This study addresses the dynamics of backscatter of kinetic energy in the context of large-eddy simulations (LES) of high-speed turbulent reacting flows. A priori analyses of direct numerical simulations (DNS) of reacting and inert supersonic, time-developing, hydrogen–air turbulent mixing layers with complex chemistry and multicomponent diffusion are conducted here in order to examine the effects of compressibility and combustion on subgrid-scale (SGS) backscatter of kinetic energy. The main characteristics of the aerothermochemical field in the mixing layer are outlined. A selfsimilar period is identified in which some of the turbulent quantities grow in a quasi-linear manner. A differential filter is applied to the DNS flow field to extract filtered quantities of relevance for the large-scale kinetic-energy budget. Spatiotemporal analyses of the flow-field statistics in the selfsimilar regime are performed, which reveal the presence of considerable amounts of SGS backscatter. The dilatation field becomes spatially intermittent as a result of the high-speed compressibility effect. In addition, the large-scale pressure-dilatation work is observed to be an essential mechanism for the local conversion of thermal and kinetic energies. A joint probability density function (PDF) of SGS dissipation and large-scale pressure-dilatation work is provided, which shows that backscatter occurs primarily in regions undergoing volumetric expansion; this implies the existence of an underlying physical mechanism that enhances the reverse energy cascade. Furthermore, effects of SGS backscatter on the Boussinesq eddy viscosity are studied, and a regime diagram demonstrating the relationship between the different energy-conversion modes and the sign of the eddy viscosity is provided along with a detailed budget of the volume fraction in each mode. A joint PDF of SGS dissipation and SGS dynamic-pressure dilatation work is calculated, which shows that high-speed compressibility effects lead to a decorrelation between SGS backscatter and negative eddy viscosities, which increases for increasingly large values of the SGS Mach number and filter width. Finally, it is found that the combustion dynamics have a marginal impact on the backscatter and flow-dilatation distributions, which are mainly dominated by the high-Mach-number effects.

Key words: high-speed flows, shear layers, turbulent reacting flows

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1. Introduction

Richardson’s energy-cascade hypothesis (Richardson 1922) predicts that turbulent kinetic energy is generated at the largest scales in a flow and then transferred to progressively smaller and smaller scales until it is dissipated by molecular viscosity. While this energy cascade typically holds in a statistically-averaged sense, it does not always describe the local behaviour of a turbulent flow. The turbulent dissipation associated with the smallest, viscous scales, is actually the difference between two energy fluxes, namely, the ‘forwardscatter’, corresponding to the classical energy cascade, and the ‘backscatter’, a reversal of this process in which energy is transferred from the small scales back to the large scales (Lesieur & Métai 1996).

The backscatter of energy can be understood by analysing energy fluxes in wavenumber space or in physical space, although there may not be a simple relation between them (Domaradzki & Saiki 1997). In spectral space, backscatter arises as a negative rate of energy change of an individual wavenumber mode, and it is associated with triadic interactions between large and small scales in a flow (Brasseur & Wei 1994). However, spectral analyses and their formulations become exceedingly complex when additional physics such as compressibility or combustion are considered. In physical space, local backscatter of kinetic energy is often observed as negative values of the subgrid-scale (SGS) dissipation upon filtering velocity fields obtained from direct numerical simulations (DNS) (Piomelli et al. 1991; Domaradzki, Liu & Brachet 1993; Härtel et al. 1994; Kerr, Domaradzki & Barbier 1994; Domaradzki & Saiki 1997) or from experiments (Liu, Meneveau & Katz 1994; Tao, Katz & Meneveau 2002). In physical-space analyses of energy fluxes, the negative value of the SGS dissipation is interpreted as the reverse flux of energy from small to large scales that is required to preserve the resolved turbulent motion once the small eddies have been filtered out.

If the SGS turbulent-momentum transfer in large-eddy simulations (LES) is represented using the Boussinesq eddy-viscosity hypothesis, the eddy-viscosity coefficient carries information of the net dissipation dynamics. By construction, in low-speed flows the Boussinesq eddy viscosity becomes negative in regions where backscatter occurs. In fact, the presence of local backscatter in the flow is representative of a poor correlation between SGS stress and filtered strain-rate tensors (Moser & Jiménez 2000). The consequences of the occurrence of SGS backscatter in numerical simulations are well known, particularly in LES of low-Mach-number flows. Specifically, the SGS backscatter acts as a source term in the kinetic-energy equation; if it persists, kinetic energy will tend to accumulate in the supergrid by means of a reverse turbulent-diffusion process, causing computations to become numerically unstable (Lund, Ghosal & Moin 1993). Despite the numerical difficulties that backscatter may pose, it is a commonly observed phenomenon in DNS and experiments. In fact, in incompressible turbulent channel flows, as much as 40% of the flow volume may be undergoing backscatter in physical space at any given time; yet in the mean, the classical direct energy cascade is observed (Piomelli et al. 1991).

Purely dissipative SGS models based on the Boussinesq eddy-viscosity hypothesis, such as the widely used models of Smagorinsky (1963) or Vreman (2004), do not account for backscatter. The dynamic Smagorinsky models developed by Germano et al. (1991) and Moin et al. (1991) for incompressible and compressible turbulent flows, respectively, in principle allow for backscatter by calculating the Smagorinsky constant in a dynamic procedure as a function of space and time. To compensate for large variations of the dynamic constant that may lead to numerical instabilities, in the original dynamic procedure the numerator and denominator of the expression...
for the dynamic constant were averaged over homogeneous directions (Germano et al. 1991). This averaging results in some loss of information of the sign and magnitude of the local SGS dissipation, and, in practice, generally suppresses backscatter. An extension of the dynamic procedure was proposed by Ghosal et al. (1995), where the dynamic constant was calculated in a more mathematically rigorous manner, resulting in a dynamic localization model that calculates local backscatter in amounts which are limited by a SGS kinetic-energy transport equation.

Backscatter has also been accounted for in SGS models by using stochastic forcing (Leith 1990; Mason & Thomson 1992; Carati, Ghosal & Moin 1995). However, it could be argued that backscatter is not a purely random quantity, in that it is generated by physical processes described by conservation laws. In fact, as shown in this study, backscatter is, in some situations, strongly correlated to observable physical phenomena such as volumetric expansion. The fact that backscatter is ubiquitously observed in a priori studies of DNS calls into question whether the unresolved turbulent transport computed from LES is dynamically correct if it is calculated by a SGS model incapable of predicting local backscatter. Therefore, studies of the physical mechanisms leading to the production of backscatter in turbulent flows are warranted to foster the development of improved SGS closures that incorporate the physics while preserving numerical stability. An extensive description of relevant SGS models and their capabilities with regard to predicting backscatter is given by Menevau & Katz (2000).

Compressibility and combustion phenomena often occur simultaneously in turbulent flows for engineering applications in hypervelocity propulsion such as supersonic combustion ramjets (Curran, Heiser & Pratt 1996). These effects complicate the dynamics of turbulence and may lead to generation or destruction of turbulent kinetic energy. For instance, in supersonic flows, shock waves can amplify vorticity and turbulent kinetic energy, or decrease them depending on the shock inflow characteristics (Lele 1994). In addition, the presence of eddy shocklets in compressible turbulent flows considerably steepens the dilatation field at the microscale and tend to dissipate turbulent kinetic energy (Lee, Lele & Moin 1990). In these flows, compressibility effects lead to significant amounts of flow dilatation, which plays an important role in the transfer of kinetic energy (Samtaney, Pullin & Kosović 2001; Aluie, Li & Li 2012; Shi et al. 2013).

In turbulent reacting flows, thermal energy is deposited at the smallest scales. In these scales, molecular diffusion dominates and fuel and oxidizer burn in flames releasing chemical heat. In fact, combustion represents an additional source of flow dilatation driven by thermal expansion or variable-density effects. Instabilities intrinsic to the propagation of flames can lead to self-turbulization of the reacting front and of the surrounding gas (Williams 1985). Similarly, other investigations have highlighted the importance of the pressure-dilatation flux induced by combustion as a source of turbulent kinetic energy in reacting flows (Luo 1999; Jaberi, Livescu & Madnia 2002). Nonetheless, the increase of the kinematic viscosity with temperature tends to damp turbulence in combusting flows at moderate Reynolds numbers (Takagi, Shin & Ishio 1980). These considerations suggest the existence of a complex interplay between backscatter of energy, flow dilatation and chemical–heat conversion in turbulent reacting flows.

The present study extends the understanding of backscatter phenomena to both compressible and reacting flows by performing an a priori study of DNS results of a time-developing supersonic turbulent mixing layer. Mixing layers are pivotal for the understanding of turbulent non-premixed combustion (Peters 2000). The
Diffusion flame
Fuel stream
Air stream
x3L2
L1
L3
x2
x1

**Figure 1.** (Colour online) Sketch of the computational set-up: a turbulent mixing layer develops between two supersonic streams of air and hydrogen diluted with nitrogen. For the reacting cases, the mixing of fuel and air leads to combustion chemical reactions and diffusion flames (shown in red online) in the mixing layer. The symbols are defined in the main text.

