Simulation and flow physics of a shocked and reshocked high-energy-density mixing layer

Supplementary material

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Appendix G. Experimental data

This appendix collects the NIF experimental data used in the present study. Table 9 gives the axial shock position data—from three NIF shots—used to constrain the radiation temperature boundary conditions, as described in the main paper. As implemented in two of those NIF shots, the VISAR diagnostic returned the temporal history of shock speed in the quartz, not just the main-shock or reshock breakout time. Those histories were used qualitatively to improve the boundary-condition tuning process.

Table 10 gives the mixing-layer width data—from six NIF shots—used to constrain the interface initial perturbation. The target designs for those NIF shots were nominally identical; in particular, the nominal density of all foam components was $\rho_{L,\text{nom}} =$ 0.085 g cm⁻³. However, the foam densities in the actual targets exhibited deviations of ~ 0–15% from the nominal value, leading to variations in the main-shock and reshock velocities. For making comparisons with simulations using only the nominal density, we can estimate an adjusted experimental mixing-layer width $W_{\text{exp,adj}}$, which corrects for the off-nominal foam densities associated with the measured experimental mixing-layer width $W_{\text{exp,mea}}$:

$$\mathcal{W}_{\text{exp,adj}} = \mathcal{W}_{\text{exp,mea}} \left[1 + \frac{\mathcal{W}_{\text{sim}}(\rho_{L,\text{nom}}) - \mathcal{W}_{\text{sim}}(\rho_{L,\text{mea}})}{\mathcal{W}_{\text{sim}}(\rho_{L,\text{mea}})} \right].$$
(G1)

Here, $W_{\rm sim}$ is the simulated mixing-layer width, expressed as a function of foam density ρ_L and obtained from a series of 1-D simulations using a tuned Reynolds-averaged turbulence model (Morgan & Wickett 2015) to treat $\mathbb{M}_H - \mathbb{M}_L$ mixing. Those 1-D simulations are not detailed here, though they are based on the 1-D simulations described in the appendices of the main paper. The quantity $\rho_{L,\rm mea}$ is the averaged foam density in the NIF target, based on measured masses and volumes of the foam components. The adjustment of

ID	t_{exp}	$x_{h,\exp}$	Shock	Diagnostic
N180425-003	$\begin{array}{c} 10.7 \pm 0.2 \\ 30.3 \pm 0.1 \end{array}$	$550. \pm 10$	Main shock	VISAR
N170322-002		1819. ± 50	Main shock	X-ray radiography
N171024-004	$(2.3) \pm 0.2 \\ 30.3 \pm 0.1$	$4650. \pm 10$	Reshock	VISAR (inferred)
N170322-002		$1735. \pm 50$	Reshock	X-ray radiography

TABLE 9. Measurements of the axial shock positions $x_{h,exp}$ at several times t_{exp} in the Reshock Campaign experiments. Times are in ns and positions are in μ m. The measurements are from three different NIF shots, each referenced by an identifier (ID). The first shot, a focused study of the main drive, used the VISAR diagnostic (Celliers *et al.* 2004) to measure the main-shock breakout time. The second shot, a focused study of the reshock drive, used the VISAR diagnostic to infer the reshock breakout time, with the support of 1-D simulations not detailed here. The third shot used X-ray radiography to measure (Huntington *et al.* 2020) both the main shock and reshock positions in the foam region at a common instant in time. See the main paper for definitions of the main-shock and reshock breakout times. Experimental uncertainties in the values of time and position are estimates based on broad assessments of the diagnostic techniques, and they are not based on statistical analysis of ensembles.

ID	$t_{\rm exp}$	$\mathcal{W}_{\mathrm{exp,mea}}$	$\mathcal{W}_{\mathrm{exp,adj}}$	$d\mathcal{W}_{\exp}$ [±]
N170322-002	30.3	73.	73.	10.
N170322-003	36.3	78.	80.	12.
N161128-003	40.3	110.	120.	20.
N170220-002	42.3	116.	115.	11.
N161213-001	44.3	138.	141.	13.
N161129-001	48.3	126.	124.	12.

TABLE 10. Measured and adjusted values of the experimental mixing-layer width at several times $t_{\rm exp}$ in the Reshock Campaign experiments. Times are in ns and widths are in μ m. The data are from six different NIF shots, each referenced by an identifier (ID). The shots used nominally identical targets. For each time, $W_{\rm exp,mea}$ is the mixing-layer width measured using the X-ray radiography technique of Huntington *et al.* (2020); $W_{\rm exp,adj}$ is the mixing-layer width adjusted via (G1) to approximately account for as-built densities of the foam components; and $dW_{\rm exp}$ is an estimate of experimental uncertainty in the mixing-layer widths (including contributions of $\pm 10 \ \mu$ m associated with diagnostic uncertainty and ± 0 -10 μ m associated with deviation of the as-built foam densities from the nominal value). The experimental uncertainty on each time is estimated to be ± 0.1 ns. The uncertainties reported here are estimates, and they are not based on statistical analysis of ensembles. In the main paper, $W_{\rm exp}$ always refers to $W_{\rm exp,mea}$.

(G1) is crude. It does not account for two- or three-dimensional spatial variation of the foam density across multiple blocks in the target assembly.

We provide the adjusted experimental mixing-layer widths only to illustrate the potential impact of shot-to-shot variation in the experimental data. Pending further analysis, the values of $W_{exp,adj}$ reported in table 10 should be treated as preliminary, unlike the values of $W_{exp,mea}$. In the main paper, W_{exp} always refers to the measured data $W_{exp,mea}$.

Appendix H. Validity of the continuum assumption

This appendix provides evidence that the HED mixing layers in the present study are reasonably described by the formalisms of fluid mechanics. To test the validity of the continuum assumption, we estimate the Knudsen number $Kn = \lambda_{nn}/\mathcal{L}$, where λ_{nn} is the mean free path for ion–ion collisions in the mixing plasmas and \mathcal{L} is a characteristic macroscopic length. Generally, if $Kn \ll 1$, then the continuum assumption is valid and a full Boltzmann-equation analysis is unnecessary.

