# Statistical behavior of turbulent kinetic energy transport in boundary layer flashback of hydrogen-rich premixed combustion

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A direct numerical simulation (DNS) database for boundary layer flashback of a premixed hydrogen-air flame with an equivalence ratio of 1.5 in a fully developed turbulent channel flow has been considered for this analysis. The nonreacting part of the channel flow is representative of the friction velocity based Reynolds number  $Re_{\tau} = 120$ . A skeletal chemical mechanism with 9 chemical species and 20 reactions is employed for representing hydrogen-air combustion. In this work the flow configuration and the turbulence and flame characteristics are similar to those of Gruber et al. [J. Fluid Mech. 709, 516 (2012)]. The interaction between the flame structure and the turbulent flow has been investigated for boundary layer flashback for a comparison with the earlier work of Gruber et al. [J. Fluid Mech. 709, 516 (2012)]. The statistics of wall shear stress, turbulent kinetic energy, and its dissipation have been analyzed to probe the influence of the flame on the underlying turbulence in the channel flow configuration. Furthermore, the budgets for the individual terms in the turbulent kinetic energy transport equation have also been investigated at a given plane in the channel. It is found that the propagation of the flame into the upstream part of the fully developed turbulent boundary layer introduces a flow reversal in some regions upstream of the flame and these regions lead to negative wall shear stress. Interrogation of the DNS data for the budgets of the turbulent kinetic energy transport has revealed that the aforementioned local flow reversal regions have significant influences on the turbulent kinetic energy production, pressure dilatation, and pressure transport terms. It has been found that the flame propagation into the upstream reactants leads to some weak local compressibility effects as demonstrated by the changes in the pressure related terms in the turbulent kinetic energy transport equation. These results indicate that the pressure dilatation and turbulent transport due to pressure are the two dominant terms in the turbulent kinetic energy equation in the case of wall bounded flashback flames.

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# I. INTRODUCTION

To mitigate climate change, hydrogen is considered as an alternative fuel for clean and efficient large-scale power generation with carbon capture and storage (CCS) where the original fuel is either reformed natural gas or gasified coal added to a synthetic fuel mixture [1]. Hydrogen-rich combustion offers a lower environmental impact and higher energy efficiency [2]. Hydrogen is mainly produced by the steam reforming, partial oxidation, and self-heating reforming methods from natural gas or coal [3], and recently alternative methods using biomass instead of natural gas and coal have been investigated [4]. Hydrogen is used as a fuel of choice in this case as it

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remains stable across a range of fuel concentrations during combustion and can be ignited with relative ease; as hydrogen has a high flammable range and high burning velocity. However, the aforementioned characteristics of hydrogen lead to a risk of flashback, which is an uncontrolled transient upstream propagation of a flame, and therefore make the development of hydrogen combustors much more difficult [2]. Hydrogen flames become even more complicated in the case of their interaction with the boundary layers formed near combustor walls. Flame-wall interaction (FWI) plays a pivotal role in the design of modern combustion equipment, as the new combustors are being made smaller to increase energy density and reduce weight. Many combustion devices (e.g., spark ignition (SI) engines, gas turbines), operate in wall-bounded flows and FWI can have strong effects on fuel consumption and pollutant formation which are both important concerns for automotive, civil aviation, and power generation industries.

While boundary layer flashback is a minor issue for natural gas fired gas turbines, evidence involving premixed combustion of hydrogen-rich syngas at gas turbine conditions (high pressure, high reactant temperature) indicates that boundary layer flashback presents a key challenge [2,5]. It should be noted here that the increased reactivity of hydrogen-rich syngas complicates the problem of boundary layer flashback considerably. Specifically, compared with hydrocarbon-air flames, hydrogen-air premixed flames are able to propagate three times (in relation to the flame thickness) closer to the wall before the heat loss to the solid surface leads to quenching [6]. This implies that when compared with their methane-air counterparts, hydrogen-air flames can propagate closer to the wall in regions of the boundary layer characterized by very low flow velocities. This also leads to increased heat transfer, which can potentially damage the combustor walls, and thus consequently leading to a failure of the combustion equipment. Current modeling methodologies, usually relying on Reynolds averaged Navier-Stokes (RANS) or large eddy simulation (LES) techniques, used to simulate industrial scale combustors cannot accurately account for the aforementioned physical phenomena involved in boundary layer flashback.

In turbulent reacting flows, the unclosed Reynolds stresses  $\rho u''_i u''_i$  are usually closed using a gradient hypothesis which relies on the turbulent eddy viscosity  $\mu_t$ . The eddy viscosity is usually evaluated in terms of the turbulent kinetic energy  $k = \rho u_1^{\prime\prime} u_1^{\prime\prime} / 2\overline{\rho}$  and its dissipation rate  $\widetilde{\epsilon} = \mu \partial u''_i / \partial x_i \partial u''_i / \overline{\rho}$  via the well-known  $k - \epsilon$  [7] model. There are several studies available in the literature [8,9] which deal with the closure of the transport equation for turbulent kinetic energy and its dissipation rate for nonreacting flows. In the case of premixed turbulent combustion, the problem of closing turbulent kinetic energy transport becomes more complicated due to flame generated turbulence [10], as the flame normal acceleration due to thermal expansion strongly influences the transport of turbulent kinetic energy. Flame generated turbulence in premixed flames has been linked with the mean velocity gradient due to flame normal acceleration by Bray and Libby [11] and was confirmed experimentally by Moreau and Boutier [12]. It is important to note that the preferential acceleration of low density burned products in comparison to the higher density unburned reactants in response to the self-induced pressure gradient within the flame brush significantly affects the contribution of the mean pressure gradient to the turbulent kinetic energy transport. This behavior is closely related with counter gradient transport of scalars in turbulent premixed flames [13–15]. Further experimental validation of this behavior has been provided by Borghi and Escudie [16] and Chomiak and Nisbet [17]. The importance of the effects of the fluctuating pressure gradient on turbulent kinetic energy transport has been indicated by several direct numerical simulation (DNS) analyses [18–22]. These effects were addressed in the context of RANS modeling by Bray et al. [13] and produced satisfactory agreement with experimental data for flames stabilised in stagnating flows. The contributions of pressure gradient to the transport of the Reynolds stresses has also been studied in detail and modeled based on conditional mean pressure values by Domingo and Bray [23].

