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Effects of combustion heat release on velocity and scalar statistics in turbulent premixed jet flames at low and high Karlovitz numbers

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ABSTRACT

Theoretical scaling arguments for turbulent premixed combustion indicate that the pressure-dilatation source of turbulent kinetic energy becomes significant at low Karlovitz numbers, leading to potential invalidation of commonly-used turbulence models developed for non-reacting flow. Based on these arguments, a critical Karlovitz number is defined, below which dilatation effects are expected to become significant. Velocity and scalar statistics are obtained from Direct Numerical Simulation (DNS) calculations of low Mach number spatially-evolving turbulent premixed planar jet flames. At fixed bulk Reynolds number and stoichiometric equivalence ratio, two simulations are performed at Karlovitz numbers above and below the critical Karlovitz number. Hydrogen combustion with detailed transport is modeled using a detailed nine-species chemical kinetic mechanism, and coflows of combustion products are used to ensure flame stability at uniform equivalence ratio. The analysis of these statistics focuses on three key areas. First, the influence of the velocity-pressure gradient source of turbulent kinetic energy is confirmed at a low Karlovitz number, and the unimportance of these effects is confirmed at a high Karlovitz number. Similar effects are observed for the chemical source term in the scalar variance budgets. Second, the degree of alignment between the Reynolds stress tensor (scalar flux) and the strain-rate tensor (scalar gradient), the foundation of a majority of the turbulence models used in reacting flows, is assessed with the DNS databases. Additionally, consistency of anisotropic Reynolds stress and strain-rate tensor invariants is assessed using invariant maps. While good alignment and consistency are obtained for statistics and invariants at a high Karlovitz number, both alignment and consistency degrade at a low Karlovitz number. Third, turbulence models formulated for non-reacting flow are modified algebraically in the Bray–Moss–Libby (BML) formalism for turbulent premixed combustion. A variable efficiency function is defined to capture the regime dependence of heat release effects in these models. Model performance is evaluated at Karlovitz numbers above and below the critical Karlovitz number using the DNS databases, and satisfactory prediction of counter-gradient transport in the flame-normal direction is obtained. However, heat release effects are also observed in the flame-parallel directions in the low-Karlovitz number simulation, and the models developed in the formalism for statistically planar flames fail to capture these effects. Furthermore, in the low-Karlovitz number case, redistributive effects are active on the shear components of the Reynolds stress, which are not considered in the BML formalism. More advanced turbulence models are therefore necessary for turbulent premixed jet flames below the critical Karlovitz number.

1. Introduction

Most turbulence models for Reynolds-Averaged Navier Stokes (RANS) simulations and Large Eddy Simulation (LES) rely on the assumption of small-scale isotropy, the validity of which may be questioned in certain regimes of turbulent premixed combustion. For example, in the wrinkled laminar flames regime (thin flames relative to turbulence scales), experimental measurements have revealed that the (mean shear) production term becomes a sink of turbulent kinetic energy (TKE) [1]. This so-called "negative production" is balanced in TKE budgets by flame-induced pressure-dilatation [2]. This dilatation arises from volumetric expansion due to heat release and occurs roughly on the scales of the flame thickness. Turbulence models formulated for non-reacting flows neglect this effect of heat release but are still nonetheless widely used in simulations of reacting flows. Determining the conditions under which this neglect is valid and what additional effects must be included in turbulence models for reacting flows is critical for developing predictive computational tools for reacting flows.

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The relative influence of turbulence-induced strain ("production") and combustion-induced pressure-dilatation on the turbulence structure is governed by the relative scales of turbulence and combustion. Bilger [3] provided a theoretical framework in which this length scale dependence may be characterized. With the dilatation due to heat release taken to be of order $\tau_B s_L/\delta_F$ and the turbulence-induced strain-rate of order $(\epsilon/\nu)^{1/2}$, the turbulence strain-rate is expected to dominate over dilatation when

$$\left(\frac{\epsilon}{\nu}\right)^{1/2} \gg \frac{\tau_B s_L}{\delta_F}, \tag{1}$$

where ϵ is the TKE dissipation rate, ν is the kinematic viscosity of the fluid, $\delta_F = \Delta T/\max(|\nabla T|)$ is the thickness of the laminar premixed flame, and s_L is its burning velocity. The heat release parameter is defined as $\tau_B = \rho_u/\rho_b - 1$, where ρ_u and ρ_b are the densities of the unburned reactants and burned products, respectively.

The Karlovitz number, defined as $Ka \equiv t_F/t_\eta = \delta_F/s_L(\epsilon/\nu)^{1/2}$, where t_F is the laminar flame time scale and t_η is the Kolmogorov time scale, is the appropriate parameter to quantify this regime dependence in turbulent premixed combustion [4–9]. By rearranging Eq. (1), the criterion in Eq. (1) for dominance of turbulence-induced strain over combustion-induced dilatation may be expressed in terms of the Karlovitz number, with the right-hand side (RHS) defining a *critical Karlovitz number*, Ka_{cr}:

$$Ka \equiv \frac{\delta_F}{s_L}\left(\frac{\epsilon}{\nu}\right)^{1/2} \gg \tau_B \equiv Ka_{cr}. \tag{2}$$

For most flames at atmospheric conditions, Ka_{cr} is approximately ten. When $Ka \gg Ka_{cr}$, turbulence-induced strain is expected to dominate over pressure-dilatation as the main source of TKE. However, when $Ka \ll Ka_{cr}$, pressure-dilatation is expected to become a significant source of TKE [2,3]. Because the pressure-dilatation represents a small-scale source of TKE, the validity of the assumption of small-scale turbulence isotropy is questionable in the latter regime.

