Assessment of subgrid-scale stress statistics in non-premixed turbulent wall-jet flames

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We investigate the heat-release effects on the characteristics of the subgrid-scale (SGS) stress tensor and SGS dissipation of kinetic energy and enstrophy. Direct numerical simulation (DNS) data of a non-premixed reacting turbulent wall-jet flow with and without substantial heat release is employed for the analysis. This study comprises, among others, an analysis of the eigenvalues of the resolved strain rate and SGS stress tensors, to identify the heat-release effects on their topology. An assessment of the alignment between the eigenvectors corresponding to the largest eigenvalues of these two tensors is also given to provide further information for modelling of the SGS stress tensor. To find out the heat-release effects on the dynamics of the turbulent kinetic energy and enstrophy dissipation, probability density functions (PDFs) and mean values are analyzed.

The mean SGS shear stress and turbulent kinetic energy both slightly increase in the buffer layer and substantially decrease further away from the wall, due to the heat-release effects. Contrary to the kinetic energy, heat release decreases the mean SGS dissipation of enstrophy in the near-wall region. Moreover, differences in the shapes of the PDFs between the isothermal and exothermic cases indicate changes in the intermittency level of both SGS dissipations. Heat release also increases the SGS stress anisotropy in the near-wall region. Although, the structure of the mean resolved strain-rate tensor only marginally differs between the isothermal and exothermic cases in the near-wall region, substantial differences are observed in the jet area, where compressibility effects are important and heat-release effects are found to promote compression states. The differences in the relative alignment between the SGS stress and resolved strain-rate tensors in the isothermal and exothermic cases are discussed in connection with the differences in the SGS dissipation of kinetic energy.

1. Introduction

Subgrid-scale (SGS) modelling for large-eddy simulation (LES) of turbulent combustion is a challenging issue, owing to the complexity of its physics [1, 2]. Understanding the combustion effects on the dynamics of the SGS stresses and their interactions with the resolved scales is one of the main topics in this field that needs to be further explored. Although, SGS models for the scalar fluxes are naturally of prime importance in LES of combustion, SGS stress models also play an important role, since they influence the flow field predictions and hence the accuracy of the advected scalar predictions. Moreover, the SGS scalar flux dynamics are coupled with those of the SGS stress tensor [3–6]. To provide valuable data for assessment of SGS models, SGS statistics are often extracted from direct numerical simulation (DNS) data using a filtering operation. *A priori* computation of the SGS statistics provides both information on the physics of the subgrid-scales, especially in complex combustion applications and plays an important role in the design of new SGS models [7].

Combustion heat release significantly changes the turbulence dynamics at the

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large scales, through the gas expansions [8–10], and subsequently at the small scales [9]. The heat-release effects on the topology of the turbulence and scalar fields have been previously investigated for premixed and non-premixed flames [11, 12]. However, heat-release effects on the structure of the SGS stress tensor has not been explored much so far. In this study, the approach by Tao *et. al* [13], see also [14], is used to analyze the structure of the resolved strain-rate, $\tilde{S}_{ij}$ and SGS stress, τ_{ij} tensors under the influence of heat release. This study is followed by an analysis of the relative alignment of $\tilde{S}_{ij}$ and $-\tau_{ij}$ and the anisotropy of τ_{ij} , signifying the importance of anisotropy-resolving SGS modelling [15]. The role of the SGS stresses is reflected in the dynamics of the SGS dissipation of kinetic energy and enstrophy. The former explains how turbulent kinetic energy is exchanged between the resolved and subgrid-scales and the latter account for the enstrophy generation/dissipation by the subgrid-scales. Mean values, probability density functions (PDFs) and length scale of the SGS dissipation of kinetic energy and enstrophy are given and the heat-release effects are addressed. The role of the SGS enstrophy dissipation for non-reacting flows has been previously explored [see 16, 17] and here this analysis is extended to the case of reacting flows with heat release.

DNS data of a non-premixed turbulent wall-jet flame [18] is used in this study. The wall-jet flow is an interesting canonical flow problem, which once combined with the non-premixed flame, enables us to study the heat-release effects on the SGS quantities and their interactions with the wall effect. In our previous studies on reacting turbulent wall-jet flows, DNS has been employed with both isothermal and exothermic reactions [8, 19]. In Pouransari *et. al* (2014) [20], DNS of an isothermal reacting wall-jet flow was performed to study the dynamics of the flow and the embedded scalar fields and the Reynolds number effects on the statistics and structure of the flow. DNS of an exothermic reacting wall-jet flow was performed by Pouransari *et. al* (2014) [8] to analyze the heat-release effects on the different mixing scales of the flow, in particular on the vortex structures, turbulence scales and also the triple interactions of the wall, turbulence and reaction. The current study extends our previous investigations on the heat-release effects on different scales of the flow that are present in the turbulent wall-jet configuration. Recently, the heat-release effects on the small-scale anisotropy levels have been discussed [see 9], where the structure of the small scales of turbulence are represented by higher-order moments of the gradient fields. Here, we instead separate the turbulence scales, by performing a filtering operation on the DNS datasets of isothermal and exothermic reacting wall-jet flows and analyze the heat-release effects on the SGS stress statistics. A phenomenological analogy between the small-scale characteristics, observed via the statistical analysis of the flow, and those concerning the SGS statistics is expected.

The paper is organized as follows. The DNS database is explained in section 2. Details of the filtering and averaging operations are given in section 3. The governing equations of LES are explained in section 4. In section 5, the large-scale statistics are discussed. The statistics of the SGS stress tensor, SGS dissipation of kinetic energy and enstrophy are given and discussed in sections 6, 7 and 8, respectively. Conclusions are drawn in section 9.