Recently some work has been done to identify the behavior of flame flow interaction and pressure fluctuations in the case of boundary layer flashback in a fully turbulent channel flow by Gruber *et al.* [6]. In this work Gruber *et al.* [6] discussed the overall physics of the flame flow

interaction, including the behavior of the flame structure during the boundary layer flashback and the occurrence of local flow reversal pockets upstream of the flame in the near wall region induced by the Darrieus-Landau instability. The existence of pressure fluctuations triggered by the flame propagation upstream into the nonreacting channel flow was also explained. However, the detailed behavior of the turbulent kinetic energy, wall shear stress, the detailed budget of the turbulent kinetic energy transport and the influence of the mean pressure gradient on the turbulent kinetic energy transport in the case of wall bounded flames has not been explored in the case of boundary layer flashback of turbulent premixed flames. This information is fundamentally important for the modeling of flame-wall interaction in turbulent boundary layers and in particular boundary layer flashback.

Several studies have focused on closing the turbulent kinetic energy transport equation for statistically planar freely propagating turbulent premixed flames under different turbulence [24] and Lewis number [25] conditions. Recently, Lai *et al.* [26] analyzed the behavior of different terms in the turbulent kinetic energy transport equation in the context of head-on quenching premixed flames at different turbulence intensities and Lewis numbers. However, limited effort has been directed to the fundamental understanding of the statistics of turbulent kinetic energy transport in the case of flames interacting with fully developed boundary layers under flashback conditions. The main objectives of the present work are to understand the statistical behaviors of the different mechanisms, which control the evolution of the turbulent kinetic energy in boundary layer flashback of turbulent hydrogen premixed flames.

The paper is organized as follows. In the next two sections the details for the DNS data and the mathematical background for the current analysis are provided. This is followed by the results, and the conclusions are summarized in the final section.

## **II. DIRECT NUMERICAL SIMULATION DATA**

The DNS data of boundary layer flashback performed by Kitano et al. [27] has been considered in this study. This DNS is representative of flashback in a channel flow at bulk Reynolds  $Re_b =$  $\rho u_b h/\mu = 3500$ , where  $u_b = 1/2h \int_0^{2h} u \, dy$ , and Reynolds number based on the channel half height and friction velocity  $\operatorname{Re}_{\tau} = \rho u_{\tau} h/\mu = 120$ , where  $u_{\tau} = \sqrt{\tau_w/\rho}$  and  $\tau_w = \mu \partial u/\partial y|_{y=0 \text{ or } y=2h}$  is the wall shear stress. The simulation has been performed using the code known as  $FK^3$ , which has been used in several previous studies on turbulent, reacting, and multiphase flows [28-32]. The code solves conservation equations for mass, momentum, enthalpy, and chemical species in the context of finite volume methodology. A skeletal chemical mechanism comprising of 9 chemical species and 20 reactions proposed by Miller and Bowman [33] is used to account for the chemistry involved in hydrogen combustion. It should be noted here that the flow configuration and the turbulence and flame characteristics are similar to the one used in the earlier work of Gruber et al. [6]. In the present calculation the chemical reactions are calculated using the multitimescale (MTS) method in every time step with a minimum time resolution of  $1 \times 10^{-9}$  s. The spatial derivatives for the momentum equation are evaluated via a forth-order centered scheme. The convective terms of enthalpy and species mass fractions are calculated by using a third-order quadratic upstream interpolation for convective kinematics (QUICK) scheme as proposed by Ref. [34]. A second-order centered scheme is employed to calculate all the other terms in the scalar transport equations. The fractional-step method for compressible flows proposed by Moureau et al. [35] is used to solve the equations and time advancement for the convective terms is performed by using a third-order Runge-Kutta method.

The computational domain for the DNS is divided into two regions, namely, the channel flow region and the buffer region, as shown in Fig. 1. The channel flow region is subdivided into two parts, the turbulence generation region and the flashback region, as shown in Fig. 2. In the turbulence generation region of the channel flow, a fully developed wall-bounded turbulent flow is generated by imposing a pressure drop and a periodic boundary condition in the *x* direction. In the flashback region of the channel flow, the outflow characteristics of the upstream channel are introduced and a



FIG. 1. Computational grid used for the Direct Numerical Simulation shown on the x-y midplane.

freely propagating planar flame is initialized in the domain after 100 ms of the flow becoming fully turbulent in the channel. The no-slip isothermal boundary condition at 750 K is applied on the walls in the *y* direction, while the *z* direction is treated as periodic. The initial gas temperature, pressure and equivalence ratio are 750 K, 0.1 MPa, and 1.5, respectively. The laminar burning velocity  $S_L$  and the thermal flame thickness  $\delta_{th} = (T_{ad} - T_R)/\max|\nabla T|_L$  (where  $T_R$  is the reactant temperature,  $T_{ad}$ is the adiabatic flame temperature and the subscript *L* represents the laminar flame quantities) under these conditions are determined to be 14 m/s and 0.48 mm, respectively [36]. The grid resolution in the flashback region of the simulation is 50  $\mu$ m which in nondimensional wall units is  $\Delta x^+ =$  $\Delta y^+ = \Delta z^+ = 0.6$ . This level of resolution is appropriate for boundary layers as recommended by Moser *et al.* [37] and also ensures that the laminar flame thermal thickness  $\delta_{th}$  is resolved in at least 10 grid points. Note that larger grid spacing of 700  $\mu$ m ( $\Delta x^+ = 8.4$ ) is used in the *x* direction of the turbulence generation region of the simulation, as this level of resolution is sufficient to resolve the nonreacting turbulence at the conditions used in this work. A total of approximately 0.4 billion grid points are used in the simulation of which 1150 × 400 × 600 are in the flashback region of the simulation.

Mean velocity and Reynolds stresses in the nonreacting/turbulence generation region of the channel flow have been compared with the results of Tsukahara *et al.* [38,39] at  $\text{Re}_{\tau} = 110$  in Fig. 3. It should be noted here that very small differences in the mean velocity and Reynolds stresses exist between  $\text{Re}_{\tau} = 110$  and  $\text{Re}_{\tau} = 120$ , hence this comparison provides a good check for the turbulence statistics in the nonreacting/turbulence generation part of the channel flow. In this case, the Reynolds averaged quantities (denoted by  $\overline{\lambda}$ ) and fluctuations (denoted by  $\lambda' = \lambda - \overline{\lambda}$ ) have been time averaged and then space averaged in the periodic (x and z) directions. It can be noticed that an excellent agreement has been obtained for the nonreacting turbulence in the present



FIG. 2. Computational domain in the channel flow region.



FIG. 3. Mean velocity and Reynolds stresses in the turbulence generation region of the channel.

work and the published data. This establishes the fact that the turbulence interacting with the flame in the flashback region of the channel is free from inlet and numerical discretisation artefacts.