The computational setup involves two supersonic free streams of air and fuel flowing in opposite directions at the same velocity $U$, as depicted in figure 1. The fuel stream is composed of 6.7% of gaseous hydrogen ($H_2$) by mass, balanced with gaseous nitrogen ($N_2$). The temperature of the air stream, $T_A = 1500$ K, is above the crossover temperature (for ignition of $H_2$) at the initial static pressure $p_\infty = 2$ bar, and the temperature of the fuel stream is close to ambient conditions, $T_F = 500$ K. During its development, the mixing layer grows, and at sufficiently high Reynolds numbers, transitions to a turbulent state, in which large eddies engulf fresh gases and break down into smaller eddies. An approximate equilibrium state is reached farther in time, in which the effect of the initial conditions is partially lost and the first- and second-order statistics of turbulence become selfsimilar with respect to the transverse spatial coordinate rescaled with the instantaneous mixing-layer thickness. The calculations shown here consider reacting and non-reacting mixing layers. In the reacting case, the macroscopic entrainment of oxygen and hydrogen in the mixing layer leads to diffusive combustion once the large eddies have broken down into small-size eddies, in which molecular diffusion becomes important. The numerical results used in this study extend earlier works on DNS of turbulent temporal mixing layers of inert (Rogers & Moser 1994; Vreman, Sandham & Luo 1996; Pantano & Sarkar 2002) and reacting (Miller, Madnia & Givi 1994; Luo 1999; Pantano, Sarkar & Williams 2003; Mahle et al. 2007; Knaus & Pantano 2009) mixtures, to complex chemistry, multicomponent diffusion and higher convective Mach numbers.

The remainder of this paper is organized as follows. The formulation and computational details are outlined in § 2. The main simulation results are described in § 3. An analysis of the SGS backscatter dynamics is carried out in § 4, including effects on the eddy viscosity. Finally, conclusions are drawn in § 5.
2. Formulation

For obtaining the DNS results analysed in this study, the Navier Stokes and species conservation equations

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \quad \frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j},
\]

were integrated numerically together with the equation of state \( p = \rho R_0 T / W \). In this formulation, \( u_i \) are the velocity components, \( \rho \) is the static pressure, \( T \) is the static temperature, \( \rho \) is the density, \( R_0 \) is the universal gas constant, \( W \) is the total energy (including thermal, kinetic and chemical energy) and \( N \) is the number of species. Similarly, \( \tau_{ij} = 2\mu(S_{ij} - \Delta_v \delta_{ij}/3) \) is the viscous stress tensor, with \( \mu \) the molecular viscosity of the mixture, \( S_{ij} = (1/2)(\partial u_i/\partial x_j + \partial u_j/\partial x_i) \) is the strain-rate tensor, and \( \Delta_v = S_{ii}/3 \) is the flow dilatation. The variables \( Y_k \) and \( \dot{\omega}_k \) denote the mass fraction and rate of production of species \( k \), respectively. The diffusion velocities \( V_{i,k} \) are calculated using the Curtiss–Hirschfelder approximation (Hirschfelder, Curtiss & Bird 1954). The heat flux \( q_i \) is computed from the expression

\[
q_i = -\lambda \partial T / \partial x_i + \sum_{k=1}^{N} \rho h_k Y_{i,k},
\]

where \( \lambda \) is the thermal conductivity and \( h_k \) the sensible enthalpy of species \( k \). In these calculations, the Dufour effect and the thermodiffusion and barodiffusion mechanisms of heat and mass transport are neglected. The dynamic viscosity \( \mu \) of the mixture depends on temperature and is obtained from Wilke’s mixing rule based on the individual viscosities of the species, which are calculated from collision parameters (Hirschfelder et al. 1954). The specific heat capacities are computed from NASA polynomials (McBride, Gordon & Reno 2005). Lastly, the mass diffusivities are calculated by imposing constant Lewis numbers, whose values are given in §2.3.

The \( \mathrm{H_2}/\mathrm{O_2} \) mechanism by Hong, Davidson & Hanson (2010), which consists of 20 steps and \( N = 9 \) species (i.e. \( \mathrm{H_2}, \mathrm{O_2}, \mathrm{H_2O}, \mathrm{OH}, \mathrm{HO_2}, \mathrm{H_2O_2}, \mathrm{O}, \mathrm{H} \) and \( \mathrm{N_2} \)) is used to describe the reaction chemistry. In the inert case, the chemistry is inhibited by turning off all chemical sources in the species conservation equations (2.3).

The bulk-viscosity coefficient, which accounts for the relaxation time needed to equilibrate translational and internal energies in the gas volume, is neglected in this study. However, under some conditions this coefficient can be, at least, of the same order of magnitude as the molecular viscosity (Cramer 2013), and its effects may become important in dilatational flows (Fru, Janiga & Thévenin 2012). In this work, these effects may be hindered since the fuel stream is highly diluted, and hydrogen is the species that exhibits the largest bulk-viscosity coefficient in the mixture. Further investigations of these additional non-equilibrium phenomena are warranted, including the assessment of uncertainties in the reported bulk-viscosity coefficients.

2.1. Averaging and filtering operators

The Reynolds-averaged Navier–Stokes (RANS) mean of any variable \( f \) is defined here as \( \bar{f} = \int_{-\infty}^{+\infty} f \, dx_1 \, dx_3 / (L_1 L_3) \), and its perturbation from the mean is denoted by \( f' \). The
density-weighted (Favre) average of $f$ is obtained by computing $\tilde{f} = \rho f / \rho$, and $f''$ is the corresponding perturbation. In this way, $\tilde{f}$ and $f''$ represent averages over large scales in the homogeneous directions $x_1$ and $x_3$.

In this study, the DNS database is filtered to obtain quantities of relevance for LES. The filtered value of $f$ is given by $\tilde{f} = \int_{-\infty}^{+\infty} f(\alpha') G(\mathbf{x}, \mathbf{x}'; \Delta) \, d\alpha'$, where $\mathbf{x} = (x_1, x_2, x_3)$ is the position vector, $G$ is the kernel of the LES filter and $\Delta$ is a characteristic filter size. An analogous Favre-filtered version of $f$ can be defined as $\tilde{f} = \rho \tilde{f} / \rho$.

The three-dimensional differential filter of Germano (1986), which exhibits a second-order commutation error, is used in this study (see also Bose (2012)). The filter kernel of Germano (1986), $G = \exp(-r/b)/(4\pi rb^2)$, with $r = |\mathbf{x} - \mathbf{x}'|$, corresponds to the Green’s function of the partial differential equation $f = \tilde{f} - b^2 \nabla^2 \tilde{f}$, in which $b$ is a free parameter that can be related to an effective cutoff scale $\Delta$ by, for instance, equating the second moment of the filter kernel to the second moment of a spherical top-hat filter with diameter $\Delta$, as suggested by Marsden, Vasilyev & Moin (2002). This procedure yields the characteristic filter width $\Delta = b\sqrt{\Omega}$. In this study, the filter width $\Delta$ is chosen to be constant and uniform along the three spatial directions. Furthermore, in order to preserve the total momentum, the parameter $b$ is chosen to drop linearly to zero within 2.5% from the edges of the computational domain. The transfer function of the differential filter, $\tilde{f}/f = 1/(1 + b^2|\kappa|^2)$, with $\kappa$ the wave number vector, decays in wavenumber space in a continuous manner. In this analysis the dependence of the results on the filter width is examined in detail.

Lastly, the planar average of $f$ over the $\{x_1, x_3\}$ plane is denoted as $\langle f \rangle$, which coincides with the RANS average $f$ defined above, but it is kept here as a separate operator for avoiding confusion between RANS quantities and planar averages of filtered quantities.

### 2.2. Initial and boundary conditions

Equations (2.1)–(2.4) are integrated subject to the following boundary conditions. Periodic boundary conditions are enforced at $x_1 = \{0, L_1\}$ and $x_3 = \pm L_3/2$. At $x_2 = \pm L_2/2$, characteristic non-reflecting boundary conditions (Poinsot & Lele 1992) are used to suppress the reflection of acoustic waves.