Using a similar critical Karlovitz number, O'Brien et al. [10] identified the most active regions of "cross-scale" energy transfer as those corresponding to $1 < Ka \lesssim 10$ and approximately unity Damköhler number, defined as

$$Da = \frac{s_L}{\delta_F}\frac{\ell}{u'}, \tag{3}$$

where $\ell = k^{3/2}/\epsilon$ is the local pseudo-integral scale, $k = \widetilde{u_i''u_i''}/2$ is the TKE, and u' is the root-mean-square (rms) of the velocity fluctuations. (The decomposition of the velocity components u_i into means and fluctuations is defined subsequently.) Additionally, a modification of the classical turbulent premixed combustion regime diagram was introduced [10], in which Da and u'/s_L were chosen as the parameters to characterize "cross-scale" turbulent energy transfer. These parameters are related to Ka (through the Reynolds number) but were chosen in Ref. [10] specifically to describe the regimes in which combustion-induced energy transfer is active at the large scales of turbulence. These large-scale effects result in a "scale cutoff" below which the effects of combustion heat release are no longer important, and, when the LES filter width is larger than this cutoff, no effects of combustion would need to be included in LES subfilter turbulence models. In this work, the focus will be the effects of combustion heat release on the small scales of the turbulence. The present study then considers only the Karlovitz number scaling proposed by Bilger [3] in order to isolate the effects of combustion heat release arising specifically from modifications to the small-scale turbulence.

The relative influence of turbulence-induced strain and combustion-induced dilatation has been assessed in Direct Numerical Simulation (DNS), and elements of the above theory have been confirmed, albeit with some limitations. At low Karlovitz numbers, the pressure-dilatation term becomes the dominant source of TKE in decaying turbulence [2] and in forced isotropic turbulence [10], and the chemical source term likewise becomes the dominant source of scalar variance [11]. Furthermore, under certain conditions at low Karlovitz number, the spectral transfer of kinetic energy exhibits a reversal (*i.e.*, reverse-cascade transfer) near the combustion products at the scale of the laminar flame thickness [12]. At higher Karlovitz numbers, the pressure-dilatation source of TKE becomes weaker compared to viscous dissipation [5]. In enstrophy budgets, the influence of dilatation is eliminated at high Karlovitz numbers [8], although this could be influenced by the turbulence forcing in the cited work. Furthermore, in the high Karlovitz number regime, the scalar variance production term becomes comparable in magnitude to the chemical source term [6].

However, none of these studies considered the influence of mean shear. In the absence of mean shear, there is limited production, and the off-diagonal Reynolds stress components are zero. For full characterization of the effects of combustion on turbulence, mean shear effects must be included. Recent work utilizing shear-generated turbulence has confirmed the influence of the pressure-dilatation source in TKE spectra at low Karlovitz numbers [13] and the lack of dilatation effects on enstrophy budgets at high Karlovitz numbers [9], but a study of turbulence statistics parameterized on the Karlovitz number has yet to be performed. The present study addresses this need with two DNS calculations of turbulent premixed jet flames at Karlovitz numbers above and below Ka_{cr}.

Statistical alignment provides another measure of the influence of combustion heat release on turbulence. In experimental measurements [14,15] and DNS calculations [16] of low Karlovitz number premixed flames, the most extensive principal strain-rate was observed to become preferentially aligned with the flame-normal vector. This behavior is contrary to the preferential alignment of the most compressive principal strain-rate with a passive scalar gradient observed in homogeneous turbulence [17]. At higher Karlovitz numbers, DNS calculations of statistically planar flames [16] and a jet flame [9] show that the alignment of the most compressive principal strain-rate with the flame-normal vector is recovered. While these previous studies (as well as others recently reviewed by Sabelnikov and Lipatnikov [18]) have considered alignment of the strain-rate eigenvectors with the flame-normal vector, the alignment of the Reynolds stress tensor with the strain-rate tensor, the foundation of most commonly used turbulence models, has not been investigated in turbulent premixed combustion.

In the context of RANS (LES), the density-weighted Reynolds (subfilter) stress $R_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j = \widetilde{u_i''u_j''}$ and the (subfilter) scalar flux $F_{j,k} = \widetilde{u_j Y_k} - \widetilde{u}_j\widetilde{Y}_k = \widetilde{u_j''Y_k''}$ appear as unclosed terms in the Favre-averaged (filtered) momentum and scalar evolution equations, respectively. In these expressions and all that follow, tildes denote density-weighted averaging (filtering), $\widetilde{\phi} = \overline{\rho\phi}/\overline{\rho}$, and double-primes denote density-weighted fluctuations (residuals), $\phi'' = \phi - \widetilde{\phi}$. The Reynolds (subfilter) stress is typically modeled using the Boussinesq hypothesis,

$$R_{ij} \approx -2\nu_t\left(\widetilde{S}_{ij} - \frac{1}{3}\widetilde{S}_{kk}\delta_{ij}\right) + \frac{2}{3}k\delta_{ij}, \tag{4}$$

where $\widetilde{S}_{ij}$ is the Favre-averaged (filtered) strain-rate tensor and δ_{ij} is the Kronecker delta. The eddy viscosity ν_t is obtained by solving transport equations for k and ϵ in the RANS context or from Smagorinsky-type models [19,20] in the LES context. The scalar flux is typically modeled using the analogous gradient diffusion hypothesis,