In the post-processing of the reacting data, the Reynolds averaged quantities (denoted by  $\overline{\lambda}$ ), Favre averaged quantities (denoted by  $\overline{\lambda} = \overline{\rho\lambda}/\overline{\rho}$ ), and Favre fluctuations (denoted by  $\lambda'' = \lambda - \overline{\lambda}$ ) have been time averaged for  $2.2 \times 10^{-5}$  s and space averaged for 1 mm in the periodic *z* direction at each point. This has been done because of the existence of the three-dimensional turbulent features present in the flashback flame. Note that in the results presented below only the flashback region of the channel is considered.

## **III. MATHEMATICAL BACKGROUND**

The transport equation for the Favre averaged turbulent kinetic energy is given by [20]

where  $\rho$  is the density, p is the pressure,  $u_j$  is the *j*th component of velocity, and  $\tau_{ij} = \mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i) - (2/3)\mu \cdot \delta_{ij}(\partial u_k/\partial x_k)$  is the viscous stress tensor in which  $\mu$  is the dynamic viscosity. In Eq. (1) the first term on the right hand side  $T_1 = -\overline{\rho u_i'' u_j''} \partial \tilde{u}_i/\partial x_j$  represents the production of turbulent kinetic energy by mean velocity gradients [20]. The term  $T_2 = -\overline{u_i''} \partial \overline{p}/\partial x_i$  represents production by the mean pressure gradient [21] while  $T_3 = \overline{p' \partial u_i''/\partial x_i}$  is the pressure dilatation term [20,21]. The term  $T_4 = \overline{u_i'' \partial \tau_{ij}/\partial x_j}$  describes the combined effects of molecular diffusion and viscous dissipation of turbulent kinetic energy. The final two terms  $T_5 = -\overline{\partial (p' u_i'')/\partial x_i}$  and  $T_6 = -\partial (\overline{\rho u_i'' u_k'' u_k''}/2)/\partial x_i$  represent the transport of turbulent kinetic energy by pressure fluctuations and turbulent velocity fluctuations, respectively. It should be noted here that in the context of the  $k - \epsilon$  model all the terms  $T_1$  to  $T_6$  are unclosed and need models. In this work, we aim to investigate the statistical behaviors of the aforementioned terms under boundary layer flashback conditions. In the following analysis, the reactive flow field is expressed in terms of the progress variable c based



FIG. 4. Instantaneous distributions of isosurfaces of the temperature at 1700 K (colored in red) and second invariant of the velocity gradient tensor (colored by instantaneous vorticity normalized by  $u_{\tau R}/h$ ). Top left figure shows the isometric view, bottom left figure shows the side view, top right figure shows the instantaneous normalized vorticity and negative flow velocity regions (colored in green) and the bottom right figure shows the region near the top wall where dotted ellipses show the regions of flame generated turbulence.

on the water vapor mass fraction as

$$c \equiv \frac{Y_{\rm H_2O} - Y_{\rm H_2O_R}}{Y_{\rm H_2O_P} - Y_{\rm H_2O_R}},\tag{2}$$

where the subscripts *R* and *P* represent the reactant and product side of the flame. Note that all the results in the following subsections are normalized by nonreacting density  $\rho_R$ , nonreacting friction velocity  $u_{\tau R}$  and the channel half height *h*.

#### **IV. FLOW AND FLAME BEHAVIOR**

Figure 4 shows the instantaneous isosurfaces of the temperature at 1700 K and the second invariant of the velocity gradient tensor (i.e.,  $Q = (-S_{ij}S_{ij} + P^2 + \omega_{ij}\omega_{ij})/2$ , where  $P = -\nabla \cdot \mathbf{u}$ ,  $S_{ij} = 0.5(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$  and  $\omega_{ij} = (\partial u_i/\partial x_j - \partial u_j/\partial x_i)$  are the first invariant, strain rate, and the rotation rate tensor, respectively), which represents the turbulent flow structure with Q > 0 and Q < 0 indicating vorticity-dominated and strain rate-dominated regions, respectively. It can be seen from Fig. 4 that the flame alters the boundary layer structure and the turbulence decays across the flame in the near wall region (top and bottom left of Fig. 4), whereas the turbulence (i.e., vorticity) is generated in the middle of the channel in the wake of the flame. This happens due to the interaction of the two different flame branches in the middle of the channel where the turbulence level is lower on the nonreacting side of the flame.

Figure 4 (bottom right) also shows the top view of the channel, the iso-surfaces of the temperature close to the wall are removed to show the second invariant of the velocity gradient tensor more clearly. It can be noticed in Fig. 4 (bottom right) that the local cusp formation toward the product



FIG. 5. Turbulence behavior in the in the flashback case. Top figure shows the wall shear stress normalized by  $\mu_R u_{\tau R}/h$  on the top wall, black lines represent  $0.1 \le \tilde{c} \le 0.9$ , regions demarcated by white lines represent negative wall shear stress/flow recirculation regions. Figure on the bottom shows the Favre averaged turbulent kinetic energy  $\tilde{k}/u_{\tau R}^2$  on log scale (left) and its Favre averaged dissipation  $\tilde{\epsilon} \times h/u_{\tau R}^3$  on log scale (right) on the *x*-*y* plane at z/h = 2.5. In figures on the bottom row the green lines indicate progress variable at  $0.1 \le \tilde{c} \le 0.9$ .

side of the flame leads to the local generation of turbulence which grows further downstream of the flame. This cusp formation occurs due to the propagation of the flame into the low velocity regions of the boundary layer formed by the oncoming flow. Figure 4 (top right) also shows the highly localized reverse flow regions of the flow (green isosurfaces), which are clearly visible immediately upstream of each flame bulge and are limited to the near-wall region. This behavior is consistent with the earlier findings of Gruber *et al.* [6]. The reason for the occurrence of these reverse flow regions upstream of the flame is due to the variation of the pressure field in the near wall region due to the existence of the flame, which in turn induces a positive (adverse) pressure gradient immediately upstream of the flame bulges and ultimately causes a flow reversal and a detailed discussion on this can be found in Ref. [6].