The mean velocity field is initialized using a hyperbolic-tangent profile for the streamwise mean velocity, $u_1/U = \tanh[x_2/(2\delta_0^0)]$ which is based on the initial momentum thickness, $\delta_0^0$ defined in §3, and on the free-stream velocity, $U$, with the remaining components set to zero, $u_2 = u_3 = 0$. For the non-reacting case, a similar initialization for the mean density is used. For the reacting case, the temperature and mass fractions are initialized using the results of a one-dimensional simulation of an unstrained laminar mixing layer subject to the same boundary conditions as in the three-dimensional case at $x_2 \to \pm \infty$. The one-dimensional mixing layer evolves in time until ignition occurs, and the resulting species and energy profiles are used to initialize the full three-dimensional numerical simulation. Further details are given in Saghafian (2013). The streamwise velocity field is initialized with the same hyperbolic-tangent profile as in the non-reacting case.

Transition to turbulence in both the three-dimensional reacting and non-reacting cases is triggered by introducing a series of harmonic waves in the velocity field that were shown in earlier work to excite instabilities in mixing layers at various Mach numbers (Vreman, Geurts & Kuerten 1995b). The amplitude of the initial perturbations is set to 5% of the free-stream velocity at the centreline, and decays exponentially in the transverse direction. After a simulation time $500\delta_0^0/U$, the
kinetic-energy spectrum was fully developed, showing about four orders of magnitude of decay along one and a half decades of wave numbers.

2.3. Dimensionless parameters

In this study, the dimensionless parameters \( Re_\theta^0 = U \delta_\theta^0 / \nu_A \), \( Ma_A = U / c_A \), \( Ma_F = U / c_F \), \( Ma_C = 2U / (c_A + c_F) \), \( s = \rho_F / \rho_A \), \( Pr \) and \( Le_k \), remain fixed in all of the simulations. The values of these parameters are listed in table 1. In this formulation, \( Re_\theta^0 \) is the Reynolds number based on the initial momentum thickness \( \delta_\theta^0 \) and the kinematic viscosity of air \( \nu_A \). Similarly, \( Ma_A \) and \( Ma_F \) are the Mach numbers of the air and fuel streams, respectively, which are based on the corresponding speeds of sound \( c_A \) and \( c_F \) in each stream. The symbol \( Ma_C \) denotes the convective Mach number (Papamoschou & Roshko 1988). In addition, \( Pr \) and \( Le_k \) are, respectively, the Prandtl number and the Lewis number of species \( k \), which are based on local values of the kinematic viscosity, thermal diffusivity and mass diffusivities. The Reynolds number based on the initial vorticity thickness, \( \delta_w^0 = 4 \delta_\theta^0 \), is \( Re_w^0 = U \delta_w^0 / \nu_A \), which is also listed in table 1. Definitions of the vorticity and momentum thicknesses are given in § 3.

One of the objectives of this study is to assess the effect of combustion on the dynamics of backscatter in the supersonic mixing layer. It should be emphasized first that isolating the effects of non-premixed combustion in turbulent reacting flows is not trivial. For instance, the turbulent non-premixed combustion in a triply-periodic domain leads to continuous temperature increase and reactant depletion. In decaying turbulence and temporal mixing layers, both combustion and turbulence dynamics are statistically unsteady, thereby rendering the choice of a time instant for comparison not clearly defined. In high-speed spatially developing flows, such as jets, wakes or mixing layers, chemically-frozen zones coexist with burning regions as ignition is needed to establish the diffusion flames. In addition, in these configurations, the temperature of the oxidizer stream must be sufficiently large to warrant ignition, which indicates that even in the inert case the flow will be subject to variable-density effects. These are examples that illustrate some of the challenges of comparing inert and reacting flows.

In this investigation, a simple (and perhaps the simplest) approach is taken in which reacting and inert flows are compared under the criteria that (i) they are in the selfsimilar regime as described in § 3, (ii) the instantaneous momentum thicknesses are the same, which translates into the same instantaneous Reynolds number \( Re_\theta^* \) as defined below in (2.5), and (iii) the joint dimensionless parameters in table 1 are the same at the beginning of the computations. By using this procedure, some degree of dynamic similarity between the instantaneous solutions selected for the reacting and inert mixing layers is expected, in which the history of the initial conditions is lost once the selfsimilar period begins and the exact value of the time coordinate becomes irrelevant. However, it should be noted that this is not the only possible choice for making comparisons, nor does this selection allow for a completely spatiotemporal and statistically fair comparison between reacting and inert mixing layers. For instance, the Reynolds number based on the vorticity thickness, the Reynolds number based on the mean kinematic viscosity (to account for the increase in viscosity caused by chemical heat release), the Reynolds number based on the Taylor microscale or the total turbulent kinetic energy could have been used as matching parameters instead. Nonetheless, matching all of these parameters simultaneously is an intricate endeavor that may require iterative procedures and interpolation of solutions, which are outside the scope of this study.
### Parameters at the end of the simulations:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value (inert)</th>
<th>Value (reacting)</th>
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<tr>
<td>$Re^*_\theta$</td>
<td>Final Reynolds number (momentum-based)</td>
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<td>1044</td>
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<td>Final Reynolds number (vorticity-based)</td>
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<td>8746</td>
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<td>$Re^*_t$</td>
<td>Taylor Reynolds number</td>
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<td>$\eta^*$</td>
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### Joint parameters:

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**Table 1.** Dimensionless parameters used in the simulations.

The DNS data were analysed at the final momentum-thickness Reynolds number

$$Re^*_\theta = \frac{U\delta^*_\theta}{v_A} = 1044 \quad (2.5)$$

in both the inert and reacting cases, where $\delta^*_\theta = 18.6\delta^0_\theta$ is the final momentum thickness. At this time instant, both flows are in the selfsimilar regime, but the Reynolds numbers based on the vorticity thickness of the inert and reacting mixing
layers are different. In particular, \( \text{Re}_{w}^* = 8746 \) and \( \text{Re}_{w}^* = 6352 \) for the reacting and inert cases, respectively. It should be emphasized that, contrary to the low-Mach number limit, the vorticity thickness in these highly-compressible simulations exhibits substantial fluctuations because the compression and expansion waves in the mixing layer produce strong variations in the maximum value of the planar-averaged spanwise vorticity. This effect has also been noted in earlier numerical simulations at lower convective Mach numbers (see, for instance, figure 2 of Vreman, Geurts & Kuerten (1995a)). Therefore, the alternate choice of equating the inert and reacting vorticity thicknesses may not be appropriate for this highly compressible flow.

At \( \delta_0 = \delta_0^* \), the corresponding Reynolds number based on the Taylor microscale evaluated at the centreline, \( \text{Re}_{\lambda}^* = q^2 \sqrt{5}/\nu \epsilon \), where \( q^2 = u_i'' u_i'' \tilde{\epsilon} \) is twice the turbulent kinetic energy and \( \epsilon = \tau_{ik} \partial u_i''/\partial x_k \) is the turbulent dissipation. Similarly, the turbulent Mach number, defined here as \( \text{Ma}_t^* = (q/3)^{1/2}/\xi \), which is evaluated at the centreline of simulations. Values of \( \text{Re}_{\lambda}^* = q^2 \sqrt{5}/\nu \epsilon \) and \( \text{Ma}_t^* \) are given in table 1 for the reacting and inert simulations.

### 2.4. Computational set-up

The numerical solver is based on a finite-volume scheme that minimizes dissipation error while still preserving stability (You, Ham & Moin 2008; Khalighi et al. 2011). It consists of a hybrid-shock capturing scheme that switches from fourth-order central differences to a second-order essentially non-oscillatory (ENO) when shocks are detected. For the tested configuration, this corresponds to roughly 2–3 % of the gridpoints at any time. Time integration is performed using a third-order Runge–Kutta method without operator splitting with direct evaluation of the chemical sources. This is a feasible method for this high-speed flow, in which the large-scale straining time does not differ appreciably from the acoustic and chemical time scales. The temperature field is found iteratively from the total-energy field via a Newton–Raphson solver.

The numerical simulations are performed on a Cartesian grid of 768 \( \times \) 320 \( \times \) 192 elements in the \( x_1 \), \( x_2 \) and \( x_3 \) directions, respectively, with side lengths \( L_1/\delta_0^* = 315 \), \( L_2/\delta_0^* = 211 \) and \( L_3/\delta_0^* = 79 \), as depicted in figure 1. The computational domain is sufficiently large such that the integral length scales in the spanwise and streamwise directions at the final time of the simulations, which are given here by \( \ell_i^* = (1/\nu_1^2) \int_{-\infty}^{+\infty} u_1(x) u_1(x - e_i r) \, dr \) with \( i = 1, 3 \), respectively, are small compared with \( L_1 \) and \( L_3 \), as shown in table 1.

The minimum grid spacing \( h \) is within the viscous subrange of the turbulence in the mixing layer. In particular, calculations at the end of the simulations show that the average ratio of the characteristic Kolmogorov thickness \( \eta^* = (\nu^3/\epsilon)^{1/4} \) within the mixing layer to the minimum grid spacing \( h \) is 1.0 and 0.7 at the end of the reacting and inert simulations, respectively.