2. Description of the DNS data of the turbulent reacting wall-jet flow

Governing equations of the total mass, momentum, energy and species concentrations for compressible flows, following the summation convention over the repeated

indices, read

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}, \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_j E}{\partial x_j} = -\frac{\partial q_j}{\partial x_j} + \frac{\partial u_i (\tau_{ij} - p \delta_{ij})}{\partial x_j} + \dot{\omega}_T, \quad (3)$$

$$\frac{\partial \rho \theta_i}{\partial t} + \frac{\partial \rho \theta_i u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial \theta_i}{\partial x_j} \right) + \dot{\omega}_i, \quad (4)$$

where ρ is the total mass density, u_i are the three velocity components, p is the pressure, E is the total energy and θ_i are the mass fractions. In the energy Equation (3), $\dot{\omega}_T$ is the heat-release term and $\dot{\omega}_i$ are the reaction rates of the fuel and oxidizer, in the species equation (4). The heat fluxes, q_i are approximated using the Fourier's law and $\tau_{ij} = 2\mu S_{ij} - \frac{2}{3}\mu \Delta_v \delta_{ij}$ is the viscous stress tensor, where δ_{ij} is the Kronecker delta, μ is the dynamic viscosity, S_{ij} is the strain-rate tensor

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (5)$$

and $\Delta_v = S_{kk}$ is the dilatation. The fluid is assumed to be calorically perfect and obey the ideal gas law with a specific heat ratio 1.4. The viscosity is obtained through the Sutherland's law and the diffusion coefficient, D is assumed to be equal for all the species. The reaction is simplified as a single-step irreversible reaction between an oxidizer O and fuel species F that react to form a product P , whose rate is expressed with an Arrhenius law

$$\dot{\omega}_f = -K_r \rho^2 \theta_o \theta_f \exp\left(-\frac{Ze}{T}\right), \quad (6)$$

written here for the fuel species, where K_r is the pre-exponential constant, Ze is the Zeldovich number and θ_o and θ_f are the oxidizer and fuel concentrations.

The numerical method employed for the DNSs uses a sixth-order compact finite-difference scheme for the spatial discretization and a third-order Runge-Kutta scheme for the temporal integration [see 21]. The computational domain is a rectangular box, see figure 1(a). The size of the computational domain, number of grid points and other simulation parameters are given in Table 1. At the wall, no-slip

Table 1. Summary of the DNSs. L_x , L_y and L_z are the dimensions in the streamwise, wall-normal and spanwise directions, respectively and h is the inlet jet height. N_x , N_y and N_z are the number of grid points in the x , y and z directions, respectively. Da is the Damköhler number, M is the Mach number, Sc is the Schmidt number and Pr is the Prandtl number.

Case	$L_x \times L_y \times L_z$	$N_x \times N_y \times N_z$	Da	Ze	Re	M	Sc	Pr
Isothermal [22]	$48h \times 23h \times 9.6h$	$480 \times 288 \times 192$	3	0	2000	0.5	0.7	0.7
Exothermic [22]	$48h \times 23h \times 9.6h$	$480 \times 288 \times 192$	1100	8	2000	0.5	0.7	0.7

and no-flux conditions for the velocity and scalars are applied. Periodic boundary conditions are used in the spanwise direction. The ambient flow above the jet has a constant co-flow velocity of $U_c = 0.1U_j$, where U_j is the jet inlet velocity. For the plane wall-jet with co-flow, the velocity half-height $y_{1/2}$ is defined as the distance from the wall to the position where the mean velocity is half of the maximum

Figure 1. Contour plots of the instantaneous (a) streamwise velocity in a x-y plane and the computational domain and (b) passive scalar concentration in a x-y plane.

excess value, i.e. $U(y_{1/2}) = \frac{1}{2}(U_m - U_c) + U_c$. The Reynolds number based on U_j and inlet jet height is $Re = U_j h / \nu = 2000$ and the Mach number is $M = 0.5$. At the top of the domain, an inflow velocity of $0.026U_j$ is used to account for the jet entrainment. The initial temperature of the jet stream, co-flow and wall are equal to $750K$. At the inlet, fuel and oxidizer enter the domain separately in a non-premixed manner. Fuel is injected through the jet, $\theta_{f,j} = 1$, while oxidizer is injected in the co-flow, $\theta_{o,c} = 0.5$. Two DNS data sets are analyzed. The first one has an isothermal reaction and the second one has an exothermic reaction with heat release, see Table 1. In both cases, the Prandtl and Schmidt numbers are constant and equal $Pr = Sc = 0.7$. The Damköhler number, $Da = K_r \rho_j h / U_j$ is equal to 3 in the isothermal case, while it is 1100 in the exothermic case.

Contour plots of the instantaneous velocity and passive scalar concentration for the isothermal case are given in Figures 1(a) and 1(b), showing the downstream development of the jet.

3. Averaging and filtering operations

Density-weighted (Favre) averaging for the statistical mean of a quantity ϕ is defined as

$$\underline{\phi} = \frac{\rho \phi}{\underline{\rho}}, \quad (7)$$

where $\underline{\phi}$ represents the Reynolds averaged ϕ . The Reynolds decomposition for the Favre averaging gives $\phi = \underline{\phi} + \phi''$, where ϕ'' is the fluctuation around the Favre-averaged value, $\underline{\phi}$.