Figure 5 (top) shows the behavior of the averaged shear stress induced on the top channel wall. The wall shear stress increases across the flame due to an increase in the velocity on the product side of the flame. In this case, negative wall shear stress can be seen upstream of the flame in the regions of reverse flow. This implies that the reverse flow introduced by the flame in the boundary layer has an influence on the turbulent kinetic energy. Figure 5 (bottom left) shows the behavior of the Favre averaged turbulent kinetic energy extracted on the *x*-*y* plane at z/h = 2.5 location, as the flow reversal regions exist on both walls at this location. It can be seen that the turbulent kinetic energy is low in the nonreacting part of the channel upstream of the flame until it is attenuated in the far wake of the flame due to the dissipation rate induced by flame generated vorticity. Similar trends are observed for the Favre averaged turbulent kinetic energy and its dissipation within the flame brush at different locations away from the wall. The turbulent kinetic energy is zero at the wall and reaches a relatively high value at y/h = 0.1 due to the generation of turbulence caused by shear within the boundary layer. Further away from the wall, the turbulent kinetic energy decreases toward the



FIG. 6. The variation of turbulent kinetic energy (left) and turbulent dissipation (right) across the flame brush at different wall distances in the channel on the x-y plane at z/h = 2.5.

middle of the channel at y/h = 1.0. The turbulent dissipation is maximum at the wall and decreases toward the center of the channel as shown in Fig. 6. The high level of turbulent kinetic energy and its dissipation within the flame are consistent with the earlier findings of Chakraborty *et al.* [24] for unconfined statistically planar turbulent flames in the corrugated flamelets regime. It should be noted here that the flame in the middle of the channel nominally lies in the corrugated flamelets regime due to lower turbulence intensity and large length scales encountered in low Re<sub> $\tau$ </sub> channel flows.

The behavior of the Favre averaged Reynolds stresses across the flame brush at different locations in the channel is shown in Fig. 7. It should be noted that six components of  $u_i'' u_i''$  have been plotted as  $u_i^{\prime\prime} u_i^{\prime\prime}$  is a symmetric tensor. In a classical nonreacting channel flow only  $u_1^{\prime\prime} u_1^{\prime\prime}$ ,  $u_2^{\prime\prime} u_2^{\prime\prime}$ ,  $u_3^{\prime\prime} u_3^{\prime\prime}$ , and  $\widetilde{u_1''u_2''}$  components assume nonzero values [40], whereas in the case of boundary layer flashback all six components of  $u''_i u''_i$  have nonzero values within the flame brush. An increase in the values of Reynolds stresses toward the middle of the flame brush can be noticed at y/h = 0.1 and this trend continues up to y/h = 0.5 which implies that the generation of turbulence due to the formation of local shear layers within the flame brush. This phenomenon has previously been observed in statistically planar weakly turbulent premixed flames by Lipatnikov et al. [41]. At y/h = 1.0 an increase in the Reynolds stresses at the trailing edge of the flame can be seen due to the merging of the flame branches from the top and bottom walls. In the case of nonreacting channel flows, the Reynolds stresses are at the lowest levels at y/h = 1.0 (i.e., middle of the channel) [40], whereas in the case of boundary layer flashback, at y/h = 1.0 the flame induces turbulence due to local shear layer formation and also due to the large scale low frequency oscillations at the center of the channel caused by merging of the two flame branches which leads to an increase in the values of Reynolds stresses and consequently the turbulent kinetic energy.

Figure 8 shows the behavior of Favre averaged Reynolds stresses within the flame brush on the Lumley triangle, where  $\eta$  and  $\xi$  represent the second and third invariants of the normalized anisotropy tensor for  $u_i''u_i''$  defined as

$$6\eta^2 = b_{ij}b_{ji}$$
, and  $6\xi^3 = b_{ij}b_{jk}b_{ki}$ , (3)

where  $b_{ij}$  is defined as  $b_{ij} = u_i'' u_j' / u_i'' u_i'' - (1/3)\delta_{ij}$  [9]. The Reynolds stresses in the case of boundary layer flashback remain relatively anisotropic across the flame brush at all locations within the channel. This is contrary to the behavior of the Reynolds stresses in the nonreacting channel flows as the Reynolds stresses tend to isotropy toward the center of the nonreacting channel [9,40]. At y/h = 0.1,  $u_i''u_i''$  is highly anisotropic and reaches one component limit due to the proximity of



FIG. 7. Reynolds stress profiles across the flame brush at different wall distances in the channel on the x-y plane at z/h = 2.5.

the flow to the wall [9] and also due to the anisotropy induced by the thermal expansion caused by the weakly turbulent premixed flame [42]. Further away from the wall, at y/h = 0.5, the Reynolds stresses tend to move toward a more isotropic state, but the flame induces anisotropy and one component limit behavior is observed at this level. At y/h = 1.0, the merging of the two flame branches induce turbulence into the flow and cause high levels of anisotropy in this region of the channel leading to one and two component limit behavior. The individual behavior of the terms controlling turbulent kinetic energy transport are discussed in detail in the following subsections. It should be noted here that the procedure for averaging used in the reacting part of the channel ensures that the unsteady term in the turbulent kinetic energy transport equation [Eq. (1)] remains two orders of magnitude smaller in comparison to the other leading order terms (e.g., dissipation rate of turbulent kinetic energy) and consequently this term is not discussed in the subsequent sections of this paper.

#### V. BEHAVIOR OF THE MEAN VELOCITY GRADIENT TERM T<sub>1</sub>

The behavior of the mean velocity gradient term  $T_1$  in Eq. (1) is shown on the *x*-*y* plane at z/h = 2.5 location in Fig. 9. It can be seen from Fig. 9 that  $T_1$  remains slightly negative/close to zero or positive upstream of the flame in the nonreacting part of the channel and the intensity of  $T_1$  increases in the near wall region at the leading edge of the flame. This is attributed to the local flow recirculation regions shown in Figs. 4 and 5. The term  $T_1$  becomes significantly negative within the flame structure and then reaches very low values in the immediate wake of the flame. Further downstream a rapid increase in  $T_1$  can be seen which results from the interaction of the two flame branches in the middle of the channel. Figure 10 shows the behavior of  $T_1$  within the flame brush at



FIG. 8. Lumley triangle on the plane of the invariants  $\xi$  and  $\eta$  of the Reynolds stress anisotropy tensor across the flame brush at different wall distances in the channel on the *x*-*y* plane at z/h = 2.5. 1*C*, 2*C* and iso mean one-component limit, two-component limit, and isotropic, respectively.

different locations away from the channel wall. The term  $T_1$  remains zero at the wall and becomes positive at the leading edge of the flame at y/h = 0.1. This is due to the local flow recirculation regions formed upstream of the flame caused by the adverse pressure gradient in the boundary layer. Further away from the wall the magnitude of  $T_1$  increases within the flame brush up to y/h = 0.5and then decreases toward the middle of the channel. The behavior of  $T_1$  at y/h = 0.5 is consistent with that of an unconfined statistically planar premixed flame in the corrugated flamelets regime as shown by Chakraborty *et al.* [24]. The change in the sign of  $T_1$  within the flame at y/h = 0.1 and



FIG. 9. Mean velocity gradient term  $T_1$  normalized by  $\rho_R u_{\tau R}^3/h$  on the *x*-*y* plane at z/h = 2.5. The green lines indicate progress variable at  $0.1 \le \tilde{c} \le 0.9$ .