Consider a gas of identical hard-sphere particles, each with mass m. A simple relation can be derived for the mean free path λ in such a gas as a function of its viscosity μ . From kinetic theory, the mean free path for particle–particle collisions is (see Chapman & Cowling (1970, (5.21.4)) and McQuarrie (2000, (16.5) and discussion))

$$\lambda = \frac{1}{\pi n \, d^2 \sqrt{2}} \,, \tag{H1}$$

where $n = \rho/m$ is the number density, ρ is the density and d is the sphere diameter. An analytic approximation for the viscosity is (see Chapman & Cowling (1970, (10.21.1)) and McQuarrie (2000, (16.36) and (19.25)))

$$\mu = \frac{5}{16 d^2} \left(\frac{m k_b T}{\pi}\right)^{1/2},\tag{H2}$$

where T is the temperature and k_b is the Boltzmann constant ($\approx 1.381 \times 10^{-16} \text{ erg K}^{-1}$). Combining these results to eliminate d gives

$$\lambda = \frac{16\mu}{5\rho} \left(\frac{m}{2\pi k_b T}\right)^{1/2}.$$
 (H3)

The expression (H3) can be used to estimate λ_{nn} in the present study by using the mass of a single atom for m (computable from the atomic weight), the simulated ion temperature for T, the simulated density for ρ and the simulated viscosity for μ . We claim that this approach gives approximate order-of-magnitude values for λ_{nn} , despite the fact that the plasmas under consideration are not hard-sphere gases. This use of (H3) does partially account for HED phenomena via the viscosity model described in the main paper. In the shocked and reshocked mixing layers, λ_{nn} ranges from $\sim 3 \times 10^{-4}$ to $7 \times 10^{-4} \ \mu\text{m}$. By comparison, the mixing-layer width ranges from ~ 4 to 200 μm , the smallest characteristic wavelength in the initial $\mathbb{M}_H - \mathbb{M}_L$ interface perturbation is 2 μm and the standard deviation of the smallest initial perturbation component is $\sim 0.07 \ \mu\text{m}$. Therefore, Knudsen numbers based on various macroscopic lengths are indeed small, supporting the claim that a continuum Navier–Stokes-based methodology is reasonable.

Appendix I. Magnetohydrodynamic phenomena

The present study did not consider magnetohydrodynamic phenomena, i.e. the coupling of electric and magnetic fields with the fluid equations of motion. Magnetohydrodynamics can be important in turbulent flows of contemporary interest (Davidson 2015) and in HED plasmas generated at facilities like the NIF. This appendix provides quantitative support for the neglect of magnetohydrodynamics in the present study. We show that pressures associated with self-generated magnetic fields are small relative to total pressures in the mixing layer. This appendix uses the Gaussian (rather than SI) system of units.

Let E_i be the electric field, B_i the magnetic field, J_i the current density and r the resistivity. Then the electron momentum equation can be written as a generalized Ohm's law, after expressing the electron fluid velocity in terms of the current density and

neglecting electron inertia (Goldston & Rutherford 1995, (8.13)):

$$\mathsf{E}_{i} + \frac{1}{c_{o}} \epsilon_{ijk} \, u_{j} \mathsf{B}_{k} = \mathsf{r} \mathsf{J}_{i} + \frac{1}{e \, n_{e}} \left(\frac{1}{c_{o}} \, \epsilon_{ijk} \, \mathsf{J}_{j} \mathsf{B}_{k} - \frac{\partial p_{e}}{\partial x_{i}} \right). \tag{I1}$$

Faraday's law is (Goldston & Rutherford 1995, (8.16))

$$\epsilon_{ijk} \frac{\partial \mathsf{E}_j}{\partial x_k} = -\frac{1}{c_o} \frac{\partial \mathsf{B}_i}{\partial t}.$$
 (I2)

The magnetic field pressure is (Goldston & Rutherford 1995, (9.8))

$$\mathsf{p} = \frac{\mathsf{B}_i \mathsf{B}_i}{8\,\pi}.\tag{I3}$$

Here, as in the main paper, e is the charge of an electron ($\approx 4.803 \times 10^{-10}$ statcoulombs), n_e is the electron number density, p_e is the electron pressure and c_o is the speed of light in a vacuum. Suppose that $B_i = 0$ and $J_i = 0$. Then an estimate for the magnetic field self-generation rate is

$$\frac{\partial \mathsf{B}_i}{\partial t} \approx -\frac{c_o}{e \, n_e^2} \,\epsilon_{ijk} \,\frac{\partial p_e}{\partial x_j} \frac{\partial n_e}{\partial x_k}.\tag{I4}$$

We can use this relation to obtain order-of-magnitude estimates for the self-generated magnetic field pressures associated with the first shock and reshock traversals of the $\mathbb{M}_{H}-\mathbb{M}_{L}$ mixing layer, using pre- and post-shock p_{e} and n_{e} values at the mixing-layer edges; mixing-layer averages of local gradient scale lengths of density and total pressure; and traversal times based on the shock velocities. We assume, conservatively, that the gradients $\partial p_{e}/\partial x_{j}$ and $\partial n_{e}/\partial x_{k}$ are orthogonal. The procedure yields **p** values of $\sim 3 \times 10^{-5}$ and 0.04 Mbar for the first shock and reshock traversals, respectively. Since **p** is much less than total pressures in the mixing layer ($\sim 2-35$ Mbar), induced magnetic fields likely do not have a significant impact on the flow dynamics of interest.

Appendix J. Enstrophy analysis: supplementary results

To support the analysis of enstrophy in the main paper, recall the evolution equation

$$\frac{\partial}{\partial t} (\rho \Omega) + \frac{\partial}{\partial x_j} (\rho \Omega u_j) = \underbrace{\left(\rho \omega_j S_{ij} \omega_i\right)}_{\mathbb{E}_{\mathrm{I}}} + \underbrace{\left(-2 \rho \Omega \frac{\partial u_j}{\partial x_j}\right)}_{\mathbb{E}_{\mathrm{II}}} + \underbrace{\left(\frac{\omega_i}{\rho} \epsilon_{ijk} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k}\right)}_{\mathbb{E}_{\mathrm{III}}} + \underbrace{\left(\rho \omega_i \epsilon_{ijk} \frac{\partial}{\partial x_j} \left[\frac{1}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l}\right]\right)}_{\mathbb{E}_{\mathrm{III}}}.$$
(J1)

Figure 23 plots early- and late-time normalized mixing-layer integrals of each term on the right-hand side of (J1), from all three baseline simulations. The finest-resolution results were already presented in the main paper; they are shown again for comparison. See the associated discussion of mesh sensitivity in the main paper. A complete derivation of (J1) is provided below.



FIGURE 23. Evolution of the mixing-layer integrals of each term \mathbb{E}_{I} , ..., \mathbb{E}_{IV} in the enstrophy evolution equation (J 1), normalized by $\lfloor \rho \Omega \rfloor$, in the three baseline simulations. The figure headers state $\mathcal{N}_{yz,2}$ as defined in the main paper. Figures in the left column display early-time results before reshock, and figures in the right column display late-time results after reshock. The ordinate limits of the left-column figures are different from those of the right-column figures. The main paper defines the mixing-layer integral.