The filtering operation in LES can be defined as [23]

$$\overline{\phi}(x, t) = \int_D G(x - x') \phi(x', t) dx', \quad (8)$$

where $\bar{\phi}(x, t)$ is the filtered quantity, $\phi(x, t)$ is the variable to be filtered, G is the kernel of the convolution and D is the domain of integration. We use the differential form of the filter [24, 25], obtained by a Taylor series expansion of the function $\phi(x, t)$ in powers of the filter size, $\bar{\Delta}$ as

$$\bar{\phi}(x, t) = \sum_{k=0}^{\infty} \frac{1}{k!} \mathcal{M}_k \frac{\partial^k}{\partial x^k} \phi(x, t), \quad (9)$$

where M_k are the moments of the filter kernel

$$\mathcal{M}_k = \int_D x^k G(x) dx. \quad (10)$$

The box filter is used in this study, which can be written in the differential form as [26]

$$\bar{\phi}(x, t) = \phi(x, t) + \frac{\bar{\Delta}^2}{24} \frac{\partial^2}{\partial x^2} \phi(x, t) + \frac{\bar{\Delta}^4}{1920} \frac{\partial^4}{\partial x^4} \phi(x, t). \quad (11)$$

The filtering is recursive and three-dimensional. An analogous Favre-filtering operation is used as

$$\tilde{\phi} = \frac{\bar{\rho\phi}}{\bar{\rho}}. \quad (12)$$

The SGS statistics are computed at a filter size $\bar{\Delta}$ four times the DNS grid size.

4. The filtered governing equations

The momentum equation for LES is obtained by filtering Equation (2), using the definition (8), as

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}. \quad (13)$$

The last term on the right-hand side is the divergence of the SGS stress tensor, τ_{ij} defined as

$$\tau_{ij} = \bar{\rho}(\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j), \quad (14)$$

which is not known and needs to be modeled to close the equations.

The governing equation for the large-scale kinetic energy $\mathcal{K} = \frac{1}{2}\bar{\rho}\tilde{u}_i\tilde{u}_i$ can be deduced from Equation (13) as [27]

$$\frac{\partial \bar{\rho}\mathcal{K}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\mathcal{K}) = \frac{\partial}{\partial x_i}(\bar{\tau}_{ij}\tilde{u}_j - \tau_{ij}\tilde{u}_j - \bar{p}\tilde{u}_i) + \bar{p}\tilde{\Delta}_v - \bar{\tau}_{ij}\tilde{S}_{ij} + \tau_{ij}\tilde{S}_{ij}, \quad (15)$$

where the Favre-filtered strain-rate tensor is given as

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \quad (16)$$

Figure 2. Downstream development of the friction Reynolds number, $Re_\tau = u_\tau y_{1/2} / \nu$ (a) and jet half height $y_{1/2}$ (b). Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

The first term on the right-hand side of Equation (15) is the diffusion term, which does not dissipate or produce energy in a volume-averaged sense. The second and third terms represent the pressure dilatation and viscous dissipation, respectively, where $\tilde{\Delta}_v = \tilde{S}_{ii}$ is the dilatation of the resolved velocity field. The last term is the negative of the SGS dissipation, $\Pi = -\tau_{ij} \tilde{S}_{ij}$ and its mean value is negative and dissipates the resolved kinetic energy.

Enstrophy is defined as half the square of the vorticity [28]. It is a useful quantity in the study of turbulent flows in propulsive devices and combustion applications. It describes how the fluid flow acts to dissipate energy in terms of kinetic energy. However, the physical meaning conveyed by the enstrophy equation can be argued to be more direct than the dissipation equation. The distribution of energy and enstrophy in wave number space are analogous to the mass and moment of inertia in the physical space, respectively and the wave number plays the role of the inverse of distance. In addition, the anisotropic behavior of enstrophy may be related to the local homogeneity of the vorticity field. The resolved vorticity, $\tilde{\omega}_i = \epsilon_{ijk} \frac{\partial}{\partial x_j} \tilde{u}_k$ is obtained by taking the curl of the filtered Navier–Stokes equations, Equation (13) as

$$\frac{\partial \tilde{\omega}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\omega}_i}{\partial x_j} = \tilde{\omega}_j \frac{\partial \tilde{u}_i}{\partial x_j} - \tilde{\omega}_i \tilde{\Delta}_v + \frac{\epsilon_{ijk}}{\bar{\rho}} \frac{\partial \bar{p}}{\partial x_j} \frac{\partial \bar{p}}{\partial x_k} + \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\bar{\rho}} \frac{\partial \bar{\tau}_{kl}}{\partial x_l} \right) - \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\bar{\rho}} \frac{\partial \bar{\tau}_{kl}}{\partial x_l} \right), \quad (17)$$

where ϵ_{ijk} is the permutation symbol. The resolved enstrophy, $\tilde{\mathcal{E}} = \frac{1}{2} \tilde{\omega}_i \tilde{\omega}_i$ transport equation is obtained as

$$\begin{aligned} \frac{\partial \tilde{\mathcal{E}}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\mathcal{E}}}{\partial x_j} &= \tilde{\omega}_i \tilde{\omega}_j \tilde{S}_{ij} - \tilde{\mathcal{E}} \tilde{\Delta}_v - \frac{\epsilon_{ijk}}{\bar{\rho}} \tilde{\omega}_i \frac{\partial \bar{p}}{\partial x_j} \frac{\partial \bar{p}}{\partial x_k} - \\ &\bar{\tau}_{ik} \left[\frac{\partial}{\partial x_k} \left(\frac{1}{\bar{\rho}} \frac{\partial \tilde{\Delta}_v}{\partial x_i} \right) - \nabla^2 \tilde{S}_{ik} \right] + \tau_{ik} \left[\frac{\partial}{\partial x_k} \left(\frac{1}{\bar{\rho}} \frac{\partial \tilde{\Delta}_v}{\partial x_i} \right) - \nabla^2 \tilde{S}_{ik} \right] + \frac{\partial Q_j}{\partial x_j}. \end{aligned} \quad (18)$$