FIG. 10. The variation of mean velocity gradient term  $T_1$  normalized by  $\rho_R u_{\tau R}^3 / h$  across the flame brush (top left), leading edge of the flame (top right) and trailing edge of the flame (bottom) at different locations away from the wall on the x-y plane at z/h = 2.5.

y/h = 1.0 can be explained by the stress-strain lag caused by unsteady straining due to the recirculation upstream of the flame at y/h = 0.1 and the low frequency oscillations due to merging of the two flame branches at y/h = 1.0. The phase lag between the Reynolds stress and strain rate tensor has been shown in several previous studies involving nonreacting flows containing recirculation regions or flows under unsteady straining [43–45]. In these cases the turbulence intensity grows until inertial effects are large enough such that the stress tensor no longer follows the strain rate tensor, thus leading to changes in turbulence production mechanism [44].

The phase lag between the Reynolds stress and strain rate tensor in the recirculation zone upstream of the flame at y/h = 0.1 and in the middle of the channel at y/h = 1.0 can be confirmed by analyzing the relative alignment of the Reynolds stress and the mean velocity gradient tensor. The tensors  $u_i''u_j''$  and  $\partial \tilde{u}_i/\partial x_j$  can be decomposed into base eigenvectors using eigendecomposition as

$$\frac{\partial \bar{u}_i}{\partial x_i} = \alpha_s \boldsymbol{\alpha}_s \boldsymbol{\alpha}_s^T + \beta_s \boldsymbol{\beta}_s \boldsymbol{\beta}_s^T + \gamma_s \boldsymbol{\gamma}_s \boldsymbol{\gamma}_s^T, \tag{4}$$

$$-u_{i}^{\prime\prime}u_{j}^{\prime\prime} = \alpha_{-\tau}\boldsymbol{\alpha}_{-\tau}\boldsymbol{\alpha}_{-\tau}^{T} + \beta_{-\tau}\boldsymbol{\beta}_{-\tau}\boldsymbol{\beta}_{-\tau}^{T} + \gamma_{-\tau}\boldsymbol{\gamma}_{-\tau}\boldsymbol{\gamma}_{-\tau}^{T}, \qquad (5)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are the eigenvalues and  $\alpha$ ,  $\beta$ , and  $\gamma$  are the respective eigenvectors; the subscripts *s* and  $-\tau$  represent the respective eigenvalues and eigenvectors of the mean velocity gradient tensor and the negative of Reynold stress tensors, respectively, and the transposed vector is represented by the superscript *T*. The eigenvalues are ordered as  $\alpha > \beta > \gamma$ , and the corresponding eigenvectors  $\alpha$ ,  $\beta$  and  $\gamma$  are labeled as the extensive, intermediate, and compressive eigenvectors, respectively. Note that following the earlier investigation of Ahmed *et al.* [42] the negative sign has been included



FIG. 11. Direction cosines between the eigenvectors of  $\partial \tilde{u}_i / \partial x_j$  and  $-u_i'' u_j''$  across the flame brush at different y/h locations on the x-y plane at z/h = 2.5.

in the Reynolds stresses in Eq. (5). The term  $T_1$  can now be expressed as

$$T_{1} = \alpha_{-\tau}\alpha_{s}(\boldsymbol{\alpha}_{-\tau}\cdot\boldsymbol{\alpha}_{s})^{2} + \alpha_{-\tau}\beta_{s}(\boldsymbol{\alpha}_{-\tau}\cdot\boldsymbol{\beta}_{s})^{2} + \alpha_{-\tau}\gamma_{s}(\boldsymbol{\alpha}_{-\tau}\cdot\boldsymbol{\gamma}_{s})^{2} + \beta_{-\tau}\alpha_{s}(\boldsymbol{\beta}_{-\tau}\cdot\boldsymbol{\alpha}_{s})^{2} + \beta_{-\tau}\beta_{s}(\boldsymbol{\beta}_{-\tau}\cdot\boldsymbol{\beta}_{s})^{2} + \beta_{-\tau}\gamma_{s}(\boldsymbol{\beta}_{-\tau}\cdot\boldsymbol{\gamma}_{s})^{2} + \gamma_{-\tau}\alpha_{s}(\boldsymbol{\gamma}_{-\tau}\cdot\boldsymbol{\alpha}_{s})^{2} + \gamma_{-\tau}\beta_{s}(\boldsymbol{\gamma}_{-\tau}\cdot\boldsymbol{\beta}_{s})^{2} + \gamma_{-\tau}\gamma_{s}(\boldsymbol{\gamma}_{-\tau}\cdot\boldsymbol{\gamma}_{s})^{2},$$
(6)

where  $(a.b) = \cos\theta$  and  $\theta$  is the angle between the vectors a and b. Thus, the behavior of  $T_1$  can be determined by the joint statistics of geometric alignments of the Reynolds stress and the mean velocity gradient tensors and their respective eigenvalues. Figure 11 shows the direction cosines between the two eigensystems across the flame brush at different y/h locations. It can be seen that the alignment of the eigenvectors for the Reynolds stress and the mean velocity gradient tensor changes with distance away from the wall within the flame brush. At y/h = 0.1,  $\alpha_s$  aligns with  $\beta_{-\tau}$ ,  $\beta_s$  aligns with  $\gamma_{-\tau}$  and  $\gamma_s$  with  $\alpha_{-\tau}$  at the leading edge of the flame  $(0 < \tilde{c} < 0.1)$  and then the alignment changes and the eigenvectors for  $-u''_i u''_j$  and  $\partial \tilde{u}_i/\partial x_j$  become fully aligned in the rest of the flame brush until  $\tilde{c} = 0.8$ . The alignment changes again at  $\tilde{c} > 0.8$  toward that found at the leading edge of the flame due to the influence of the boundary layer interacting with the flame. Further away from the wall at y/h = 0.5 the two eigensystems remain completely aligned throughout the flame brush as found in an earlier investigation of turbulent statistically planar flames in the corrugated flamelets regime [42]. At the middle of the channel (y/h = 0.5) the alignment between the eigenvectors of  $-u''_i u''_j$  and  $\partial \tilde{u}_i/\partial x_j$  changes again and behaves in a similar manner to that found closer to the wall at y/h = 0.1.



FIG. 12. Mean pressure gradient term  $T_2$  normalized by  $\rho_R u_{\tau R}^3/h$  on the *x*-*y* plane at z/h = 2.5 (left). Relative mean pressure normalized by  $\rho_R u_{\tau R}^2$  on the *x*-*y* plane at z/h = 2.5 (right). Green lines indicate progress variable at  $0.1 \leq \tilde{c} \leq 0.9$ .