The computations were validated against the high-Mach-number simulations of the three-dimensional non-reacting turbulent mixing layer of Pantano & Sarkar (2002). The results of the test case are deferred to the appendix A.

Since combustion in the reacting mixing layer occurs predominantly in the non-premixed mode, the flames are embedded in the Kolmogorov eddies, which are dominated by molecular diffusion. The thickness of the reaction layers is, however, generally smaller than the thickness of the layers in which molecular diffusion prevails (Liñán 1974). An assessment of the capabilities of the present numerical resolution
to resolve the reaction zones is made in appendix B. In addition, studies have been performed that confirm the insensitivity of planar-averaged radical concentration profiles to the grid resolution (Saghafian 2013).

3. Overall characteristics of the aerothermochemical flow field in the mixing layer

In this section, the main simulation results are outlined for their later use in the analysis of backscatter. Focus is directed to overall quantities that indicate selfsimilar behaviour, compressibility and combustion.

3.1. The selfsimilar mixing layer

After a transient, in which the influences of the initial conditions are noticeable, a quasi-linear regime is observed in the growth of the momentum thickness $\delta_\theta$, the vorticity thickness $\delta_w$ and, for the reacting cases, in the mean chemical-production rate of water vapour per unit of in-plane surface $\dot{\mathcal{W}}_{H_2O}$, as shown in figure 2 and figure 3. Here, $\delta_\theta$ and $\delta_w$ are computed from the definitions

$$\delta_\theta = \frac{1}{2(1+s)} \int_{-\infty}^{\infty} \rho \left[ 1 - \left( \frac{\bar{u}_1}{U} \right)^2 \right] \, dx_2,$$

(3.1)

and

$$\delta_w = \frac{1}{|\omega_3_{\text{max}}|} \int_{-\infty}^{+\infty} |\omega_3| \, dx_2,$$

(3.2)

with $\omega_3 = \partial u_1 / \partial x_2$ the mean spanwise vorticity (Brown & Roshko 1974). For the reacting cases, $\dot{\mathcal{W}}_{H_2O}$ is calculated as

$$\dot{\mathcal{W}}_{H_2O} = \int_{-\infty}^{+\infty} \dot{w}_{H_2O} \, dx_2,$$

(3.3)

where $\dot{w}_{H_2O}$ is the production rate of water-vapour mass per unit volume. The period of quasi-linear growth of $\delta_\theta$ and $\dot{\mathcal{W}}_{H_2O}$ is defined here as the period of selfsimilar evolution, during which the turbulence characteristics are approximately selfsimilar when non-dimensionalized with the instantaneous large spatial scale $\delta_\theta$ and the long time scale $\delta_\theta/U$. The choice of $\delta_\theta$ as spatial scale is convenient here because it is an integral quantity that varies smoothly and takes explicitly into account the density variations in the mixing layer.

The vorticity and momentum mixing-layer thicknesses grow in time as a result of the momentum transfer between the free streams and the corresponding vorticity generation. In the first approximation, the relation

$$\frac{1}{U} \frac{d\delta_\theta}{dt} = C_\theta$$

(3.4)

represents the growth of the momentum thickness in the selfsimilar region, with $C_\theta$ a dimensionless constant that depends in a complex manner on the aerothermochemical parameters of the problem. In particular, these DNS results show that $C_\theta = 7.6 \times 10^{-3}$ and $C_\theta = 1.4 \times 10^{-2}$ for the reacting and inert mixing layers, respectively. At the end of the simulations, the ratio $\delta_w/\delta_\theta$ is 6.1 and 8.3 for the inert and reacting cases, respectively. Specifically, figure 2 shows that $\delta_\theta$ and $\delta_w$ grow more slowly for
Figure 2. Time variations of (a) momentum thickness and (b) vorticity thickness for inert (solid lines) and reacting (dashed lines) simulations. The time instants denoted by the symbols ◦, ▷, ◀ and □, are spaced $U \Delta t / \delta_0^* = 71.2$ time units (i.e. 2.84 times the strain time $\delta_0^*/U$). Quantities denoted by the symbol □ correspond to the final momentum thickness $\delta_0 = \delta_0^*$.

Figure 3. Mean rate of water-vapour mass production per unit of in-plane surface $\dot{\nabla} \text{H}_2\text{O}$ as a function of time in the reacting mixing layer. Refer to caption in figure 2 for the symbols ◦, ▷, ◀ and □. The characteristic chemical time $t_q$ is estimated from the low-pressure limit of the rate constant of the recombination step $\text{H} + \text{O}_2 + \text{N}_2 \rightarrow \text{HO}_2 + \text{N}_2$ at the air-stream temperature $T_A$.

the reacting simulations, a trend which is in agreement with earlier investigations at smaller convective Mach numbers (Miller et al. 1994; Luo 1999; Pantano et al. 2003; Knaus & Pantano 2009). This effect is most likely due to the decrease in the Reynolds stresses as shown by Mahle et al. (2007). Furthermore, it is observed in figure 2(a) that the momentum thickness at the end of the simulations, $\delta_0 = \delta_0^*$, lies within the quasi-linear growth zone that is representative of the selfsimilar period in both inert and reacting cases.
The selfsimilarity of the mixing layer is also revealed by the collapse of the profiles of mean streamwise velocity $u_1$ and streamwise Reynolds stress $\rho\overline{u'\overline{u}'}$, as shown in figure 4. These overall trends in first- and second-order statistics are also in agreement with earlier studies in non-reacting (Brown & Roshko 1974; Papamoschou & Roshko 1988; Rogers & Moser 1994; Vreman et al. 1996; Pantano & Sarkar 2002) and reacting (Miller et al. 1994; Luo 1999; Pantano et al. 2003; Knaus & Pantano 2009) turbulent mixing layers at smaller convective Mach numbers with either one-step or infinitely-fast chemistry and Fickian diffusive-transport descriptions.

3.2. Compressibility and combustion

The high Mach numbers used in these simulations imply that the acoustic time scale $\delta_{\theta}/c_A$ is of the same order as the characteristic eddy-straining time $\delta_{\theta}/U$. This causes the pressure to undergo strong variations that are of the same order as the characteristic dynamic pressure $\rho_A U^2$ during a turnover time of the large eddies, which, in turn, leads to strong density variations in the mixing layer.

As the supersonic fuel stream is entrained in the mixing layer, it encounters regions of decreasing velocity and, more specifically, subsonic zones. Sometimes these decelerations to subsonic conditions occur abruptly in between eddies carrying supersonic and subsonic flows. These zones of strong variations in the Mach number have been termed eddy shocklets in earlier works (Lee et al. 1990; Miller et al. 1994; Vreman et al. 1996; Samtaney et al. 2001), and develop more prominently on
the fuel-side edge of the mixing layer because of the higher Mach number in that region, as observed in the dark-colour corrugations of the density-gradient contours shown in figure 5(a,c). In fact, the high-speed compressibility effect causes a strong spatial intermittency in the flow dilatation, which develops large-magnitude cusps at the smallest scales.

Furthermore, the high-speed compressibility effect causes a partial recovery of the free-stream kinetic energy as the gas reaches the nearly-stagnant central region of the mixing layer, by which the local temperature increases by a factor of 1.5 with respect to the air-stream static temperature \( T_A \) even in the absence of chemical reactions, as observed in figure 5(b). In the reacting case, the chemical heat released leads to an additional increase in the gas temperature by a factor of 1.3 with respect to the maximum temperature in the inert flow, as shown in figure 5(d). It is therefore clear that the temperature rise in the flow has a strong component that is due to compressibility effects. This is an important consideration for the physical interpretation of backscatter in the present mixing-layer configuration, as detailed in § 4.

The contours of the production rate of hydroxyl radical (OH) in the reacting mixing layer are shown in figure 5(c) (see also figure 15 in appendix B). The presence of OH appears to be more frequent on the air-side edge of the mixing layer, which is where the mixture is nearly stoichiometric, as observed in figure 5(d). Some of the zones where OH is produced are located downstream from highly compressed regions, where the temperature increases sharply in amounts of order unity with respect to itself, and which appear to be reacting eddy shocklets. The resulting flame brush resembles a thick layer in mixing-layer scales, along which the temperature fluctuates strongly due to effects of turbulent mixing and compressibility.