The first, second, third, fourth and fifth terms on the right-hand side are the vortex stretching, vorticity expansion, baroclinic, viscous and SGS dissipation terms,

Figure 3. Favre-averaged streamwise velocity profiles in (a) outer scaling, where U_j is the inlet jet velocity, and (b) inner scaling at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case; --- : logarithmic law of the wall.

respectively. The last term is the enstrophy flux, Q_j defined as

$$Q_j = \left[-\tilde{\omega}_i \epsilon_{ijk} \frac{1}{\rho} \frac{\partial \tau_{kl}}{\partial x_l} + \epsilon_{ilk} \frac{1}{\rho} \tau_{kj} \frac{\partial \tilde{\omega}_i}{\partial x_l} \right] + \left[\tilde{\omega}_i \epsilon_{ijk} \frac{1}{\rho} \frac{\partial \bar{\tau}_{kl}}{\partial x_l} - \epsilon_{ilk} \frac{1}{\rho} \bar{\tau}_{kj} \frac{\partial \tilde{\omega}_i}{\partial x_l} \right], \quad (19)$$

where the terms in the first and second brackets are enstrophy SGS and viscous diffusion terms.

In the following sections, large-scale and SGS statistics are presented. Most of the statistics are given at $x/h = 33$, where the exothermic and isothermal cases have a comparable Re_τ , see figure 2 (a). However, most of the conclusions drawn are valid for $20 < x/h < 40$.

5. Large-scale statistics

5.1. Mean velocity, shear stress and turbulent kinetic energy

Figures 2(a) and (b) show the downstream development of the friction Reynolds number, $Re_\tau = u_\tau y_{1/2} / \nu = y_{1/2}^+$ and $y_{1/2}$ for the isothermal and exothermic cases, where the friction velocity is defined as $u_\tau = \sqrt{\tau_{wall} / \bar{\rho}_{wall}}$. Figure 2(a) demonstrates the delay in transition to turbulence due to the heat release [see 8] and Figure 2(b) shows that in the exothermic case $y_{1/2}$ development is slower.

Figure 4. Favre-averaged (a) shear stress and (b) turbulent kinetic energy in inner scaling at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

The mean velocity profiles are given in Figures 3(a) and 3(b) in inner and outer

Figure 5. Contour plots of the Reynolds averaged s_s^* for the region $20 < x/h < 40$ for (a) isothermal and (c) exothermic cases. (b) shows a comparison between the two cases at the downstream position $x/h = 30$. Line styles are as follows; —□— : isothermal case; —■— : exothermic case.

scalings. The flow is accelerated due to the heat release and the maximum excess velocity $U_m - U_c$ is increased about 40%, see Figure 3(a). The mean velocity profiles in inner units are also remarkably different. The slope of the logarithmic law that fits the profiles is steeper in the exothermic case than the isothermal one, see Figure 3(b), indicating a sharper velocity gradient in the logarithmic region for the exothermic case, although the log-region is here very limited due to the relatively low Reynolds number.

The Favre averaged shear stress $\underline{\rho u''v''}$ and turbulent kinetic energy $\underline{K} = 1/2 \underline{\rho u''u''}$ profiles are given in inner units in Figures 4(a) and 4(b), respectively. Due to the sharp velocity gradients in the inner layer, $y/h < 1$, a high turbulent kinetic energy production and shear stress exist in this region. The profiles of $\underline{\rho u''v''}$ and $\underline{K}$ have peaks in the inner layer, $y/h < 1$, which are not affected by the heat release. However, large differences are observed between the two cases in the jet area, located in the middle of the reaction zone, where the heat-release effects dominate. Both $\underline{\rho u''v''}$ and $\underline{K}$ decrease with the heat release in this region, which indicates a reduction in the turbulent kinetic energy production inside the flame [see also 8].

5.2. Structure of the resolved strain-rate tensor

Figure 6. Probability density functions of s_s^* at (a) $y^+ \approx 15$ and (b) $y = y_{1/2}$ at the downstream position $x/h = 33$. Line styles are as follows; —□— : isothermal case; —■— : exothermic case. PDFs are scaled to unit area.

In this section, the heat-release effects on the structure of the resolved strain-rate tensor $\tilde{S}_{ij}$ are examined. Following Lund and Rogers [29], the structure of the deviatoric part of the filtered strain-rate tensor $\tilde{S}_{ij}^d = \tilde{S}_{ij} - \tilde{\Delta}_v/3 \delta_{ij}$ is characterized

Figure 7. Reynolds averaged (a) SGS shear stress, τ_{xy}^+ and (b) SGS kinetic energy K_{SGS}^+ in wall units at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

using the dimensionless parameter s_s^* defined as

$$s_s^* = -\frac{3\sqrt{6}\alpha_s\beta_s\gamma_s}{(\alpha_s^2 + \beta_s^2 + \gamma_s^2)^{3/2}}, \quad (20)$$

where $\alpha_s > \beta_s > \gamma_s$ are the eigenvalues of $\tilde{S}_{ij}^d$ and follow the relation $\alpha_s + \beta_s + \gamma_s = 0$. Hence, α_s , β_s and γ_s correspond to the most extensive, intermediate and most contracting eigenvalues of $\tilde{S}_{ij}^d$, respectively. By its definition, s_s^* is bounded between -1.0 and 1.0. The lower bound indicates axisymmetric contraction and the upper bound indicates axisymmetric extension, which is also the most probable strain state in isotropic turbulence [29].