The misalignment between the two eigensystems at y/h = 0.1 and y/h = 1.0 is representative of the phase lag between the Reynolds stress and strain rate tensor caused by the recirculation zones (at y/h = 0.1) and cyclic unsteadiness in the flow (at y/h = 1.0). The perfect alignment of the eigenvectors for the two tensors in the regions of heat release can be explained by the fact that in the case of reacting flows with heat release, the effects of dilatation play an important role as shown in many previous studies involving scalar gradient alignment with the principal directions of the strain rate [46–48]. In the case of premixed combustion, the relative alignment of the eigenvectors for  $-u''_i u''_i$  and  $\partial \tilde{u}_i / \partial x_i$  is influenced by the competition between the thermochemical and fluid dynamic processes. This implies that the chemical reactions releasing heat cause dilatation and flame normal acceleration which competes with the local turbulent fluid dynamics processes [42] and tends to reduce the lag between the Reynolds stress and the strain rate tensor. In this case the flow remains highly anisotropic as shown in Fig. 8 due to the perfect alignment of the two eigensystems caused by heat release across a large part of the flame brush. This results in a situation where the Reynolds stress tensor has only one significant component, and this is reflected in the one component like behavior across the flame brush [42]. These effects should be explicitly accounted for in the closure of term  $T_1$  for accurate modeling of premixed turbulent combustion.

### VI. BEHAVIOR OF THE MEAN PRESSURE GRADIENT TERM T<sub>2</sub>

The variation of the mean pressure gradient term  $T_2$  is shown in Fig. 12 on the x-y plane at z/h = 2.5 location. The term  $T_2$  takes mostly positive or small negative values in the boundary layer upstream of the flame 0 < x/h < 0.8 due to the local compressibility caused by the propagation of the flame into the oncoming reactants. This can be confirmed by the contours of the relative pressure field in Fig. 12. At the leading edge of the flame the term  $T_2$  assumes negative values as shown in Fig. 13 for different locations away from the wall within the flame brush and then switches to mostly positive values in the rest of the flame structure. It can be noticed in Fig. 13 that  $T_2$  becomes negative at y/h = 1.0, this is due to the pressure drop induced by the interaction of the two flame branches extending from the top and bottom walls of the channel. The overall changes in  $T_2$  exist due to the pressure drop and local compressibility effects and then slowly decays to zero in the far wake of the flame as shown in Fig. 12.

# VII. BEHAVIOR OF THE PRESSURE DILATATION TERM T<sub>3</sub>

Figure 14 shows the pressure dilatation term  $T_3$  in Eq. (1) on the x-y plane at z/h = 2.5 location. The pressure dilatation effects remain negligibly small away from the flame. However, within the flame brush, the pressure dilatation term changes sign depending on the proximity to the wall. Figure 15 shows that in the near wall region, the pressure dilatation term remains positive at the leading edge of the flame and assumes negative values in the trailing edge of the flame, whereas



FIG. 13. Mean pressure gradient term  $T_2$  normalized by  $\rho_R u_{\tau R}^3/h$  across the flame brush at different locations away from the wall on the x-y plane at z/h = 2.5.

toward the middle of the channel this behavior switches and the pressure dilatation term takes negative values at the leading edge of the flame and becomes positive with increasing values of  $\tilde{c}$ . These changes in the behavior of term  $T_3$  at different channel heights exist due to the combination of pressure drop within the flame and an increase in the magnitude of the individual diagonal elements of the velocity gradient tensor in the dilatation rate induced by thermal expansion effects. Note that the pressure dilatation term is one of the biggest terms in terms of the magnitude and is consistent with the earlier findings in freely propagating premixed turbulent planar flames [18,22,24,25] and head-on quenching flames [26].

#### VIII. BEHAVIOR OF THE MOLECULAR DIFFUSION AND DISSIPATION CONTRIBUTION T4

The viscous dissipation term can be expressed as

$$T_{4} = \overline{u_{i}^{\prime\prime} \frac{\partial \tau_{ij}}{\partial x_{j}}} = \underbrace{-\overline{\rho}\widetilde{\epsilon}}_{T_{41}} + \underbrace{\left[ u_{i}^{\prime\prime} \frac{\partial}{\partial x_{k}} \left( \mu \frac{\partial u_{k}^{\prime\prime}}{\partial x_{i}} \right) - \frac{2}{3} \overline{u_{i}^{\prime\prime} \frac{\partial}{\partial x_{i}} \left( \mu \frac{\partial u_{k}^{\prime\prime}}{\partial x_{k}} \right)} \right]}_{T_{42}} + \underbrace{\frac{\partial}{\partial x_{j}} \left( \overline{\mu} \frac{\partial \widetilde{k}}{\partial x_{j}} \right)}_{T_{43}}.$$
 (7)

The variation of the viscous dissipation term  $T_4$  and all the individual terms in Eq. (7) are shown in Fig. 16. The behavior of  $T_4$  is primarily driven by the behavior of turbulent dissipation (term  $T_{41}$ ) and the contributions from  $T_{42}$  and  $T_{43}$  are very small in comparison to  $T_{41}$  as shown in Figs. 16 and 17. This behavior is expected in the limit of high Reynolds number and is consistent with the earlier findings for reacting [24] and nonreacting [8] flows. In the region upstream of the flame  $T_{41}$ 



FIG. 14. Pressure dilatation term  $T_3$  normalized by  $\rho_R u_{\tau R}^3/h$  on the *x*-*y* plane at z/h = 2.5. The green lines indicate progress variable at  $0.1 \le \tilde{c} \le 0.9$ .



FIG. 15. Pressure dilatation term  $T_3$  normalized by  $\rho_R u_{\tau R}^3 / h$  across the flame brush at different locations away from the wall on the x-y plane at z/h = 2.5.

has the largest value at the wall, which is again consistent with the classical channel flow behavior [8,40], while  $T_{42}$  approaches zero (i.e.,  $T_{42} \rightarrow 0$ ) at the wall due to no slip condition and  $T_{43}$  takes large values at the wall due to steep gradients of turbulent kinetic energy in the boundary layer. All the terms contributing to  $T_4$  become large near the walls within the flame due to steep velocity and viscous gradients introduced by heat release. Toward the middle of the channel within the flame all the terms behave similar to an unconfined statistically planar flame [24].

#### IX. BEHAVIOR OF THE PRESSURE TRANSPORT TERM T<sub>5</sub>

The distribution of the pressure transport term  $T_5$  on the x-y plane at z/h = 2.5 location is shown in Fig. 18. The pressure transport is negative upstream of the flame (0 < x/h < 1) and then progressively becomes positive towards the flame. This happens due to the compressibility effects caused by the propagating flame. Figure 19 shows that in the near wall region, the pressure



FIG. 16. Molecular diffusion and dissipation contribution  $T_4$  (top left),  $T_{41}$  (top right),  $T_{42}$  (bottom left), and  $T_{43}$  (bottom right). All terms are shown on the *x*-*y* plane at z/h = 2.5 and are normalized by  $\rho_R u_{\tau R}^3/h$ . The green lines indicate progress variable at  $0.1 \leq \tilde{c} \leq 0.9$ .