In order to locate the overall stoichiometric condition in figure 5, the stoichiometric value \( Z_{st} = 1/(1 + S) = 0.31 \) of the H-element mixture fraction

\[
Z_H = \frac{W_{H_2}}{2Y_{H_2,F}} \left( \frac{2Y_{H_2}}{W_{H_2}} + \frac{Y_H}{W_H} + \frac{2Y_{H_2O}}{W_{H_2O}} + \frac{Y_{OH}}{W_{OH}} + \frac{Y_{HO_2}}{W_{HO_2}} + \frac{2Y_{H_2O_2}}{W_{H_2O_2}} \right) \tag{3.5}
\]

is used, where \( S = rY_{H_2,F}/Y_{O_2,A} = 2.30 \). In this formulation, \( Y_{H_2,F} = 0.067 \) is the mass fraction of hydrogen in the fuel stream, \( Y_{O_2,A} = 0.233 \) is the mass fraction of oxygen in the air stream and \( r = 8 \) is the stoichiometric mass ratio for \( H_2/O_2 \) combustion. Additional information regarding conditional probability density functions (PDFs) of the temperature and reactant mass fractions in H-element mixture-fraction space is given in appendix B.

### 4. Dynamics of SGS backscatter of kinetic energy

In this section, the spatial distribution of backscatter is investigated by filtering the DNS data of the reacting and inert mixing layers described above. For this purpose, the source terms in the large-scale kinetic-energy conservation equation are evaluated, including the contribution from the large-scale pressure-dilatation work. In addition, the Boussinesq eddy viscosity is calculated and its spatial distribution is analysed in conjunction with the dissipation, flow dilatation and mixture fraction.

#### 4.1. Distributions of SGS backscatter and large-scale pressure-dilatation work

In the following analysis, the relevant aerothermochemical variables are normalized with the instantaneous momentum thickness \( \delta_\theta^* \) as the unit of spatial scale, the
SGS backscatter in supersonic hydrogen–air turbulent mixing layers

Figure 5. (a,c) Midplane contours of the density-gradient modulus normalized with its maximum value $|\nabla \rho|/|\nabla \rho|_{\text{max}}$, including contours of OH production (red lines, reacting case) and stoichiometric line $Z_H = Z_{st}$ (green lines, reacting case). (b,d) Midplane streamwise contours of the dimensionless temperature $(T - T_F)/(T_A - T_F)$ including the stoichiometric line $Z_H = Z_{st}$ (green lines, reacting case). These snapshots correspond to the final momentum thickness $\delta_\theta^*$. 
characteristic strain time $\delta^*/U$ as the unit of time, $\rho_A$ as the unit of density, $U$ as the unit of velocity, $\rho_A U^2$ as the unit of pressure and $\mu_A$ the unit of dynamic viscosity.

In these variables, the filtered version of the momentum equation (2.2) becomes

$$\frac{\partial}{\partial t}(\tilde{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j}(\tilde{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{1}{Re^*_o} \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} - \frac{\partial \tilde{T}_{ij}}{\partial x_j},$$  

(4.1)

where the tensor $\tilde{T}_{ij} = \tilde{\rho} \tilde{u}_i \tilde{u}_j - \tilde{\rho} \tilde{u}_i \tilde{u}_j$ describes the dimensionless residual stresses, which are evaluated from the DNS data.

A conservation equation for the large-scale kinetic energy, $k = \tilde{u}_i \tilde{u}_i/2$, can be obtained by multiplying (4.1) by $\tilde{u}_i$ and using the continuity equation (2.1), which gives

$$\frac{\partial \tilde{\rho} k}{\partial t} + \frac{\partial}{\partial x_i}(\tilde{\rho} \tilde{u}_i k) = \alpha + \Pi - \epsilon_v - \epsilon_{SGS}. $$

(4.2)

In this formulation, the quantity denoted by $\alpha$ is given by

$$\alpha = \frac{\partial}{\partial x_i} \left( \frac{\tilde{\tau}_{ij} \tilde{u}_j}{Re^*_o} - \tilde{T}_{ij} \tilde{u}_j - \tilde{p} \tilde{u}_i \right).$$

(4.3)

The volumetric integral of $\alpha$ over the computational domain can be written as a closed surface integral along the boundaries, which vanishes in free-shear flows, indicating that $\alpha$ is just a transport term that redistributes kinetic energy. However, the last three terms on the right-hand side of (4.2) are sources and sinks of large-scale kinetic energy.

In particular, $\Pi$ is the dimensionless pressure-dilatation work, given by

$$\Pi = \tilde{p} \tilde{\Delta}_v,$$

(4.4)

with $\tilde{\Delta}_v = \partial \tilde{u}_i / \partial x_i$ being the dilatation of the Favre-filtered velocity field. The pressure-dilatation work $\Pi$ depends explicitly only on resolved quantities and therefore no model closure is needed to compute it. Depending on the sign of the flow dilatation, $\Pi$ can transform resolved kinetic energy into thermal energy in compression regions $\tilde{\Delta}_v < 0$, or drain thermal energy and transfer it into the large-scale kinetic-energy field in expansion regions $\tilde{\Delta}_v > 0$. In addition, $\epsilon_v$ represents the dimensionless viscous dissipation

$$\epsilon_v = \frac{\tilde{\tau}_{ij} \tilde{S}_{ij} / Re^*_o}{(2\mu(\tilde{S}_{ij} - \Delta_v \delta_{ij}/3))\tilde{S}_{ij}}.$$

(4.5)

which is a sink of large-scale kinetic energy. In this formulation, $\tilde{S}_{ij} = (1/2)(\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i)$ is the rate of strain of the Favre-filtered velocity field. Lastly, $\epsilon_{SGS}$ is the non-dimensional SGS dissipation

$$\epsilon_{SGS} = -\tilde{T}_{ij} \tilde{S}_{ij},$$

(4.6)

which represents the rate at which kinetic energy is transferred from the resolved motion to the subgrid. The SGS dissipation $\epsilon_{SGS}$ is not a viscous dissipation, in that the energy transfer that it represents is due entirely to inertial processes at the filter level. In fact, contrary to the viscous dissipation $\epsilon_v$, the SGS dissipation $\epsilon_{SGS}$ may be locally positive, which indicates dissipation of large-scale kinetic energy or forwardscatter to the subgrid, or negative, which corresponds to the transfer of kinetic energy.
energy from the subgrid scales to the filtered velocity field. The latter case, namely \( \epsilon_{SGS} < 0 \) or energy transfer from the subgrid to the supergrid, is referred to as SGS backscatter of kinetic energy (Germano et al. 1991; Piomelli et al. 1991; Lesieur & Métais 1996; Domaradzki & Saiki 1997; Menevau & Katz 2000). The physical phenomenon represented by \( \epsilon_{SGS} < 0 \) bears a strong resemblance with the reverse energy-transfer process described by the backscatter flux term that appears in the kinetic-energy equation in wavenumber space, although spectral backscatter and SGS backscatter are not strictly equivalent in inhomogeneous flows or when the spectral cutoff filter is not employed for calculating \( \epsilon_{SGS} \).

In order to isolate positive and negative local contributions to the SGS dissipation and pressure-dilatation work prior to planar averaging, the definitions

\[
\text{forwardscatter: } \epsilon_{SGS}^+ = \frac{1}{2}(\epsilon_{SGS} + |\epsilon_{SGS}|) \geq 0, \tag{4.7}
\]

\[
\text{backscatter: } \epsilon_{SGS}^- = \frac{1}{2}(\epsilon_{SGS} - |\epsilon_{SGS}|) \leq 0, \tag{4.8}
\]

are used here in analogy to Piomelli et al. (1991), although a reverse sign is employed here to denote the more intuitive positive values of \( \epsilon_{SGS} \) as forward-dissipating dynamics. Specifically, if \( \epsilon_{SGS} \) becomes negative as in backscattering regions, then \( \epsilon_{SGS}^+ \) becomes zero, and vice versa. In addition, the integral of the planar-averaged SGS dissipation in the cross-shear direction,

\[
E_{SGS} = \int_{-\infty}^{+\infty} \langle \epsilon_{SGS} \rangle \, dx_2, \tag{4.9}
\]

is utilized to monitor the temporal evolution of the net dissipation, forwardscatter and backscatter as the mixing layer grows. Similar to the expressions (4.10) for \( \epsilon_{SGS}^+ \) and \( \epsilon_{SGS}^- \), the SGS dissipation \( E_{SGS} \) can be decomposed into positive \( E_{SGS}^+ > 0 \) and negative \( E_{SGS}^- < 0 \) contributions, which here refer to forwardscatter and backscatter, respectively.

A similar decomposition into positive and negative pressure-dilatation work fluxes

\[
\Pi^+ = \frac{1}{2}(\Pi + |\Pi|) \quad \text{and} \quad \Pi^- = \frac{1}{2}(\Pi - |\Pi|), \tag{4.10}
\]

can be used to describe the production of large-scale kinetic energy by flow expansion, \( \Pi^+ > 0 \), and its destruction by flow compression, \( \Pi^- < 0 \).