Contour plots of the Reynolds averaged s_s^* are given in Figure 5(a-c) for the isothermal and exothermic cases. Figures show substantial differences between the two cases. In the inner-layer, i.e. $y/h < 1$, s_s^* is positive in both isothermal and exothermic cases with smaller values in the exothermic case. It is worth mentioning that regions with positive s_s^* are more correlated with regions of high SGS dissipation [29]. While s_s^* is always positive in the isothermal case, negative values are observed in the exothermic case outside the flame area, i.e. $y/h > 5$. This clearly indicates that the heat-release effects, indeed, promote the contraction states due to the gas expansions. These effects are found to be more intense further downstream of the flow, see Figure 5(c). In other words, the fuel jet in the exothermic case burns and releases heat, which results in significant compression of the fluid, both near the outer edge of the jet and in the fluid confined between the wall and the jet, i.e. close to the inner half-height of the jet. Hence, lower SGS dissipation is expected in this region for the exothermic case, compared to the isothermal one, due to the negative s_s^* . These observations are also in agreement with those of the unfiltered fields, results not presented.

A more detailed analysis of s_s^* in the near-wall region is carried out to highlight the differences between the two cases by examining the PDFs, where interesting observations are made. The PDFs of s_s^* are given in Figures 6(a) and 6(b) for two wall distances, i.e. at $y^+ \approx 15$ in the buffer layer of the inner layer and at $y = y_{1/2}$. PDFs have remarkably different characteristics close to and further away from the wall. Close to the wall at $y^+ \approx 15$, PDFs are negatively skewed due to the wall effects. The most probable state for s_s^* is 0.22 for the isothermal case, while it is reduced to 0.17 in the exothermic one. The mean values at this point are $\overline{s_s^*} = 0.1$ and 0.02 for the isothermal and exothermic cases, respectively. The PDFs are both negatively skewed with a larger skewness factor (S) in the isothermal case with

Figure 8. Contour plots of the Reynolds averaged s_τ^* for the region $20 < x/h < 40$ for (a) isothermal and (c) exothermic cases. (b) shows a comparison between the two cases at the downstream position $x/h = 30$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

$S = -0.29$ compared to -0.21 for the exothermic case. Further away from the wall at $y = y_{1/2}$, turbulence shows a more isotropic character with more extension states and the most probable strain state has $s_s^* = 0.94$ in the isothermal case, while it is slightly less for the exothermic case with $s_s^* = 0.78$ and a smaller peak value, which confirms that more compression exists for the exothermic case. The PDFs are again negatively skewed with similar skewness factors in the isothermal and exothermic cases, although the latter has a slightly lower value than the former. The mean value, $\overline{s_s^*}$ is also reduced from 0.28 in the isothermal case to 0.24 in the exothermic case. In general, heat release lowers the mean and most probable values of s_s^* . It also reduces the skewness of the PDF of s_s^* towards a Gaussian distribution.

6. Statistics of the subgrid-scale stress tensor

6.1. Mean SGS shear stress and kinetic energy

The Reynolds averaged SGS shear stress, $\overline{\tau_{xy}}$ and SGS kinetic energy, $\overline{K_{SGS}} = 1/2 \overline{\tau_{ii}}$ are given in Figures 7(a) and 7(b) in wall units. The behavior of $\overline{\tau_{xy}}$ and $\overline{K_{SGS}}$ follow those of the total (resolved plus SGS) shear stress and kinetic energy, see Figure 4(a) and 4(b), which are similar to the observations in [8] for the unfiltered fields. Heat-release reduces both $\overline{\tau_{xy}}$ and $\overline{K_{SGS}}$ in the jet area, while they remain almost unchanged in the vicinity of the wall. The similarity in the trend of the heat-release effects on the total and SGS statistics indicates that large and small-scale turbulence mixing scales are affected in a comparable manner [see also 9]. However, the reduction in $\overline{K_{SGS}}$ in the exothermic case is more substantial than what is observed in the total statistics and the outer peak in $\overline{K_{SGS}}$ profile almost vanishes. According to Figures 7(b) and 4(b), in this *a priori* LES analysis, 10% of the turbulent kinetic energy is within the SGS. A level that is representative of a well-resolved LES, however this also confirms that the range of scales present in these DNS is sufficient to perform such *a priori* analysis.

6.2. Structure of the SGS stress tensor

Similar to the resolved strain-rate tensor, a parameter s_τ^* for the deviatoric part of the SGS stress tensor, i.e. $\tau_{ij}^d = \tau_{ij} - \tau_{kk}/3 \delta_{ij}$, can be defined as [13]

$$s_\tau^* = -\frac{3\sqrt{6}\alpha_\tau\beta_\tau\gamma_\tau}{(\alpha_\tau^2 + \beta_\tau^2 + \gamma_\tau^2)^{3/2}}. \quad (21)$$

Figure 9. Probability density functions of s_τ^* at (a) $y^+ \approx 15$ and (b) $y/h = 7$ at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case. PDFs are scaled to unit area.

Similar to s_s^* , s_τ^* also varies between -1 and +1. Contour plots and a line plot of the Reynolds averaged s_τ^* , at $x/h = 30$, are given in Figures 8(a)-(c). Contrary to s_s^* , s_τ^* is always negative. Hence, the preferred state for the SGS stress is the contraction state. At $x/h = 30$, close to the wall, $\underline{s}_\tau^*$ is close to -1, implying an axisymmetric contraction state. In the jet area, $\underline{s}_\tau^*$ is increased to almost -0.5 in both isothermal and exothermic cases, indicating a decrease in the abundance of the contraction state and a different character for the SGS stress tensor, compared to the other parts of the flow. The behavior of $\underline{s}_\tau^*$ in the isothermal and exothermic cases is similar up to $y/h = 4$, with minor differences. Major differences exist in the outer edge of the wall-jet flow, i.e. $5 < y/h < 6$, see Figure 8(b). This region has similarities with the outer edge of boundary layer flow with strong inhomogeneity and intermittency at its turbulent non-turbulent interface. The small scales of the turbulent flow are more anisotropic in this region for the exothermic case [see 9], which can be parallelized with lower s_τ^* values observed in Figure 8(b). The contour plots also confirm the same behavior as what was discussed for the position $x/h = 30$.