FIG. 17. Molecular diffusion and dissipation contribution normalized by  $\rho_R u_{\tau R}^3 / h$  across the flame brush at different locations away from the wall on the *x*-*y* plane at z/h = 2.5.

transport term is negative at the front end of the flame but becomes positive toward the burnt gas side; whereas toward the middle of the channel the pressure transport term assumes positive values at the leading edge but becomes negative towards the burned gas side of the flame. The behavior of the pressure transport term towards the middle of the channel is similar to that of an unconfined statistically planer premixed flame as reported by Chakraborty *et al.* [24]. Note that the magnitude of the pressure transport term is similar to that of the pressure dilatation term and is one of the largest terms in the turbulent kinetic energy transport equation. This behavior is also consistent with the earlier findings of Lai *et al.* [26] for premixed turbulent head-on quenching flames.



FIG. 18. Pressure transport term  $T_5$  normalized by  $\rho_R u_{\tau R}^3/h$  on the *x*-*y* plane at z/h = 2.5. The green lines indicate progress variable at  $0.1 \leq \tilde{c} \leq 0.9$ .



FIG. 19. Pressure transport term  $T_5$  across the flame brush normalized by  $\rho_R u_{\tau R}^3 / h$  at different locations away from the wall on the x-y plane at z/h = 2.5.

# X. BEHAVIOR OF THE TURBULENT TRANSPORT TERM $T_6$

The turbulent transport term  $T_6$  represents the turbulent diffusion of the turbulent kinetic energy. Figure 20 shows the triple correlation term on the x-y plane at z/h = 2.5 location. The values of triple correlation term are close to zero in the region upstream and downstream of the flame. Figure 21 shows that at the front of the flame,  $T_6$  assumes negative or very close to negative values across the flame brush for all y/h locations and becomes positive for high values of  $\tilde{c}$ . This behavior is similar to that of an unconfined statistically planar flame as shown by Chakraborty *et al.* [24] for the corrugated flamelets regime, and in this case originates due to the large length scales encountered in low Re<sub> $\tau$ </sub> channel flow. The largest variation in the magnitude of  $T_6$  can be observed for y/h = 0.1 and y/h = 0.5 locations, as the turbulence generated due to the shear in the near wall region significantly influences the turbulent transport due to triple correlation of fluctuating velocity.

#### XI. TOTAL BUDGET

Figure 22 shows the budgets of the terms on the right hand side of Eq. (1) at y/h = 0, y/h = 0.1, y/h = 0.5 and y/h = 1 within the flame brush. The pressure related terms i.e., pressure dilatation  $T_3$  and the transport of turbulent kinetic energy by pressure fluctuations  $T_5$  remain dominant throughout the domain. The viscous dissipation term  $T_4$  is maximum at the wall and decreases away from the wall, while the mean pressure gradient term  $T_2$  becomes dominant away from the wall due to an increase in the velocity fluctuations and the mean pressure gradient. Furthermore, it should be noted



FIG. 20. Turbulent transport term  $T_6$  normalized by  $\rho_R u_{\tau R}^3 / h$  on the *x*-*y* plane at z/h = 2.5. The green lines indicate progress variable at  $0.1 \le \tilde{c} \le 0.9$ .



FIG. 21. Turbulent transport term  $T_6$  across the flame brush normalized by  $\rho_R u_{\tau R}^3 / h$  at different locations away from the wall on the x-y plane at z/h = 2.5.

that the magnitudes of  $T_3$  and  $T_5$  are high at the wall and in the near wall region (y/h = 0.0 and y/h = 0.1) and decrease away from the wall (y/h = 0.5) before increasing again in the middle of the channel (y/h = 1.0) due the interaction of the two flame branches from the top and bottom side of the channel which induce low frequency flow and pressure oscillations.



FIG. 22. Total budget of the turbulent kinetic energy transport equation within the flame brush at different locations away from the wall on the x-y plane at z/h = 2.5. All the terms are normalized by  $\rho_R u_{\tau R}^3/h$ .

Although the flame considered here exhibits some attributes of premixed turbulent combustion within the corrugated flamelets regime, there are some differences in the turbulent kinetic energy transport between the current analysis (i.e., turbulent boundary layer flashback of a premixed flame) and the previous analyses [20,21] on turbulent kinetic energy transport in freely propagating statistically planar premixed turbulent flames representing the corrugated flamelets regime. It is worth noting that the flames in Refs. [20,21] were free of any mean shear whereas the presence of wall induces mean shear effects in the current configuration, which consequently leads to differences in the turbulent kinetic energy budget under turbulent boundary layer flashback conditions. One of the most notable qualitative differences in the turbulent kinetic energy transport in the current configuration in comparison to those in Refs. [20,21] is the sign change of the mean velocity gradient term  $T_1$  in this configuration (see Fig. 10) due to flow reversal, whereas  $T_1$  remained negative throughout the flame brush in Refs. [20,21]. The other major qualitative difference lies in the negative values of the pressure dilatation term  $T_3$  in the current configuration, whereas this term was reported to be positive in Refs. [20,21]. It was explained by Chakraborty et al. [24,25] that the pressure dilatation term  $T_3$  can assume negative values for small values of Damkhöler number. In this configuration, a local Damkhöler number can be derived based on the local values of Favre averaged turbulent kinetic energy and its dissipation rate as  $Da \sim S_L k / \delta_{th} \tilde{\epsilon}$  which suggests that low Damkhöler number effects remain prevalent in the vicinity of the wall as k is damped close to the wall becase of the no-slip boundary condition, whereas  $\tilde{\epsilon}$  assumes large values at the wall as shown in Fig. 6. This further indicates that the modeling of the turbulent kinetic energy transport for turbulent boundary layer flashback of premixed turbulent flames needs to be developed in such a manner that it remains valid for a range of different Damkhöler numbers across different combustion regimes.