Appendix K. MDTKE analysis: supplementary results

To support the analysis of MDTKE in the main paper, recall the evolution equation

$$\frac{\partial}{\partial t} \left(\mathcal{K} \right) + \frac{\partial}{\partial x_{j}} \left(\mathcal{K} \, \tilde{u}_{j} \right) = \underbrace{\left(- \overline{\rho u_{i}^{\prime\prime} u_{j}^{\prime\prime}} \frac{\partial \tilde{u}_{i}}{\partial x_{j}} \right)}_{\mathbb{T}_{\mathrm{I}}} + \underbrace{\left(\overline{u_{i}^{\prime\prime}} \left[\frac{\partial \bar{\sigma}_{ij}}{\partial x_{j}} - \frac{\partial \bar{p}}{\partial x_{i}} \right] \right)}_{\mathbb{T}_{\mathrm{II}}} + \underbrace{\left(\overline{\rho^{\prime}} \frac{\partial u_{i}^{\prime\prime}}{\partial x_{i}} \right)}_{\mathbb{T}_{\mathrm{III}}} + \underbrace{\left(- \frac{\partial}{\partial x_{j}} \left[\frac{1}{2} \, \bar{\rho} \left(\widetilde{u_{i}^{\prime\prime} u_{i}^{\prime\prime\prime} u_{j}^{\prime\prime}} \right) + \overline{\rho^{\prime} u_{j}^{\prime\prime}} - \overline{\sigma_{ij}^{\prime} u_{i}^{\prime\prime}} \right] \right)}_{\mathbb{T}_{\mathrm{IV}}} + \underbrace{\left(- \overline{\sigma_{ij}^{\prime}} \frac{\partial u_{i}^{\prime\prime}}{\partial x_{j}} \right)}_{\mathbb{T}_{\mathrm{V}}}. \tag{K1}$$

Figure 24 plots early- and late-time normalized mixing-layer integrals of each term on the right-hand side of (K1), from all three baseline simulations. The finest-resolution results were already presented in the main paper; they are shown again for comparison. See the associated discussion of mesh sensitivity in the main paper. A complete derivation of (K1) is provided below.



FIGURE 24. Evolution of the mixing-layer integrals of each term $\mathbb{T}_{I}, ..., \mathbb{T}_{V}$ in the MDTKE evolution equation (K 1), normalized by $|\mathcal{K}|$, in the three baseline simulations. The figure headers state $\mathcal{N}_{yz,2}$ as defined in the main paper. Figures in the left column display early-time results before reshock, and figures in the right column display late-time results after reshock. The ordinate limits of the left-column figures are different from those of the right-column figures. The main paper defines the mixing-layer integral.

Appendix L. Fluid mechanics fundamentals

This appendix derives several important equations used in the present study. The exposition is based on graduate-level fluid mechanics textbooks (Aris 1962; Panton 2005), material on compressible turbulence (Liou & Shih 1991; Andreopoulos *et al.* 2000; Sagaut & Cambon 2008; Chassaing *et al.* 2010; Gatski & Bonnet 2013) and a mathematical methods textbook (Riley *et al.* 2006). Our goal is to clearly and succinctly develop— starting only from basic conservation laws and using consistent definitions and notation— the key equations governing vorticity, enstrophy, the Reynolds stress tensor and MDTKE. The derivations are intended for students or non-specialists.

L.1. Preliminaries

This appendix summarizes notation, definitions and identities from tensor mathematics and elementary fluid mechanics. For further explanation, see Aris (1962), Panton (2005) and Riley *et al.* (2006).

A vector \boldsymbol{a} is written in index notation as a_i . The summation convention for repeated indices is

$$a_i a_i \equiv a_1 a_1 + a_2 a_2 + a_3 a_3. \tag{L1}$$

Two important tensors are the Kronecker delta δ_{ij} (a symmetric second-order tensor, also called the substitution tensor or identity tensor) and the Levi-Civita symbol ϵ_{ijk} (an antisymmetric third-order tensor, also called the *permutation symbol* or the alternating unit tensor):

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases}$$
(L 2)

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) = (1, 2, 3), \ (2, 3, 1), \ \text{or} \ (3, 1, 2), \\ -1 & \text{if} \ (i, j, k) = (3, 2, 1), \ (2, 1, 3), \ \text{or} \ (1, 3, 2), \\ 0 & \text{otherwise.} \end{cases}$$
(L3)

A tensor is *symmetric* if the interchange of any two indices does not change the value of the component; a tensor is *antisymmetric* if the interchange of any two indices reverses the sign of the component, while leaving its absolute value unchanged (Aris 1962, §2.61). A useful identity is

$$\epsilon_{ijk} \epsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}. \tag{L4}$$

If **a** and **b** are vectors, then the cross product $c = a \times b$ is given by $c_i = \epsilon_{ijk} a_j b_k$.

Let \boldsymbol{u} be the fluid velocity vector. The *vorticity*, expressed in index and symbolic notation, is

$$\omega_i = \epsilon_{ijk} \frac{\partial u_k}{\partial x_j} \quad \Longleftrightarrow \quad \boldsymbol{\omega} = \boldsymbol{\nabla} \times \boldsymbol{u}. \tag{L5}$$

The symmetric deformation or rate of strain tensor is

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) . \tag{L 6}$$

The following identities hold, for any scalar ϕ (Aris 1962, §3.24):

$$\epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{\partial \phi}{\partial x_k} \right) = 0 \quad \iff \quad \boldsymbol{\nabla} \times (\boldsymbol{\nabla} \phi) = \boldsymbol{0} \,, \tag{L7}$$

$$\frac{\partial \omega_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\epsilon_{ijk} \frac{\partial u_k}{\partial x_j} \right) = 0 \quad \iff \quad \boldsymbol{\nabla} \cdot \boldsymbol{\omega} = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \boldsymbol{u}) = 0, \quad (L8)$$

$$u_j \frac{\partial u_i}{\partial x_j} = \epsilon_{ijk} \,\omega_j u_k + \frac{1}{2} \frac{\partial}{\partial x_i} \left(u_k u_k \right) \quad \iff \quad \left(\boldsymbol{u} \cdot \boldsymbol{\nabla} \right) \boldsymbol{u} = \boldsymbol{\omega} \times \boldsymbol{u} + \frac{1}{2} \boldsymbol{\nabla} \left(|\boldsymbol{u}|^2 \right). \quad (L 9)$$

Let T_{ij} be any tensor. Following Aris (1962, §2.45) and Panton (2005, §3.6), it can be written as a sum of symmetric and antisymmetric components:

$$T_{ij} = \underbrace{\frac{1}{2} (T_{ij} + T_{ji})}_{\text{symmetric}} + \underbrace{\frac{1}{2} (T_{ij} - T_{ji})}_{\text{antisymmetric}}$$
$$= [T_{ij}]_{\text{sym.}} + \frac{1}{2} \epsilon_{ijk} d_k, \qquad d_k = \epsilon_{klm} T_{lm}.$$
(L 10)

In particular, from the definitions above,

$$\frac{\partial u_i}{\partial x_j} = S_{ij} + \frac{1}{2} \epsilon_{ijk} \epsilon_{klm} \frac{\partial u_l}{\partial x_m} = S_{ij} - \frac{1}{2} \epsilon_{ijk} \epsilon_{klm} \frac{\partial u_m}{\partial x_l}$$
$$= S_{ij} - \frac{1}{2} \epsilon_{ijk} \omega_k.$$
(L 11)

If Q_{ij} is a symmetric tensor and R_{ij} is an antisymmetric tensor, then their inner product is zero:

$$Q_{ij}R_{ij} = 0. \tag{L12}$$

Consider any quantities a, b, c and d and any independent variable z. As noted by Liou & Shih (1991), the following identities are useful:

$$a\frac{\partial}{\partial z}(bc) + b\frac{\partial}{\partial z}(ac) = \frac{\partial}{\partial z}(abc) + ab\frac{\partial}{\partial z}(c), \qquad (L13)$$

$$a\frac{\partial}{\partial z}(b\,c\,d) + b\frac{\partial}{\partial z}(a\,c\,d) = \frac{\partial}{\partial z}(a\,b\,c\,d) + a\,b\frac{\partial}{\partial z}(c\,d)\,. \tag{L14}$$

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L.2. Equations of fluid motion

The continuity equation for conservation of mass is

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho \, u_j \right) = 0, \tag{L15}$$

where ρ is the density and u_i is the fluid velocity.