Figures 9(a) and 9(b) show the PDFs of s_τ^* at $y^+ \approx 15$ and $y/h = 7$. Figures indicate a similar behavior for s_τ^* in the isothermal and exothermic cases close to the wall, at $y^+ \approx 15$, with some differences in the tails of the PDFs. Further away from the wall at $y/h = 7$, substantial differences are observed between the two cases. The PDF for the isothermal case has a broader tail than the exothermic one. This indicates that the preferred state for the SGS stresses is a compression state, while for the isothermal case there are more expansion events.

6.3. Anisotropy of the SGS stress tensor

To further characterize the heat-release effects on the SGS stress tensor, its anisotropy invariant maps [30, 31] are presented in Figure 10(a) by cross-plotting the second II and third III invariants of the SGS stress anisotropy tensor, a_{ij} defined as

$$a_{ij} = \frac{\tau_{ij}}{\tau_{kk}} - \frac{1}{3}\delta_{ij}, \quad \text{II} = a_{ij}a_{ij}, \quad \text{III} = a_{ik}a_{kj}a_{ji}. \quad (22)$$

The limits in the anisotropy invariant map correspond to the two-component turbulence state, when $\text{II} = 2/9 + 2\text{III}$ and axisymmetric turbulence state, when $\text{II} = 3/2(4/3|\text{III}|)^{2/3}$. These limits define a triangle in the anisotropy invariant map, within which all the physically realizable turbulence states lie. In the anisotropy

Figure 10. (a) Anisotropy invariant map of the Reynolds averaged SGS stress anisotropy tensor a_{ij} and (b) Lumley flatness factor, at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$ (in a) and $\blacksquare$ (in b) : exothermic case. Circle marks indicate values at the wall and cross signs show the corresponding values at $y^+ = 30$.

invariant map, isotropic turbulence with zero anisotropy corresponds to the lower corner of the triangle. Axisymmetric turbulence corresponds to the left and right edges of the triangle. At the left edge, one component of SGS velocity fluctuations is smaller than the other two, while at the right edge, one component of velocity fluctuations dominates the other two. The latter is denoted by axisymmetric expansion and the former by axisymmetric contraction. The upper edge of the triangle corresponds to the two-component turbulence as in turbulence near solid walls.

The anisotropy invariant maps are given in Figure 10(a). The SGS anisotropy level increases due to the heat-release effects in the entire wall-normal direction. Close to the wall, the SGS dynamics have a two-dimensional turbulence character, due to the wall blocking effect, which damps the wall-normal velocity fluctuations in the near-wall region. At the vicinity of the wall, the isothermal case has a smaller anisotropy than the exothermic one with an anisotropy state closer to the left edge of the triangle, corresponding to the axisymmetric contraction state. This implies that the wall-normal and spanwise components of the SGS stress tensor are damped in the exothermic case. The trajectory of the exothermic case follows the two-component limit and its anisotropy magnitude rapidly grows, while the isothermal case has a lower anisotropy. Around $y^+ = 7$, a maximum occurs in the profiles of the two cases and the peak for the exothermic case has a substantially higher value than the isothermal one. This behavior is similar to what was observed for the total anisotropy map characteristics [see 8], but it is more accentuated for the SGS anisotropies. Further away at $y^+ = 30$, the trajectories move towards the lower part of the right edge. While the isothermal case gets very close to the lower corner of the triangle, the exothermic case lies somewhere on the right edge. This is consistent with the fact that the lower corner of the anisotropy invariant map represents an isotropic turbulence energy distribution and indeed, the flow exhibits more isotropic characteristics in the isothermal case. Hence, the SGS anisotropy is, in general, larger in the exothermic case than the isothermal one, confirming the behavior observed for the SGS stress tensor in Figure 8(b).

To further study the SGS stress characteristics, the Lumley flatness factor $\tilde{F} = 1 + 9II + 27III$ is used, see Figure 10(b). It is limited between zero and one, where small values indicate a flow with quasi-two-dimensional turbulence and values close to one indicate turbulence with an isotropic three-component behavior. Inside the boundary layer, $\tilde{F}$ is small in both cases. Compared to the isothermal case, the exothermic case has smaller $\tilde{F}$ values, hence a higher anisotropy level. Further away from the wall, $\tilde{F}$ is close to unity in the isothermal case, indicating an isotropic state, while it is lower in the exothermic case with an anisotropic state. Close

Figure 11. Probability density functions of the cosine of the angle between $\alpha_{-\tau}$ and α_s at (a) $y^+ \approx 15$ and (b) $y = y_{1/2}$ at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case. PDFs are scaled to unit area.

to $y/y_{1/2} = 1.5$, the exothermic case prediction of $\check{F}$ attains a local minimum, indicating an increase in the local anisotropy due to the heat release, which is not observed in the isothermal one.