Figure 6(a,b) shows the time evolution of \( E_{SGS} \) for inert and reacting mixing layers. Instead of the time coordinate \( t \), the momentum mixing-layer thickness \( \delta_\theta \) has been used on the horizontal axis of the plot, since the mapping between both variables is approximately linear in the selfsimilar region, \( \delta_\theta \sim C_\theta Ut \), as observed in figure 2(a), with \( C_\theta \) given by (3.4). In the selfsimilar period, the integrated SGS dissipation \( E_{SGS} \) does not undergo strong variations with time, which suggests that the characteristic value of \( \langle \epsilon_{SGS} \rangle \) decreases approximately with time as \( 1/t \), as indicated by the order-of-magnitude estimate \( E_{SGS} \sim \langle \epsilon_{SGS} \rangle \delta_\theta \) in (4.9). Figure 6(c,d) shows that at the final momentum thickness the integrated SGS backscatter \( E_{SGS}^- \) amounts to approximately 23% and 18% of the net value in the inert and reacting mixing layers, respectively. This indicates a slightly lower relative intensity of backscatter for the reacting case. During the self-similar period, this conclusion appears to be mostly insensitive to the value of the momentum thickness as well as the choice of the filter width.

For filters in the inertial subrange, the viscous dissipation \( \epsilon_v \) is small compared with the competing terms \( \epsilon_{SGS} \) and \( \Pi \) in the large-scale kinetic-energy conservation equation (4.2). Therefore, in the absence of molecular mechanisms of energy
dissipation, the SGS dissipation is responsible for the entire transfer of kinetic energy between the subgrid and the resolved motions. Although the overall planar-averaged energy transfer $\langle \epsilon_{\text{SGS}} \rangle$ occurs from the large scales to the subgrid scales in accord with the traditional turbulent cascade, figure 7(a,b) reveals that backscatter occurs locally within the mixing layer due to the non-zero contribution of $\epsilon_{\text{SGS}}^{-}$ to the net SGS dissipation. Furthermore, the levels of SGS dissipation increase with filter width (see also figure 6(a)). However, this increment in the SGS dissipation becomes proportionally smaller as the filter width becomes larger, as it may be expected from the constancy predicted by the Kolmogorov’s universal equilibrium theory for the turbulent dissipation across the inertial subrange. In inert compressible flows this invariance may only apply in a much narrower interval of small filter widths where the large-scale pressure-dilatation work ceases to be important for the kinetic-energy transfer dynamics, as suggested by recent studies (Aluie et al. 2012).

Similarly, figure 7(c,d) shows that local values of the large-scale pressure-dilatation work are comparable with the SGS dissipation. In addition, the planar average of the net large-scale pressure-dilatation work $\langle \Pi \rangle$ is found to be the result of the difference between two large fluxes of expansion $\langle \Pi^+ \rangle$ and compression $\langle \Pi^- \rangle$, which attain their maximum values near the centreline of the mixing layer where stagnation conditions are reached. These fluxes tend to cancel each other, thus indicating that a certain level of homogenization of the intense compression and expansion phenomena occurs in the mixing layer upon spatial averaging.
A correlation between backscatter and flow expansion is observed in figure 8, in which isocountours of $\epsilon_{\text{SGS}} < 0$ tend to visually follow closely those of $\Pi > 0$, this conclusion being mostly independent of the presence of chemical reactions in the mixing layer. In fact, no visible correlation in figure 8(b,d) can be simultaneously detected between pressure-dilatation work and the stoichiometric line (which is approximately indicative of the maximum flame temperature as described in § 3). Further inspection of the same phenomena is made in figure 9 over a larger computational domain by calculating the joint PDF between $\epsilon_{\text{SGS}}$ and $\Pi$. The correlation coefficient in the region of the joint PDF shown in the insets of figure 9 is $-0.69$ and $-0.48$ for the inert and reacting flows, respectively.

Figure 9 shows that the prevalent mode of energy exchange in the mixing layer is forwardscatter, which occurs in 54% and 66% by volume fraction in inert and reacting mixing layers, respectively, the remaining portion being in backscatter mode. At low values of the pressure-dilatation, which are most frequently found in the mixing layer, the most probable values of the SGS dissipation $\epsilon_{\text{SGS}}$ evolve with powers of $\Pi$ in a manner reminiscent of the quadratic trend recently proposed by Shi et al. (2013) for compressible homogeneous isotropic turbulence. These conclusions appear to be unaffected by combustion in the mixing layer.
It may be tempting to explain the correlation between large-scale pressure-dilatation work of expansion and backscatter by using the transport equation for the SGS kinetic energy, \( k_{SGS} = \frac{1}{2} (\bar{u} \bar{u}_i - \bar{u}_i \bar{u}_j) \), namely

\[
\frac{\partial \rho k_{SGS}}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i k_{SGS}) = \alpha_{SGS} + \Pi_{SGS} + \epsilon_{SGS} - \epsilon_{v,SGS},
\]

(4.11)
which can be obtained by subtracting (4.2) from the transport equation of the filtered kinetic energy, \( \tilde{K} = \tilde{u}_i \tilde{u}_i / 2 \). In this formulation, \( \alpha_{SGS} = \partial \theta / \partial \tilde{u}_i (p \tilde{u}_i \tilde{u}_i + \tau_{ij} \tilde{u}_j - \tilde{p} \tilde{u}_i \tilde{K} + \tilde{p} \tilde{u}_i \tilde{K}) \) is a redistribution term, and \( \epsilon_{v, SGS} = \tilde{u}_i \tilde{S}_{ij} - \tau_{ij} \tilde{S}_{ij} \) is the molecular dissipation. More importantly, (4.11) contains the SGS pressure-dilatation work \( \Pi_{SGS} = \tilde{p} \Delta_v - \tilde{p} \Delta_v \) and SGS dissipation \( \epsilon_{SGS} \) as source terms. Specifically, (4.11) reveals that \( k_{SGS} \) is destroyed through backscatter, this effect being of key importance in the formulation of the dynamic localization model of the Smagorinsky constant (Ghosal et al. 1995). In compressible flows, however, the SGS kinetic energy can be produced or depleted by SGS dilatation, which is represented by \( \Pi_{SGS} \) in (4.11).

A hypothetical explanation of the localization of backscatter in expanding regions observed above could be based on a balance of SGS pressure dilatation work and SGS dissipation in (4.11), which implies no accumulation of \( k_{SGS} \) in the subgrid and negligible viscous effects. In these simulations, however, only slightly more than half of the computational cells undergoing volumetric expansion have positive values of \( \Pi_{SGS} \). Since backscatter tends to occur more often than \( \Pi_{SGS} > 0 \) in regions subject to expansion, and \( \Pi > 0 \) occurs exclusively in those regions, there are additional underlying physical phenomena needed to explain the anticorrelation between \( \Pi \) and \( \epsilon_{SGS} \). Exact quantifications of these compressible subgrid dynamics are beyond the scope of this study and require further investigations.

It is worth noting that two different sources of flow dilatation \( \Delta_v \) are present in this flow. The first component of the dilatation is of order \( \Delta_v \sim \gamma_A M_A^2 U / \delta_0 \) and pertains to the compressible nature of this high-speed mixing layer, causing characteristic large-scale variations in the planar-averaged density of order \( \Delta \rho / \rho = O(\rho_A U^2 / p_\infty) \). The corresponding mechanism of energy transfer enhanced by this first component of \( \Delta_v \) tends to peak in the large scales as a result of the cancellation of compression and expansion waves, as observed in figure 7(c,d). The second component of the dilatation is of order \( \Delta_v \sim U Q Y_{F,F} Z_{st} / (c_{p,A} T_A \delta_0) \) and is related to the density fluctuations introduced by combustion, which produce characteristic large-scale variations in the planar-averaged temperature \( \Delta T / T = O(Q Y_{F,F} Z_{st} / (c_{p,A} T_A)) \), where \( Q \) is the overall heat of combustion per unit mass of fuel. The ratio of compressibility and combustion contributions to the dilatation represents an Eckert number \( Ec = \gamma_A M_A^2 c_{p,A} T_A / (Q Y_{F,F} Z_{st}) \), which becomes of order 10 for the present simulations. This indicates that the contribution of the high-speed flow compressibility to the pressure-dilatation overwhelms any addition that may be expected from the thermal expansion induced by combustion in this supersonic mixing layer, even though these two effects are most likely non-additive.