Define the substantial (or material) derivative as the sum of the local rate of change and the convective change (Panton 2005, $\S4.3$):

$$\frac{D(\cdot)}{Dt} \equiv \frac{\partial(\cdot)}{\partial t} + u_j \frac{\partial(\cdot)}{\partial x_j}.$$
 (L 16)

The Navier-Stokes equations for conservation of momentum (consisting of three scalar equations, one for each coordinate index i) are

$$\rho \, \frac{Du_i}{Dt} = \rho \, \frac{\partial u_i}{\partial t} + \rho \, u_j \frac{\partial u_i}{\partial x_j} = \frac{\partial \Sigma_{ij}}{\partial x_j},\tag{L17}$$

with

$$\Sigma_{ij} = -p\,\delta_{ij} + \sigma_{ij},\tag{L18}$$

$$\sigma_{ij} = 2\,\mu\,S_{ij} + \lambda\,\frac{\partial u_k}{\partial x_k}\,\delta_{ij} = 2\,\mu\left(S_{ij} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right),\tag{L19}$$

where Σ_{ij} is the stress tensor, p is the pressure, σ_{ij} is the deviatoric viscous stress tensor, μ is the shear viscosity and λ is the second viscosity coefficient. In (L 19), we have used the Stokes assumption that the thermodynamic and mechanical pressures are equal, which implies

$$\lambda = -\frac{2}{3}\,\mu.\tag{L20}$$

For a full discussion of the Stokes assumption, see Aris (1962, §5.24), Panton (2005, §6.1) and Gatski & Bonnet (2013, §2.2.1). Unless stated otherwise, in this supplementary material and in the main paper, the term *viscosity* refers to μ . Note that μ is sometimes called the *dynamic viscosity*, to distinguish it from the *kinematic viscosity* $\nu = \mu/\rho$ (Panton 2005, §7.7). The kinematic viscosity is also called the *momentum diffusivity*.

Let ϕ be any flow variable. From (L 15) and (L 16),

$$\rho \frac{D\phi}{Dt} = \rho \frac{\partial\phi}{\partial t} + \rho u_j \frac{\partial\phi}{\partial x_j} = \left[\frac{\partial}{\partial t} \left(\rho \phi\right) - \phi \frac{\partial\rho}{\partial t}\right] + \left[\frac{\partial}{\partial x_j} \left(\rho \phi u_j\right) - \phi \frac{\partial}{\partial x_j} \left(\rho u_j\right)\right]$$
$$= \frac{\partial}{\partial t} \left(\rho \phi\right) + \frac{\partial}{\partial x_j} \left(\rho \phi u_j\right) - \phi \left[\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho u_j\right)\right]$$
$$= \frac{\partial}{\partial t} \left(\rho \phi\right) + \frac{\partial}{\partial x_j} \left(\rho \phi u_j\right).$$
(L 21)

In particular,

$$\rho \frac{Du_i}{Dt} = \frac{\partial}{\partial t} \left(\rho \, u_i\right) + \frac{\partial}{\partial x_j} \left(\rho \, u_i u_j\right) \tag{L 22}$$

gives an alternate form of the Navier–Stokes equations:

$$\frac{\partial}{\partial t} \left(\rho \, u_i \right) + \frac{\partial}{\partial x_j} \left(\rho \, u_i u_j \right) = \frac{\partial \Sigma_{ij}}{\partial x_j}. \tag{L 23}$$

L.3. Evolution of vorticity

Take (L 17), apply the identity (L 9) and redefine indices:

Take the curl of this equation, i.e. apply the operator $\epsilon_{ijk} \partial(\cdot)_k / \partial x_j$ to all terms:

$$\underbrace{\underbrace{\epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{\partial u_k}{\partial t} \right)}_{(1)} + \underbrace{\epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\epsilon_{klm} \, \omega_l \, u_m \right)}_{(2)} = \underbrace{-\frac{1}{2} \epsilon_{ijk} \frac{\partial}{\partial x_j} \left[\frac{\partial}{\partial x_k} \left(u_m u_m \right) \right]}_{(3)} + \underbrace{\epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \Sigma_{kl}}{\partial x_l} \right)}_{(4)}.$$

Consider each of the numbered terms:

$$\begin{aligned} \widehat{\mathbf{1}} &= \frac{\partial}{\partial t} \left(\epsilon_{ijk} \frac{\partial u_k}{\partial x_j} \right) = \frac{\partial \omega_i}{\partial t}, \\ \widehat{\mathbf{2}} &= \frac{\partial}{\partial x_j} \left[\left(\delta_{il} \, \delta_{jm} - \delta_{im} \, \delta_{jl} \right) \omega_l \, u_m \right] \qquad [\text{from } (\mathbf{L} \, 4)] \\ &= \frac{\partial}{\partial x_j} \left(\omega_i \, u_j - \omega_j \, u_i \right) \\ &= \omega_i \, \frac{\partial u_j}{\partial x_j} + u_j \, \frac{\partial \omega_i}{\partial x_j} - \omega_j \, \frac{\partial u_i}{\partial x_j} - u_i \, \frac{\partial \omega_j}{\partial x_j} \\ &= \omega_i \, \frac{\partial u_j}{\partial x_j} + u_j \, \frac{\partial \omega_i}{\partial x_j} - \omega_j \, \frac{\partial u_i}{\partial x_j} \qquad [\text{from } (\mathbf{L} \, 8)] \,, \\ \widehat{\mathbf{3}} &= 0 \qquad [\text{from } (\mathbf{L} \, 7)] \,, \\ \widehat{\mathbf{4}} &= \frac{1}{\rho} \, \epsilon_{ijk} \, \frac{\partial^2 \Sigma_{kl}}{\partial x_j \partial x_l} - \frac{1}{\rho^2} \, \epsilon_{ijk} \, \frac{\partial \rho}{\partial x_j} \, \frac{\partial \Sigma_{kl}}{\partial x_l}. \end{aligned}$$