6.4. Relative alignment of the SGS stress and strain-rate tensors

Understanding the heat-release effects on the relative alignment of the SGS stress and resolved strain-rate tensors plays an important role in understanding the SGS physics, which is important in the development of SGS models [13, 15, 32]. Similar to Tao *et. al* [13], we examine the angle between the eigenvectors of the negative of the SGS stress and resolved strain-rate tensors, corresponding to their largest eigenvalue, i.e. α_s and $\alpha_{-\tau}$, in the near-wall region of the reacting turbulent wall-jet flow. The PDFs of the cosine of the angle between α_s and $\alpha_{-\tau}$, i.e. $\cos[\angle(\alpha_s, \alpha_{-\tau})]$, are given in Figures 11(a) and 11(b). In the buffer layer at $y^+ \approx 15$, where the turbulence kinetic energy production and SGS dissipation are maximum, the most probable value is $\angle(\alpha_s, \alpha_{-\tau}) \approx 43$ degrees. The peak in the PDFs is larger in the exothermic case than the isothermal one. The PDFs also have a smaller second peak with $\angle(\alpha_s, \alpha_{-\tau}) \approx 140$, which is slightly higher for the exothermic case. At $y/y_{1/2} = 1$, $\angle(\alpha_s, \alpha_{-\tau})$ is closer to 0 degrees in the isothermal case, while it is close to 49 for the exothermic case. This implies that the heat release reduces the relative alignment between $-\tau_{ij}$ and $\tilde{S}_{ij}$. This reduction could be attributed to the decrease of the local Reynolds number by the heat-release effects, which needs to be further explored using a different range of Reynolds numbers. It should also be pointed out that the increasing heat release and decreasing Reynolds number effects are not always in the same direction [see 20]. Moreover, it should also be mentioned that the results are not consistent with the eddy-viscosity concept, where a complete alignment between $-\tau_{ij}$ and $\tilde{S}_{ij}$ is assumed. This motivates the use of other SGS models that give a more realistic geometrical description of the SGS stress tensor [see e.g. 15].

7. Subgrid-scale dissipation of kinetic energy

The main role of a SGS model is to remove energy from the resolved scales [33]. This role can be best understood by observing the governing equation of the resolved kinetic energy $\mathcal{K}$ in Equation (15), where the SGS energy dissipation is defined as $\Pi = -\tau_{ij}\tilde{S}_{ij}$. The Reynolds averaged Π is given in Figure 12 (a)–(c) in wall units. The contour plots in Figures 12 (b) and (c) show the spatial development of the

Figure 12. Reynolds averaged subgrid-scale dissipation Π in inner units, at the downstream position $x/h = 33$ (a) and its contour plots for $20 < x/h < 40$ for the isothermal (b) and exothermic (c) cases. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

Figure 13. Probability density functions of the SGS dissipation in wall units at (a) $y^+ \approx 15$ and (b) $y = y_{1/2}$ at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case. PDFs are scaled to unit area.

SGS dissipation. The SGS dissipation has a peak in the buffer layer at $y^+ \approx 15$, where the kinetic energy production is maximum. The SGS dissipation is larger in the exothermic case than the isothermal one. The SGS dissipation has a second peak in the jet area, indicating the balance between the mean production and dissipation of turbulent kinetic energy. This peak is larger in the isothermal case than the exothermic one, which is consistent with the reduced alignment between $-\tau_{ij}$ and $\tilde{S}_{ij}$ in the exothermic case, observed earlier.

More detailed information about the dynamics of Π is given by its PDFs in Figure 13(a) and 13(b). The PDFs confirm the existence of backscatter of energy, i.e. $\Pi < 0$ events. It is also observed that the PDFs are positively skewed and Π is always positive. At $y^+ \approx 15$, the PDF of Π has a broader tail in the exothermic case than the isothermal one, indicating a more intermittent Π in the exothermic case. The peak of Π occurs towards smaller values in the exothermic case. On the contrary, further away from the wall at $y/y_{1/2} = 1$, Π has a wider PDF in the isothermal case, compared to the exothermic one. Hence, it has a more intermittent character in the isothermal case.

Length scale of the SGS dissipation, $L_x[\Pi]$ is a measure of its intermittency and is computed from the spatial two-point correlation of its fluctuating part as [34]

$$L_x[\Pi] = \int_0^{l_x} \frac{\overline{\Pi'(x, y, z, t) \Pi'(x + r, y, z, t)}}{\overline{\Pi'^2(x, y, z, t)}} dr, \quad (23)$$

where Π' is the fluctuating part of Π and l_x is the length at which the two-point correlation of Π' becomes reasonably close to zero. The SGS dissipation length scales computed with Equation (23) are shown in Figure 14, where they have been normalized by the grid-filter scale, i.e. $\overline{\Delta} = \sqrt[3]{\overline{\Delta_x \Delta_y \Delta_z}}$. $L_x[\Pi]$ is three times

Figure 14. Length scale of the SGS dissipation $L_x[\Pi]$, scaled with the grid-scale $\overline{\Delta} = \sqrt[3]{\overline{\Delta_x \Delta_y \Delta_z}}$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

Figure 15. Reynolds averaged SGS enstrophy dissipation χ in wall units, at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

larger than $\overline{\Delta}$ in the near-wall viscous region and is the same in both exothermic and isothermal cases. There is an increase in the length scale in the buffer layer, where $L_x[\Pi]$ is indeed larger in the exothermic case than the isothermal one. This increase indicates a decrease in the intermittency of Π , due to the heat release and the corresponding decrease in the local Reynolds number. Moreover, it indicates an increase in the size of the small scales [also pointed out in 8], which is a sign for an increased anisotropy, also mentioned earlier in the analysis of the SGS stress anisotropy. Further away from the wall, the length scale decreases in terms of $\overline{\Delta}$. It approaches $\overline{\Delta}$ in the isothermal case, as also observed in incompressible turbulent channel flow simulations [see 34], while it reaches $2\overline{\Delta}$ in the exothermic case. Many parallels can be observed here between the characteristics of the small-scale and SGS anisotropy, but a direct analogy cannot be made between the behavior of $L_x[\Pi]$ and odd higher-order moments of the velocity gradients representing the intermittency of the small-scales of turbulence [see 9].