# XII. IMPLICATIONS FOR CLOSURE MODELS

In the light of the statistical behaviors of different terms in the turbulent kinetic energy transport equation [Eq. (1)] presented in the preceding sections some implications on the closures of these terms are presented here. In the case of the mean velocity gradient term  $T_1$ , it is evident from the changes in the sign of  $T_1$  across the flame brush and the channel height that the closure strategy requires a modification to the existing approximation introduced by Boussinesq [49], which assumes that the Reynolds stresses are proportional to the mean rate of strain. This assumption does not hold in the case of boundary layer flashback and modified stress-strain lag models [44,50] or modified nonequilibrium models [51,52] are needed which account for the effects of heat release due to combustion. The mean pressure gradient term  $T_2$  becomes a leading order term within the flame as the distance from the wall increases (see Fig. 22). In this case  $\overline{u''_i}$  can be expressed as a function of turbulent scalar flux,  $\overline{u''_i c''} \sim (\rho_R^{-1} - \rho_P^{-1})\overline{\rho u''_i c''}/\overline{\rho}$  (where  $\rho_R$  and  $\rho_P$  are the densities in the unburned gas and fully burned products, respectively) [21,24,25], which implies that the turbulent scalar flux controls the behavior of  $T_2$  and appropriate damping of  $\overline{u''_i c''}$  is needed to account for the effects of the turbulent boundary layer for accurate modeling of term  $T_2$  in wall bounded premixed flames as suggested by Lai *et al.* [26].

The pressure dilatation  $(T_3)$  and the pressure transport  $(T_5)$  terms exhibit both positive and negative values within the flame brush at different channel heights. In the case of  $T_3$ , the negative values are consistent with the earlier DNS investigations [24,25], but are in contrast to the models proposed in the literature [20,21], which are only able to predict positive values for  $T_3$ , which is assumed to be proportional to  $\tau^2 S_L^3 \rho_R / \delta_{\text{th}}$ . Thus, improved models for the pressure dilatation term are needed in the case of boundary layer flashback which can account for pressure fluctuations due to heat release in wall bounded flames. The pressure transport term can be simplified as  $T_5 = -\overline{u_i''\partial p'/\partial x_i} - T_3$  and the closure for  $T_5$  relies on the closure for  $T_3$  and  $-\overline{u_i''\partial p'/\partial x_i}$ . Several closures for this term exist in the literature for nonreacting [53] and premixed reacting [20,24,25]



FIG. 23. The behavior of  $\overline{\rho u'_i u''_j u''_j} \times \partial \tilde{k} / \partial x_i$  within the flame brush at different locations away from the wall on the x-y plane at z/h = 2.5. All the terms are normalized by  $\rho_R u^5_{\tau_R} / h$ .

flows, but these closures need to be modified to include the effects of turbulent boundary layers with chemical reaction.

In the viscous dissipation and molecular diffusion term  $(T_4)$ ,  $T_{42}$  is the only unclosed term as the turbulence dissipation contribution  $(T_{41})$  is modeled by a separate transport equation in the context of the well-known  $k - \epsilon$  model [7] and the term  $T_{43}$  relies on the resolved/modeled quantities. Several closures exist for  $T_{43}$  in the literature [20,21,24,25]. These closures require appropriate near wall damping to account for wall effects as demonstrated in the case of head-on quenching flames [26] and further improvements are needed to account for the influence of the turbulent boundary layer in the case of flashback flames. The turbulent transport term is smaller than the other terms in the turbulent kinetic energy transport equation. In the case of nonreacting turbulence  $\overline{\rho u''_i u''_j u''_j}/2$  is usually modeled as  $\overline{\rho u_i'' u_i'' u_i''}/2 = -(\mu_t/\sigma_k(\partial \tilde{k}/\partial x_i))$  (where  $\sigma_k$  is the turbulent Schmidt Number) via the gradient diffusion hypothesis [8]. The variations of  $\overline{\rho u_i'' u_j'' u_i''} \times \partial \tilde{k} / \partial x_i$  are shown in Fig. 23. In this case if  $\overline{\rho u'_i u''_i u''_i} \times \partial k/\partial x_i > 1$  (here repeated *i* does not indicate summation but represents i = 1, 2 and 3 individually and repeated j indicates summation) then it implies counter gradient transport and if  $\rho u''_i u''_i \times \partial k / \partial x_i < 1$  (here repeated *i* does not indicate summation but represents i = 1, 2 and 3 individually and repeated j indicates summation) then it implies gradient type transport. It can be noticed in Fig. 23 that both gradient and counter gradient type effects exist in the near wall region (y/h = 0.1) due to the local recirculation zones formed upstream of the flame. As the distance from the wall increases a more counter gradient type transport is observed. This is consistent with the earlier findings of head-on quenching flames [26] and needs to be accounted for in the closure for  $T_6$ .

The accurate modeling of the individual terms in the turbulent kinetic energy transport equation is important from the point of view of the accurate prediction of the Favre averaged turbulent kinetic energy, which is required for closing the mean reaction rate [54–56], turbulent flame speed prediction [57,58], and the mean flame shape prediction in the case of turbulent boundary layer flashback [59]. The proposal of new models for the different terms in the turbulent kinetic energy transport equation is beyond the scope of current work. To develop robust closures, the statistical trends for the different terms in the turbulent kinetic energy transport equation at different flow conditions (i.e., boundary layer flashback in channel flows at different Re<sub> $\tau$ </sub> values) are needed, such that the model is applicable at different conditions. The development of closure models is part of the ongoing work and will be addressed in detail in the future studies.

## XIII. SUMMARY AND CONCLUSIONS

The behavior of turbulence and the transport equation for turbulent kinetic energy have been investigated by using a direct numerical simulation (DNS) database for flashback of premixed hydrogen-air flame in a fully developed turbulent channel flow. The nonreacting turbulence characteristics of the channel flow are representative of the friction velocity based Reynolds number  $Re_{\tau} = 120$ , while a hydrogen-air mixture with an equivalence ratio of 1.5 has been considered. A detailed chemical mechanism with 9 chemical species and 20 reaction is employed for an accurate representation of hydrogen-air combustion. The flow configuration and the turbulence and flame characteristics are similar to the one used in the earlier work of Gruber et al. [6]. The influence of the flame on the turbulence in the channel flow has been analyzed by investigating wall shear stress, turbulent kinetic energy and its dissipation rate. It has been found that the propagation of the flame into the upstream fully developed turbulent boundary layer introduces a flow reversal in some regions upstream of the flame, which is consistent with the earlier findings of Gruber et al. [6], and these regions lead to negative wall shear stress on the walls. The budgets of the turbulent kinetic energy transport reveal that the local flow reversal regions have an influence on the turbulent kinetic energy production, pressure dilatation and pressure transport terms. Some weak local compressibility effects have been observed as demonstrated by the changes in the mean pressure gradient, pressure dilatation and pressure transport terms in the turbulent kinetic energy equation upstream of the flame. It has also been found that the pressure dilatation and turbulent transport due to pressure are the two dominant terms in the turbulent kinetic energy equation under flashback conditions. This is consistent with the earlier findings of Lai et al. [26] for head-on quenching flames. The modeling of unclosed terms of turbulent kinetic energy transport equation will form the basis of future investigations.

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