Combining all of these results, multiplying through by ρ and rearranging terms yields an evolution equation for vorticity (compare Gatski & Bonnet (2013, (2.11))):

$$\rho \frac{D\omega_i}{Dt} = \rho \frac{\partial \omega_i}{\partial t} + \rho u_j \frac{\partial \omega_i}{\partial x_j}
= \rho \frac{\partial u_i}{\partial x_j} \omega_j - \rho \frac{\partial u_j}{\partial x_j} \omega_i - \frac{1}{\rho} \epsilon_{ijk} \frac{\partial \rho}{\partial x_j} \frac{\partial \Sigma_{kl}}{\partial x_l} + \epsilon_{ijk} \frac{\partial^2 \Sigma_{kl}}{\partial x_j \partial x_l}.$$
(L 24)

The first term in the second line of (L 24) can be re-written as $\rho \omega_j S_{ij}$, after making use of the identity (L 11) and noting that $\epsilon_{ijk} \omega_j \omega_k = 0$ from the property (L 12). Thus,

an alternate form of the vorticity evolution equation is

$$\rho \frac{D\omega_i}{Dt} = \rho \frac{\partial\omega_i}{\partial t} + \rho u_j \frac{\partial\omega_i}{\partial x_j} = \rho \omega_j S_{ij} - \rho \frac{\partial u_j}{\partial x_j} \omega_i + \rho \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \Sigma_{kl}}{\partial x_l}\right).$$
(L25)

Using (L 18), the last term in (L 25) can be written as

$$\begin{split} \rho \,\epsilon_{ijk} \, \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \Sigma_{kl}}{\partial x_l} \right) &= \rho \,\epsilon_{ijk} \, \frac{\partial}{\partial x_j} \left[\frac{1}{\rho} \frac{\partial}{\partial x_l} \left(-p \,\delta_{kl} + \sigma_{kl} \right) \right] \\ &= \rho \,\epsilon_{ijk} \, \left[-\frac{1}{\rho} \frac{\partial}{\partial x_j} \left(\frac{\partial p}{\partial x_k} \right) + \frac{1}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} \right) \right] \\ &= -\epsilon_{ijk} \, \frac{\partial}{\partial x_j} \left(\frac{\partial p}{\partial x_k} \right) + \frac{1}{\rho} \,\epsilon_{ijk} \, \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \rho \,\epsilon_{ijk} \, \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} \right) \\ &= \frac{1}{\rho} \,\epsilon_{ijk} \, \frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \rho \,\epsilon_{ijk} \, \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l} \right) \quad \text{[from (L 7)]} \,. \end{split}$$

Consequently, one additional form of the vorticity evolution equation is (compare Chassaing *et al.* $(2010, \S 6.2.1, \text{ footnote } 1)$ and Andreopoulos *et al.* (2000, (12)))

$$\rho \frac{D\omega_i}{Dt} = \rho \frac{\partial\omega_i}{\partial t} + \rho u_j \frac{\partial\omega_i}{\partial x_j}
= \rho \omega_j S_{ij} - \rho \frac{\partial u_j}{\partial x_j} \omega_i + \frac{1}{\rho} \epsilon_{ijk} \frac{\partial\rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \rho \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial\sigma_{kl}}{\partial x_l}\right). \quad (L\,26)$$

L.4. Evolution of enstrophy

Following Andreopoulos et al. (2000) and Chassaing et al. (2010), define the enstrophy

$$\Omega = \frac{1}{2} \omega_i \omega_i. \tag{L27}$$

Note that some instead define Ω without the factor of 1/2. Multiply (L 26) by ω_i to obtain

$$\rho \,\omega_i \,\frac{D\omega_i}{Dt} = \rho \,\omega_i \,\frac{\partial \omega_i}{\partial t} + \rho \,u_j \,\omega_i \,\frac{\partial \omega_i}{\partial x_j}$$
$$= \rho \,\omega_j \,S_{ij} \,\omega_i - \rho \,\frac{\partial u_j}{\partial x_j} \,\omega_i \,\omega_i + \frac{\omega_i}{\rho} \,\epsilon_{ijk} \,\frac{\partial \rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \rho \,\omega_i \,\epsilon_{ijk} \,\frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial \sigma_{kl}}{\partial x_l}\right).$$

Observe that $\partial \Omega / \partial z = \omega_i \partial \omega_i / \partial z$ for $z = x_j$ or z = t. Consequently, the following is an evolution equation for enstrophy (compare Andreopoulos *et al.* (2000, (13))):

$$\rho \frac{D\Omega_i}{Dt} = \rho \frac{\partial\Omega}{\partial t} + \rho u_j \frac{\partial\Omega}{\partial x_j}$$
(L 28)
$$= \rho \omega_j S_{ij} \omega_i - 2\rho \Omega \frac{\partial u_j}{\partial x_j} + \frac{\omega_i}{\rho} \epsilon_{ijk} \frac{\partial\rho}{\partial x_j} \frac{\partial p}{\partial x_k} + \rho \omega_i \epsilon_{ijk} \frac{\partial}{\partial x_j} \left(\frac{1}{\rho} \frac{\partial\sigma_{kl}}{\partial x_l}\right).$$

L.5. Averaging operators

This appendix reviews the concept of statistical or ensemble averaging of a flow variable. The discussion is based principally on Chassaing *et al.* (2010, \S 5.1–5.3) and Gatski & Bonnet (2013, \S 3.1–3.3).

Consider a flow variable ϕ , which in general is a function of x_i and t. The *Reynolds* decomposition of ϕ is

$$\phi \equiv \overline{\phi} + \phi', \tag{L29}$$

with $\overline{\phi}$ the *Reynolds average* of ϕ and ϕ' the *Reynolds fluctuation* of ϕ . The Reynolds average $\overline{(\cdot)}$ is defined as a mean over an ensemble of flows. However, other types of operators are often used as surrogates for ensemble averaging in practice. For example, time averaging might be used for a statistically steady flow, or spatial averaging might be used for a flow that is statistically homogeneous in one or more coordinate directions. Pope (2000, §3.8), Sagaut & Cambon (2008, §2.2.1) and Gatski & Bonnet (2013, §3.1.1) discuss these ideas in more detail. In the present study, if the mixing layer is welldeveloped, then it is reasonable to assume statistical homogeneity in the two spanwise directions, but not in the axial direction. Hence, the present study defines the Reynolds average as the spatial average over the two spanwise directions.

The Favre decomposition of ϕ is

$$\phi \equiv \widetilde{\phi} + \phi'', \qquad \widetilde{\phi} \equiv \frac{\rho \, \phi}{\overline{\rho}}, \tag{L 30}$$

with ϕ the Favre (or mass-weighted) average of ϕ and ϕ'' the Favre (or mass-weighted) fluctuation of ϕ .