8. Subgrid-scale dissipation of enstrophy

The dynamics of enstrophy is closely related to that of vorticity and the SGS stresses have a prominent role in it. The effects of the subgrid-scales on the resolved enstrophy generation and dissipation are best understood by looking at its

Figure 16. Probability density functions of the SGS enstrophy dissipation in wall units at (a) $y^+ \approx 15$ and (b) $y = y_{1/2}$ at the downstream position $x/h = 33$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case. PDFs are scaled to unit area.

transport equation (18), where the SGS dissipation of enstrophy is defined as

$$\chi = -\tau_{ij} \left[\frac{\partial}{\partial x_j} \left(\frac{1}{\bar{\rho}} \frac{\partial \tilde{\Delta}_v}{\partial x_i} \right) - \nabla^2 \tilde{S}_{ij} \right]. \quad (24)$$

In this definition, the first-term on the right-hand side is due to the compressibility effects and involves the flow dilation. In the incompressible limit, this term vanishes and the remaining term is similar to the incompressible formulation given in [35]. The Reynolds-averaged SGS dissipation of enstrophy, $\underline{\chi}$ is given in Figure 15 for the two cases in the near-wall region, i.e. $y^+ < 30$, where the differences are more obvious.

The mean SGS dissipation has a peak in the near-wall region, at $y^+ = 5$ in the isothermal and exothermic cases. The amplitude for the exothermic case is smaller than the isothermal one. This is due to the fact that the resolved enstrophy is reduced in the exothermic case and the predictions of vorticity and dynamics of streaks are also modified by the heat release [8]. The SGS dissipation of enstrophy attains a minimum at $y^+ \approx 12$. In the isothermal case, $\underline{\chi}$ approaches zero, while in the exothermic case, negative values of SGS dissipation are observed, which are due to the dilatation of the flow.

To give more information, PDFs of χ are given in Figure 16. Close to the wall at $y^+ \approx 15$, the PDFs are skewed due to the wall effects. The PDF of the exothermic case has thinner tails, indicating smaller intermittency levels compared to the isothermal case. Further away from the wall, at $y/y_{1/2} = 1$, the same trend is also observed and is even more intense, which signifies a substantial decrease in the enstrophy and its intermittency due to the heat-release and a decrease in the local Reynolds number.

To further analyze the heat-release influence on the SGS enstrophy dissipation, its length scale, $L_x[\chi]$ is computed, see Figure 17. Compared to the grid filter size, $L_x[\chi]$ is larger in the near-wall region. The exothermic and isothermal cases give comparable results in this region, but in the buffer layer $L_x[\chi]$ is larger in the exothermic case. Further away from the wall, $L_x[\chi]$ approaches $\bar{\Delta}$ in the isothermal case, while it approaches a higher value in the exothermic case. The differences between the two cases indicate an overall increase in the length scale of the SGS dissipation of enstrophy due to the heat release, hence, a subsequent increase in the anisotropy and a decrease in the intermittency of the fluctuations.

Figure 17. Length scale of the SGS dissipation of enstrophy, $L_x[\chi]$ scaled with the grid-scale $\bar{\Delta} = \sqrt[3]{\bar{\Delta}_x \bar{\Delta}_y \bar{\Delta}_z}$. Line styles are as follows; $\square$: isothermal case; $\blacksquare$: exothermic case.

9. Concluding remarks

An analysis of the subgrid-scale (SGS) stress tensor has been carried out, to study the heat-release effects, using direct numerical simulation (DNS) data of a turbulent reacting wall-jet flow. Two sets of DNSs are employed, one includes an isothermal reaction and the other an exothermic one with heat release. The study includes an analysis of the heat-release effects on the structure and relative alignment of the resolved strain-rate and SGS stress tensors. A box filter is used to obtain the SGS quantities. However, a Gaussian filter is also implemented, which gave similar results. Hence, only the results for the box filter are presented. Analysis of the eigenvectors of the resolved strain-rate tensor shows that extension is the dominant state in the isothermal case, while compression state is more dominant in the jet area of the flow in the exothermic case. Contrary to the resolved strain-rate tensor, compression state is dominant for the SGS stress tensor and the heat release has a promotive role. The heat release also has a considerable influence on the relative alignment of the SGS stress and resolved strain tensors. Analysis of the PDFs of the cosine of the angle between the eigenvectors, corresponding to the largest eigenvalue of the two tensors, shows that the alignment is increased in the buffer layer, while it is decreased away from the wall. The degree and variation of the non-alignment between the SGS stress and the resolved strain-rate tensors represents an important indication of the need for SGS stress models that are more advanced than the eddy-viscosity-based ones [36, 37]. Analysis of the SGS stress anisotropy shows that the heat release increases the SGS anisotropy everywhere in the flow.

The SGS dissipation of kinetic energy is evaluated by analyzing its mean, PDF and length scale. The mean SGS dissipation was found to increase in the near-wall region and decrease in the jet area. The PDFs show an increased intermittency in the SGS dissipation in the buffer layer in the exothermic case, while the opposite occurs further away from the wall. Further analysis of the SGS dissipation shows that its length scale is substantially affected, especially in the jet area where the heat-release effects are observed, leading to much larger length scales in the exothermic case.

Finally, the SGS dissipation of enstrophy is studied, where the heat-release effects are found to decrease the mean SGS enstrophy dissipation and its intermittency in the near-wall region.

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