The elevation of temperature caused by the chemical heat release produces, at least, two different effects in the mixing layer. First, a debilitation of the high-speed flow-compressibility effects occurs because of an increase in the speed of sound, with the pressure-dilatation work becoming smaller in the reacting case, which by the reasoning above also reverts in lower amounts of SGS backscatter for the same momentum thickness. The lower levels of \( \Pi \) in the reacting case are evidenced by comparing the planar averages in figure 7(c,d) and by the joint PDFs in figure 9(a,b). Second, the kinematic viscosity in the reacting simulations increases to roughly double its value in the inert computations, an effect which tends to damp turbulence (Takagi et al. 1980). However, this finite Reynolds-number effect tends to be cancelled by the fact that, because of the decrease in density, more vortical structures are needed in the reacting simulations to reach the same momentum thickness of the inert mixing layer, as observed in figure 2(b).
In figure 10(a–d), the joint PDFs of pressure dilatation work and SGS backscatter versus filtered H-element mixture fraction \( \tilde{Z}_H \) (introduced in § 3) also confirm that the chemical heat released by combustion has a very modest effect on these two quantities. No significant variations of \( \Pi \) and \( \epsilon_{SGS} \) are observed with respect to \( \tilde{Z}_H \) as would typically be expected near stoichiometric conditions in reacting mixing layers, where the temperature reaches the maximum values. However, this conclusion should be taken with caution, as it may only pertain to high-speed turbulent reacting flows dominated by compressibility effects. In such configurations, the temperature increment caused by combustion may just serve to relax the dominant high-speed compressibility effects on the energy-conversion dynamics, as described above.

4.2. Effects of flow dilatation and SGS backscatter on the Boussinesq eddy viscosity

In the Boussinesq approximation, the deviatoric part of the SGS stress tensor is modelled as

\[
\mathcal{T}_{ij} - \frac{1}{3} \delta_{ij} \mathcal{T}_{kk} = -2 \bar{\rho} v_t \left( \tilde{S}_{ij} - \frac{\tilde{\Lambda}_v \delta_{ij}}{3} \right)
\]  

(4.12)

(see Rogallo & Moin 1984). In the formulation, \( \delta_{ij} \) is the Kronecker tensor and \( v_t \) is a scalar eddy viscosity. In particular, the eddy-viscosity model (4.12) assumes a perfect alignment between the SGS stress and filtered strain-rate tensors.

In the high-speed flow analysed in this study, negative values of the eddy viscosity in (4.12) are not completely correlated with the occurrence of SGS backscatter. This is in contrast to low-speed turbulent flows, in which SGS backscatter is a cause of concern for numerical simulations as it is fully correlated with negative eddy viscosities (Piomelli et al. 1991; Lund et al. 1993). To illustrate this, consider contracting expression (4.12) with \( \tilde{S}_{ij} \), which gives

\[
\epsilon_{SGS} + \frac{2}{3} \tilde{\rho} k_{SGS} \tilde{\Lambda}_v = 2 \bar{\rho} v_t \left( |\tilde{S}|^2 - \frac{\tilde{\Lambda}_v^2}{3} \right),
\]

(4.13)
where $k_{SGS} = \overline{\rho} = \frac{\overline{u_k u_k} - \overline{u_k u_k}}{2}$ is the SGS kinetic energy, and $|\overline{S}|$ is the contraction of the strain tensor with itself, $|\overline{S}|^2 = \overline{S_{ij} S_{ij}}$. It is worth emphasizing that the term in brackets on the right-hand side of (4.13) is a positive-definite quadratic form, and therefore the sign of the eddy diffusivity $v_t$ is imposed solely by the sign of the left-hand side of the equation. Negative values of $v_t$ are representative of antiparallel-like alignment between the strain-rate tensor and the deviatoric part of the SGS stress tensor.

From (4.13), the eddy viscosity

$$v_t = \frac{\epsilon_{SGS}(1 + \Lambda)}{2\overline{\rho}(|\overline{S}|^2 - \frac{\Delta^2}{3})}$$

(4.14)

is obtained, where $\Lambda$ is a dimensionless ratio given by

$$\Lambda = \frac{\gamma_A M_{SGS}^2 \Pi}{\epsilon_{SGS}}$$

(4.15)

which represents the ratio of the dilatation work done by the SGS dynamic pressure to the SGS dissipation, with $\Pi$ and $\epsilon_{SGS}$ defined in (4.4) and (4.6), respectively. In this formulation, the symbol $M_{SGS}$ denotes the SGS Mach number

$$M_{SGS} = \sqrt{\frac{2\overline{\rho} k_{SGS}}{3\gamma_A \overline{\rho}}}$$

(4.16)

which represents the ratio of the characteristic SGS flow velocity $\sqrt{2k_{SGS}/3}$ to the characteristic filtered speed of sound $\sqrt{\gamma_A \overline{\rho}/\overline{\rho}}$. Note that the sign of the SGS kinetic energy is positive for non-negative filters (Ghosal et al. 1995), and therefore $M_{SGS}$ is a well-defined quantity in this analysis.

The SGS Mach number (4.16) is a measure of the importance of compressibility effects in the subgrid scales (Erlebacher et al. 1992). The value of the SGS Mach number is highly dependent on the filter width. In high-speed turbulent flows, an increasingly large amount of shocked regions of high $M_{SGS}$ are transferred from the filtered field into the subgrid as $\Delta$ increases, with $M_{SGS}$ increasing as a positive power of the filter width. On the contrary, in low-speed flows, the SGS Mach number is negligible for all filter widths and the resulting value of $\Lambda$ is small in (4.14), thereby rendering the sign of the eddy viscosity fully correlated with the sign of the SGS dissipation, with $v_t < 0$ occurring always in the presence of SGS backscatter $\epsilon_{SGS} < 0$ and vice versa (Germano et al. 1991; Piomelli et al. 1991; Carati et al. 1995; Ghosal et al. 1995; Lesieur & Métai 1996).

In the mixing layer analysed here, the SGS Mach number (4.16) is locally sufficiently large to make the dimensionless ratio $\Lambda$ an order-unity quantity for the inert and reacting cases in some locations of the flow, as observed in the planar-averaged values $\langle M_{SGS} \rangle$ and $\langle |\Lambda| \rangle$ in figure 11. It should be emphasized, however, that some information of local phenomena is lost upon planar-averaging the SGS Mach number. In the present simulations the SGS Mach number attains relatively large local values even for small filter widths because of the intense expansion and compression waves in the mixing layer, which are rapidly transferred to the subgrid scales upon filtering the flow field. This is evidenced by the strong density gradients shown in figure 5(a,c). In addition, the higher temperatures encountered in the reacting
mixing layer tend to increase the filtered speed of sound, leading to smaller values of ⟨MaSGS⟩.

In this way, competition exists in (4.14) between dissipation and dilatation work by the SGS dynamic pressure, which determines the local sign of the eddy viscosity νt. In fact, the eddy viscosity appears here as a spatially intermittent quantity whose sign is not well correlated with the presence of SGS backscatter or combustion. This is shown by the isocontours in figure 12. From this, a regime diagram can be developed that describes these synergistic dynamics, which is summarized in figure 13(a). This diagram provides a budget of volume fractions undergoing each regime in terms of the possible combinations between the signs of ϵSGS, γAMaSGS²Π and νt. In particular, the eddy viscosity is negative in approximately 32% (31%) of the sampled volume for Δ = 10h. Here values in brackets indicate the percentages in the reacting case, and the absence of brackets correspond to percentages in the inert mixing layer. The 63% (41%) of this portion of the volume fraction with νt < 0 is undergoing backscatter, with the remaining volume in a mode in which forwarsscatter and compression occur simultaneously. Equivalently, backscatter occurs in 46% (34%) of the volume, but the eddy viscosity is negative in only 43% (38%) of this portion. Increasing the filter

Figure 11. Spatial distributions of (a,b) planar-averaged SGS Mach number ⟨MaSGS⟩ and (c,d) planar-averaged absolute value of the ratio of the dilatation work done by the SGS dynamic pressure to the SGS dissipation ⟨|Λ|⟩ for different filter widths Δ (refer to the legend in (a)). The insets in (c,d) show the mesh points in the region 2 < x2/δ°/θ < 5 overlaid on the ⟨|Λ|⟩ curve for Δ = 2.5h.
width to $\Delta = 20h$ leads to a decrease in the volume fraction with $\nu_t < 0$ in backscatter mode, 38% (33%), and to an overall increase in the SGS Mach number.

Further insight is provided in figure 13(b,c) by the joint PDFs of the SGS dissipation and the dilatation work done by the SGS dynamic pressure. For small values of the dilatation work done by the SGS dynamic pressure, which are the most probable in the mixing layer, a correlation is observed between $\epsilon_{SGS}$ and $\gamma_A M_{SGS}^2$ as evidenced by the insets of figure 13(b,c), by which backscatter tends to occur in regions undergoing volumetric expansion with both positive and negative eddy viscosities. Specifically, the correlation coefficient in the region of the joint PDF shown in the insets of figure 13(b,c) is $-0.50$ and $-0.25$ for the inert and reacting cases, respectively.