Following the literature, here it is always assumed that the Reynolds-averaging operator commutes with derivatives, e.g.

$$\frac{\partial\left(\cdot\right)}{\partial x_{i}} \equiv \frac{\partial\left(\cdot\right)}{\partial x_{i}}.$$
(L 31)

In general, an analogous commutativity property does not hold for the Favre-averaging operator:

$$\frac{\widetilde{\partial(\cdot)}}{\partial x_i} = \frac{1}{\bar{\rho}} \left(\overline{\rho \frac{\partial(\cdot)}{\partial x_i}} \right) \neq \frac{\partial}{\partial x_i} \left(\overline{\frac{\rho(\cdot)}{\bar{\rho}}} \right) = \frac{\partial(\widetilde{\cdot})}{\partial x_i}.$$
 (L 32)

The following identities hold:

$$\overline{\overline{\phi}} = \overline{\phi} \,, \qquad \overline{\overline{\phi}} = \widetilde{\phi} \,, \qquad \overline{\phi'} = 0 \,, \qquad \widetilde{\phi''} = 0 \,, \qquad \overline{\rho \, \phi''} = \overline{\rho} \, \widetilde{\phi''} = 0. \tag{L33}$$

Additional properties of the averaging operators are discussed by Chassaing *et al.* (2010, $\S5.3.5$).

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L.6. Reynolds averaging of the continuity equation

Consider the continuity equation (L 15) and substitute the Favre decomposition for u_j :

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left[\rho \left(\widetilde{u}_j + u_j'' \right) \right] = 0.$$

Apply the Reynolds-averaging operator to both sides of this equation to obtain

$$0 = \overline{\frac{\partial \rho}{\partial t}} + \overline{\frac{\partial}{\partial x_j} \left[\rho \left(\widetilde{u}_j + u_j' \right) \right]} = \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} \left(\bar{\rho} \, \widetilde{u}_j + \overline{\rho \, u_j''} \right) = \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} \left(\bar{\rho} \, \widetilde{u}_j \right).$$
(L 34)

L.7. Evolution of the mean momentum

From (L23) and (L18), the Navier–Stokes equations can be written as

$$\frac{\partial}{\partial t} \left(\rho \, u_i \right) + \frac{\partial}{\partial x_j} \left(\rho \, u_i u_j \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j}. \tag{L35}$$

Substitute the Favre decompositions for u_i and u_j and apply the Reynolds-averaging operator:

$$\frac{\overline{\partial}}{\partial t}\left[\rho\left(\widetilde{u}_{i}+u_{i}^{\prime\prime}\right)\right]+\overline{\frac{\partial}{\partial x_{j}}\left[\rho\left(\widetilde{u}_{i}+u_{i}^{\prime\prime}\right)\left(\widetilde{u}_{j}+u_{j}^{\prime\prime}\right)\right]}=-\overline{\frac{\partial p}{\partial x_{i}}}+\overline{\frac{\partial \sigma_{ij}}{\partial x_{j}}}$$

The left-hand side (LHS) and right-hand side (RHS) of this equation reduce to

$$\begin{aligned} \text{LHS} &= \frac{\partial}{\partial t} \left(\rho \, \widetilde{u}_i + \rho \, u_i'' \right) + \frac{\partial}{\partial x_j} \left(\rho \, \widetilde{u}_i \widetilde{u}_j + \rho \, \widetilde{u}_i u_j'' + \rho \, \widetilde{u}_j u_i'' + \rho \, u_i'' u_j'' \right) \\ &= \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_i + \overline{\rho \, u_i''} \right) + \frac{\partial}{\partial x_j} \left(\bar{\rho} \, \widetilde{u}_i \widetilde{u}_j + \widetilde{u}_i \, \overline{\rho \, u_j''} + \widetilde{u}_j \, \overline{\rho \, u_i''} + \overline{\rho \, u_i'' u_j''} \right) \\ &= \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_i \right) + \frac{\partial}{\partial x_j} \left(\bar{\rho} \, \widetilde{u}_i \widetilde{u}_j + \overline{\rho \, u_i'' u_j''} \right), \end{aligned}$$
$$\begin{aligned} \text{RHS} &= -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\sigma}_{ij}}{\partial x_j}. \end{aligned}$$

Combining these results and replacing j with k gives an evolution equation for the mean momentum $\bar{\rho} \, \tilde{u}_i$ (compare Chassaing *et al.* (2010, (5.25)) and Sagaut & Cambon (2008, (9.57))):

$$\frac{\partial}{\partial t}\left(\bar{\rho}\,\widetilde{u}_{i}\right) + \frac{\partial}{\partial x_{k}}\left(\bar{\rho}\,\widetilde{u}_{i}\widetilde{u}_{k}\right) = -\frac{\partial\bar{p}}{\partial x_{i}} + \frac{\partial}{\partial x_{k}}\left(\bar{\sigma}_{ik} - \overline{\rho\,u_{i}^{\prime\prime}u_{k}^{\prime\prime}}\right).\tag{L 36}$$

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L.8. Evolution of the Reynolds stress tensor

Multiply (L 36) by \tilde{u}_j (Liou & Shih 1991) to obtain

$$\widetilde{u}_{j} \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_{i} \right) + \widetilde{u}_{j} \frac{\partial}{\partial x_{k}} \left(\bar{\rho} \, \widetilde{u}_{i} \widetilde{u}_{k} \right) = -\widetilde{u}_{j} \frac{\partial \bar{p}}{\partial x_{i}} + \widetilde{u}_{j} \frac{\partial}{\partial x_{k}} \left(\bar{\sigma}_{ik} - \overline{\rho \, u_{i}^{\prime \prime} u_{k}^{\prime \prime}} \right). \tag{L37}$$

Interchange the indices i and j to obtain

$$\widetilde{u}_{i}\frac{\partial}{\partial t}\left(\bar{\rho}\,\widetilde{u}_{j}\right)+\widetilde{u}_{i}\frac{\partial}{\partial x_{k}}\left(\bar{\rho}\,\widetilde{u}_{j}\widetilde{u}_{k}\right)=-\widetilde{u}_{i}\frac{\partial\bar{p}}{\partial x_{j}}+\widetilde{u}_{i}\frac{\partial}{\partial x_{k}}\left(\bar{\sigma}_{jk}-\overline{\rho\,u_{j}''u_{k}''}\right).\tag{L38}$$

Add (L37) and (L38), collect terms and apply the identities (L13) and (L14):

$$\begin{bmatrix} \widetilde{u}_j \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_i \right) + \widetilde{u}_i \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_j \right) \end{bmatrix} + \begin{bmatrix} \widetilde{u}_j \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \widetilde{u}_i \widetilde{u}_k \right) + \widetilde{u}_i \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \widetilde{u}_j \widetilde{u}_k \right) \end{bmatrix} = \\ - \begin{bmatrix} \widetilde{u}_i \frac{\partial \bar{p}}{\partial x_j} + \widetilde{u}_j \frac{\partial \bar{p}}{\partial x_i} \end{bmatrix} + \begin{bmatrix} \widetilde{u}_j \frac{\partial}{\partial x_k} \left(\bar{\sigma}_{ik} - \overline{\rho} \, \overline{u}_i'' \overline{u}_k'' \right) + \widetilde{u}_i \frac{\partial}{\partial x_k} \left(\bar{\sigma}_{jk} - \overline{\rho} \, \overline{u}_j'' \overline{u}_k'' \right) \end{bmatrix}$$

