Combust. Flame* 52 (1983) 185–202.
- [6] K. N. C. Bray, P. A. Libby, J. B. Moss, Unified modeling approach for premixed turbulent combustion—part I: General formulation, *Combust. Flame* 61 (1985) 87–102.
- [7] D. Veynante, A. Trouvé, K. N. C. Bray, T. Mantel, Gradient and counter-gradient scalar transport in turbulent premixed flames, *J. Fluid Mech.* 332 (1997) 263–293.

- [8] J. F. MacArt, T. Grenga, M. E. Mueller, Evolution of flame-conditioned velocity statistics in turbulent premixed jet flames at low and high Karlovitz numbers, *Proc. Combust. Inst.* 37 (2019) 2503–2510.
- [9] A. Y. Klimenko, R. W. Bilger, Conditional moment closure for turbulent combustion, *Prog. Energy Combust. Sci.* 25 (1999) 595–687.
- [10] N. Swaminathan, R. W. Bilger, Analyses of conditional moment closure for turbulent premixed flames, *Combust. Theory Model* 5 (2001) 241–260.
- [11] R. K. Cheng, Conditional sampling of turbulence intensities and Reynolds stress in premixed turbulent flames, *Combust. Sci. Technol.* 41 (1984) 109–142.
- [12] J. F. MacArt, Computational simulation and modeling of heat release effects on turbulence in turbulent reacting flow, Ph.D. thesis, Princeton University, 2018.
- [13] O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High order conservative finite difference scheme for variable density low Mach number turbulent flows, *J. Comput. Phys.* 227 (2008) 7125–7159.
- [14] J. F. MacArt, M. E. Mueller, Semi-implicit iterative methods for low Mach number turbulent reacting flows: Operator splitting versus approximate factorization, *J. Comput. Phys.* 326 (2016) 569–595.
- [15] S. G. Davis, A. V. Joshi, H. Wang, F. Egolfopoulos, An optimized kinetic model of H_2/CO combustion, *Proc. Combust. Inst.* 30 (2005) 1283–1292.

- [16] N. Burali, S. Lapointe, B. Bobbitt, G. Blanquart, Y. Xuan, Assessment of the constant non-unity Lewis number assumption in chemically-reacting flows, *Combust. Theory Model* 7830(July) (2016) 1–26.
- [17] R. Chartrand, Numerical differentiation of noisy, nonsmooth data, *ISRN Appl. Math.* 2011 (2011) Article ID 164564.
- [18] C. G. Speziale, Analytical methods for the development of Reynolds-stress closures in turbulence, *Annu. Rev. Fluid Mech.* 23 (1991) 107–157.