Since the SGS backscatter and the dilatation work of expansion done by the SGS dynamic pressure yield contributions of opposite sign in the eddy-viscosity equation (4.14), the correlation between these two quantities tends to moderate the effect of backscatter in generating negative amounts of eddy viscosity relative to purely incompressible flows. As shown above, the volume fraction undergoing backscatter with negative eddy viscosities decreases with filter width and SGS Mach number, a trend which is visualized in the insets of figure 13(b,c) as a decrease in the angular shift between the line $\nu_t = 0$ and the high-probability ridge of the joint PDF of $\epsilon_{SGS}$ and $\gamma_A M_{SGS}^2$. In the low-Mach-number limit, the high-probability ridge becomes a vertical line and the joint PDF has a negligible horizontal width, thereby indicating that $\nu_t < 0$ occurs exclusively in the presence of SGS backscatter and vice versa.

Notwithstanding the marginal influence of combustion on the turbulence dynamics that have been analysed in this supersonic flow, it is worth emphasizing that the interplay between the eddy diffusivity and flames may need further exploration in the context of LES of low-speed turbulent reacting flows, in which the SGS flow dilatation is enhanced by the chemical heat release deposited at the microscales.
Figure 13. (Colour online) (a) Regime diagram representative of the different energy-conversion modes, quoting the corresponding volume fractions in inert and reacting (in brackets) mixing layers. (b,c) Isocontours of the joint PDF between SGS dissipation $\epsilon_{\text{SGS}}$ and dilatation work by the SGS dynamic pressure $\gamma_{A}Ma_{\text{SGS}}^{2}I_{\delta}^{*}$ for $\Delta = 10h$. A magnification of the central zone of the joint PDF's is shown in the figure insets which includes the ridge of maximum probability (white dashed line) along with the point of global maximum probability (white ×). Refer to caption in figure 9 for the volume sampled to obtain the statistics.

(see, for instance, Libby & Bray (1981) for related counter-gradient transport effects in RANS modelling of turbulent premixed combustion).

5. Conclusions

In this study, the dynamics of backscatter of kinetic energy have been investigated in the context of LES of high-speed turbulent reacting flows of interest for hypervelocity propulsion. A priori analyses of DNS of reacting and inert supersonic, time-evolving, hydrogen–air turbulent mixing layers at high convective Mach numbers and with complex chemistry and multicomponent diffusion, were performed in order to elucidate the effects of compressibility and combustion on the SGS backscatter of kinetic energy.
The overall characteristics of the aerothermochemical field in the mixing layer were first examined, in which the importance of high-speed compressibility effects was highlighted. In addition, a self-similar period was identified in which the relevant turbulent quantities grew in a quasi-linear manner. A differential filter was applied to the DNS flow field in order to extract filtered quantities, which were used in the LES equation for the large-scale kinetic-energy budget. Spatiotemporal analyses of the flow-field statistics in the self-similar regime were performed, revealing the presence of noticeable amounts of SGS backscatter in the mixing layer.

The flow dilatation was observed to be spatially intermittent as a result of the high-speed compressibility dynamics taking place at the microscales. In addition, the large-scale pressure-dilatation work was found to be an essential mechanism for the conversion between thermal and kinetic energies. Moreover, the planar average of the large-scale pressure-dilatation work was found to be the difference between two large fluxes of opposite sign, which indicated some degree of cancellation between the compression and expansion waves in the mixing layer. A joint PDF of SGS dissipation and large-scale pressure-dilatation work was computed, which showed that backscatter occurs primarily in regions undergoing volumetric flow expansion. This implied the existence of an underlying physical mechanism that contributed to the reverse energy cascade.

Effects of SGS backscatter on the Boussinesq eddy viscosity were studied, and a regime diagram, demonstrating the relationship between the different energy-conversion modes and the sign of the eddy viscosity, was provided along with a detailed budget of volume fractions in each mode. A joint PDF of SGS dissipation and SGS dynamic-pressure dilatation work showed that high-speed compressibility effects induce a decorrelation between SGS backscatter and negative eddy viscosities which is not present in the low-speed regime. In particular, the decorrelation between backscatter and negative eddy viscosities increases for increasingly large values of the SGS Mach number and filter width.

Comparisons between reacting and inert mixing layers were conducted with regard to backscatter phenomena under dynamically-similar conditions and equal momentum thicknesses. Under these conditions, the combustion dynamics were found to have a marginal impact on the backscatter and flow-dilatation distributions, which were dominated by high-Mach-number effects. In this way, the main source of dilatation in the flow appeared to be the large-scale compressibility forcing that results from the opposing high-speed motion of the air and fuel streams. The additional dilatation caused by the chemical heat deposited by combustion at the microscales results in a negligible contribution. In fact, combustion in this supersonic mixing layer tends to reduce the high-speed compressibility effects because of an increase in the characteristic speed of sound. Therefore, the results of this study suggest that high-speed compressibility, rather than combustion, may be the key physical phenomenon that controls the energy-conversion dynamics relevant for the modelling of SGS turbulent fluxes in the reacting supersonic mixing layer in the diluted conditions studied in this work.

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FIGURE 14. Comparison of DNS of Pantano & Sarkar (2002) (dashed lines and ○ symbols) and present work (solid lines and □ symbols) for a non-reacting mixing layer at $Ma_C = 1.1$: (a) normalized momentum thickness $\delta_0/\delta^0_0$ and growth rate $\dot{\delta}_0/\delta^0_0$ (inset) as a function of the dimensionless time $tU/\delta^0_0$; (b) spatial distribution of turbulent production $\mathcal{P}$ and dissipation $\epsilon$ evaluated at $tU/\delta^0_0 = 475$, both values being normalized with $U^3/\delta_0$.

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Appendix A

The DNS of Pantano & Sarkar (2002) is used for numerical verification of the computational set-up described in § 2.4. The test case consists of a non-reacting, compressible, temporal mixing layer at a convective Mach number $Ma_C = 1.1$ (i.e. case A11 of Pantano & Sarkar (2002)). The turbulent mixing layer is formed between two gaseous streams of the same composition and at the same density and temperature flowing in opposite directions as depicted in figure 1.

The computational mesh described in § 2.4 was employed for the calculations. The initial and boundary conditions utilized in the computations were as described in § 2.2. The mixing layer was made to transition to a turbulent regime according to the method outlined in § 2.2, and evolved in time through the selfsimilar period, in which comparisons against first- and second-order statistics of Pantano & Sarkar (2002) were performed.

Figure 14(a) shows a good agreement between the results of Pantano & Sarkar (2002) and the present work in terms of the temporal evolution of the momentum thickness and its growth rate. A selfsimilar period is observed in the present simulation as indicated by the plateau in the growth rate shown in the inset of figure 14(a). Compared with the results reported by Pantano & Sarkar (2002), a 7% discrepancy in the normalized growth rate in the selfsimilar range is found in the present simulations.

The Reynolds-averaged rates of turbulent production $\mathcal{P} = \langle u_i^\prime u_k^\prime \partial u_i / \partial x_k \rangle$ and dissipation $\epsilon = \tau_{ik} \partial u_i^\prime / \partial x_k$, evaluated at the latest time of the present simulation, are shown in figure 14(b). It should be emphasized that the turbulent production and dissipation rates for the $Ma_C = 1.1$ case of Pantano & Sarkar (2002) are
time-averaged over the selfsimilar period (C. Pantano, Private communication, 2013) and computed using constant transport properties, whereas the results shown for the present simulations are planar-averaged values at a given instant of time (yet within the selfsimilar range) obtained using a different initialization procedure and temperature-dependent transport properties of gaseous nitrogen (N$_2$). In spite of these differences, there is a reasonable agreement between the two simulations.

Appendix B

The capabilities of the computational set-up described in § 2.4 for numerically resolving the flame in the present configuration are briefly described below. In particular, figure 15 shows the computational mesh superimposed on temperature and OH production-rate contours near stoichiometric conditions in the central region of the same midplane cut shown above in figure 5, where the flow velocity is predominantly in the positive streamwise direction at transonic Mach numbers. It is observed that there are typically a number of grid points across these reacting layers.

The conditional PDFs of temperature and reactant mass fractions in H-element mixture-fraction space (subject to preferential-diffusion and non-unity Lewis-number effects) are shown in figure 16 for the reacting simulations at the final momentum thickness $\delta^*_\theta$. The resulting statistics resemble a burning diffusion-flame structure with leakage of reactants, thereby indicating finite-rate chemistry effects caused by the small residence time of the reactants in the mixing layer, which is favourable for the numerical resolution of the flame.

In summary, these results suggest that the present numerical simulations employ an acceptable grid resolution for capturing the main combustion characteristics of this mixing layer.
Figure 16. Contours of the mixture-fraction-conditioned PDFs of (a) oxidizer mass fraction, (b) fuel mass fraction and (c) dimensionless temperature, with conditional mean (solid white lines) and mean ± standard deviation (white-dashed lines). Dark and light regions indicate, respectively, high and low probability.

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SGS backscatter in supersonic hydrogen–air turbulent mixing layers