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$$\begin{bmatrix} \frac{\partial}{\partial t} \left(\bar{\rho} \, \widetilde{u}_i \widetilde{u}_j \right) + \widetilde{u}_i \widetilde{u}_j \, \frac{\partial \bar{\rho}}{\partial t} \end{bmatrix} + \left[\frac{\partial}{\partial x_k} \left(\bar{\rho} \, \widetilde{u}_i \widetilde{u}_j \widetilde{u}_k \right) + \widetilde{u}_i \widetilde{u}_j \, \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \widetilde{u}_k \right) \end{bmatrix} = - \left[\widetilde{u}_i \, \frac{\partial \bar{p}}{\partial x_j} + \widetilde{u}_j \, \frac{\partial \bar{p}}{\partial x_i} \right] \\ + \left[\widetilde{u}_j \, \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \widetilde{u}_i \, \frac{\partial \bar{\sigma}_{jk}}{\partial x_k} \right] - \left[\widetilde{u}_j \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_k''} \right) + \widetilde{u}_i \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_j'' u_k''} \right) \right]$$

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$$\frac{\partial}{\partial t} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j \right) + \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j \tilde{u}_k \right) + \tilde{u}_i \tilde{u}_j \left[\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \tilde{u}_k \right) \right] = - \left[\tilde{u}_i \, \frac{\partial \bar{p}}{\partial x_j} + \tilde{u}_j \, \frac{\partial \bar{p}}{\partial x_i} \right] \\ + \left[\tilde{u}_j \, \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \tilde{u}_i \, \frac{\partial \bar{\sigma}_{jk}}{\partial x_k} \right] - \left[\tilde{u}_j \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_k''} \right) + \tilde{u}_i \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_j'' u_k''} \right) \right].$$

Applying (L 34) gives an evolution equation for $\bar{\rho} \, \tilde{u}_i \tilde{u}_j$:

$$\frac{\partial}{\partial t} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j \right) + \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j \tilde{u}_k \right) = - \left[\tilde{u}_i \, \frac{\partial \bar{p}}{\partial x_j} + \tilde{u}_j \, \frac{\partial \bar{p}}{\partial x_i} \right] + \left[\tilde{u}_j \, \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \tilde{u}_i \, \frac{\partial \bar{\sigma}_{jk}}{\partial x_k} \right] - \left[\tilde{u}_j \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_k''} \right) + \tilde{u}_i \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_j'' u_k''} \right) \right].$$
(L 39)

Next, consider again the Navier–Stokes equations (L 35). Replace j with k and multiply by u_j to obtain

$$u_j \frac{\partial}{\partial t} \left(\rho \, u_i\right) + u_j \frac{\partial}{\partial x_k} \left(\rho \, u_i u_k\right) = -u_j \frac{\partial p}{\partial x_i} + u_j \frac{\partial \sigma_{ik}}{\partial x_k}.$$
 (L 40)

Interchange the indices i and j to give

$$u_i \frac{\partial}{\partial t} \left(\rho \, u_j\right) + u_i \frac{\partial}{\partial x_k} \left(\rho \, u_j u_k\right) = -u_i \frac{\partial p}{\partial x_j} + u_i \frac{\partial \sigma_{jk}}{\partial x_k}.$$
 (L 41)

Following a procedure similar to the one used to obtain (L 39), add (L 40) and (L 41), collect terms and apply the identities (L 13) and (L 14):

$$\begin{split} \left[u_{j} \frac{\partial}{\partial t} \left(\rho u_{i} \right) + u_{i} \frac{\partial}{\partial t} \left(\rho u_{j} \right) \right] + \left[u_{j} \frac{\partial}{\partial x_{k}} \left(\rho u_{i} u_{k} \right) + u_{i} \frac{\partial}{\partial x_{k}} \left(\rho u_{j} u_{k} \right) \right] = \\ - \left[u_{i} \frac{\partial p}{\partial x_{j}} + u_{j} \frac{\partial p}{\partial x_{i}} \right] + \left[u_{j} \frac{\partial \sigma_{ik}}{\partial x_{k}} + u_{i} \frac{\partial \sigma_{jk}}{\partial x_{k}} \right] \\ \Downarrow \\ \left[\frac{\partial}{\partial t} \left(\rho u_{i} u_{j} \right) + u_{i} u_{j} \frac{\partial \rho}{\partial t} \right] + \left[\frac{\partial}{\partial x_{k}} \left(\rho u_{i} u_{j} u_{k} \right) + u_{i} u_{j} \frac{\partial}{\partial x_{k}} \left(\rho u_{k} \right) \right] = \\ - \left[u_{i} \frac{\partial p}{\partial x_{j}} + u_{j} \frac{\partial p}{\partial x_{i}} \right] + \left[u_{j} \frac{\partial \sigma_{ik}}{\partial x_{k}} + u_{i} \frac{\partial \sigma_{jk}}{\partial x_{k}} \right] \\ \downarrow \\ \frac{\partial}{\partial t} \left(\rho u_{i} u_{j} \right) + \frac{\partial}{\partial x_{k}} \left(\rho u_{i} u_{j} u_{k} \right) + u_{i} u_{j} \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{k}} \left(\rho u_{k} \right) \right] = \\ - \left[u_{i} \frac{\partial p}{\partial x_{j}} + u_{j} \frac{\partial p}{\partial x_{i}} \right] + \left[u_{j} \frac{\partial \sigma_{ik}}{\partial x_{k}} + u_{i} \frac{\partial \sigma_{jk}}{\partial x_{k}} \right] . \end{split}$$

Applying (L 15) gives an evolution equation for $\rho u_i u_i$:

$$\frac{\partial}{\partial t}\left(\rho \, u_i u_j\right) + \frac{\partial}{\partial x_k}\left(\rho \, u_i u_j u_k\right) = -\left[u_i \, \frac{\partial p}{\partial x_j} + u_j \, \frac{\partial p}{\partial x_i}\right] + \left[u_j \, \frac{\partial \sigma_{ik}}{\partial x_k} + u_i \, \frac{\partial \sigma_{jk}}{\partial x_k}\right]. \quad (L\,42)$$

Now substitute the Favre decompositions for u_i , u_j and u_k in (L 42) and apply the Reynolds-averaging operator:

$$\underbrace{\frac{\partial}{\partial t} \left[\rho \left(\widetilde{u}_i + u_i'' \right) \left(\widetilde{u}_j + u_j'' \right) \right]}_{(5)} + \underbrace{\frac{\partial}{\partial x_k} \left[\rho \left(\widetilde{u}_i + u_i'' \right) \left(\widetilde{u}_j + u_j'' \right) \left(\widetilde{u}_k + u_k'' \right) \right]}_{(6)} = \underbrace{\left[\left(\widetilde{u}_i + u_i'' \right) \frac{\partial p}{\partial x_j} + \left(\widetilde{u}_j + u_j'' \right) \frac{\partial p}{\partial x_i} \right]}_{(7)} + \underbrace{\left[\left(\widetilde{u}_j + u_j'' \right) \frac{\partial \sigma_{ik}}{\partial x_k} + \left(\widetilde{u}_i + u_i'' \right) \frac{\partial \sigma_{jk}}{\partial x_k} \right]}_{(8)}$$

Consider each of the numbered terms and substitute the Reynolds decompositions for p, σ_{ik} and $\sigma_{jk}:$

Combine all of these results to obtain

$$\begin{split} \frac{\partial}{\partial t} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j + \overline{\rho \, u_i'' u_j''} \right) + \frac{\partial}{\partial x_k} \left(\bar{\rho} \, \tilde{u}_i \tilde{u}_j \tilde{u}_k + \overline{\rho \, u_i'' u_j''} \, \tilde{u}_k \right) &= - \left[\tilde{u}_i \, \frac{\partial \bar{p}}{\partial x_j} + \tilde{u}_j \, \frac{\partial \bar{p}}{\partial x_i} \right] \\ &+ \left[\tilde{u}_j \, \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \tilde{u}_i \, \frac{\partial \bar{\sigma}_{jk}}{\partial x_k} \right] - \left[\tilde{u}_j \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_k''} \right) + \tilde{u}_i \, \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_j'' u_k''} \right) \right] \\ &- \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_j'' u_k''} \right) - \left[\overline{\rho \, u_i'' u_k''} \, \frac{\partial \tilde{u}_j}{\partial x_k} + \overline{\rho \, u_j'' u_k''} \, \frac{\partial \tilde{u}_i}{\partial x_k} \right] \end{split} \tag{L 43} \\ &- \left[\overline{u_i''} \, \frac{\partial \bar{p}}{\partial x_j} + \overline{u_j''} \, \frac{\partial \bar{p}}{\partial x_i} \right] - \left[\frac{\partial}{\partial x_j} \left(\overline{p' u_i''} \right) + \frac{\partial}{\partial x_i} \left(\overline{p' u_j''} \right) \right] + \left[\overline{p'} \, \frac{\partial u_i''}{\partial x_j} + \overline{p'} \, \frac{\partial u_j''}{\partial x_i} \right] \\ &+ \left[\overline{u_j''} \, \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \overline{u_i''} \, \frac{\partial \bar{\sigma}_{jk}}{\partial x_k} \right] + \left[\frac{\partial}{\partial x_k} \left(\overline{\sigma_{ik}' u_j''} \right) + \frac{\partial}{\partial x_k} \left(\overline{\sigma_{jk}' u_i''} \right) \right] \\ &- \left[\overline{\sigma_{ik}'} \, \frac{\partial u_j''}{\partial x_k} + \overline{\sigma_{jk}'} \, \frac{\partial u_i''}{\partial x_k} \right]. \end{split}$$

Subtracting (L39) from (L43) gives

$$\begin{split} \frac{\partial}{\partial t} \left(\overline{\rho \, u_i'' u_j''} \right) &+ \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_j''} \, \widetilde{u}_k \right) = -\frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_j'' u_k''} \right) - \left[\overline{\rho \, u_i'' u_k''} \, \frac{\partial \widetilde{u}_j}{\partial x_k} + \overline{\rho \, u_j'' u_k''} \, \frac{\partial \widetilde{u}_i}{\partial x_k} \right] \\ &- \left[\overline{u_i''} \, \frac{\partial \overline{p}}{\partial x_j} + \overline{u_j''} \, \frac{\partial \overline{p}}{\partial x_i} \right] - \left[\frac{\partial}{\partial x_j} \left(\overline{p' u_i''} \right) + \frac{\partial}{\partial x_i} \left(\overline{p' u_j''} \right) \right] + \left[\overline{p' \, \frac{\partial u_i''}{\partial x_j}} + \overline{p' \, \frac{\partial u_j''}{\partial x_i}} \right] \\ &+ \left[\overline{u_j''} \, \frac{\partial \overline{\sigma}_{ik}}{\partial x_k} + \overline{u_i''} \, \frac{\partial \overline{\sigma}_{jk}}{\partial x_k} \right] + \left[\frac{\partial}{\partial x_k} \left(\overline{\sigma_{ik}' u_j''} \right) + \frac{\partial}{\partial x_k} \left(\overline{\sigma_{jk}' u_i''} \right) \right] \\ &- \left[\overline{\sigma_{ik}'} \, \frac{\partial u_j''}{\partial x_k} + \overline{\sigma_{jk}'} \, \frac{\partial u_i''}{\partial x_k} \right]. \end{split}$$

Rearranging terms yields an evolution equation for the *Reynolds stress tensor* $\overline{\rho u''_i u''_j} = \overline{\rho u''_i u''_j}$ (compare Sagaut & Cambon (2008, (9.62)), Chassaing *et al.* (2010, (5.36) and (11.1)) and Gatski & Bonnet (2013, (5.23) and (5.24))):

$$\frac{\partial}{\partial t} \left(\overline{\rho \, u_i'' u_j''} \right) + \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_j''} \, \widetilde{u}_k \right) = - \left[\overline{\rho \, u_i'' u_k''} \, \frac{\partial \widetilde{u}_j}{\partial x_k} + \overline{\rho \, u_j'' u_k''} \, \frac{\partial \widetilde{u}_i}{\partial x_k} \right] \tag{L44}$$

$$+ \overline{p' \left(\frac{\partial u_i''}{\partial x_j} + \frac{\partial u_j''}{\partial x_i} \right)} - \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_j'' u_k''} + \delta_{jk} \, \overline{p' u_i''} + \delta_{ik} \, \overline{p' u_j''} - \overline{\sigma_{ik}' u_j''} - \overline{\sigma_{jk}' u_i''} \right)$$

$$+ \left[\overline{u_i''} \left(\frac{\partial \overline{\sigma}_{jk}}{\partial x_k} - \frac{\partial \overline{p}}{\partial x_j} \right) + \overline{u_j''} \left(\frac{\partial \overline{\sigma}_{ik}}{\partial x_k} - \frac{\partial \overline{p}}{\partial x_i} \right) \right] - \left[\overline{\sigma_{ik}'} \, \frac{\partial u_j''}{\partial x_k} + \overline{\sigma_{jk}'} \, \frac{\partial u_i''}{\partial x_k} \right].$$

L.9. Evolution of MDTKE

Define the local turbulent kinetic energy (LTKE)

$$\mathcal{I} = \frac{1}{2} u_i'' u_i'',\tag{L45}$$

and the mean density-weighted turbulent kinetic energy (MDTKE)

$$\mathcal{K} = \frac{1}{2} \overline{\rho \, u_i'' u_i''} = \frac{1}{2} \, \overline{\rho} \, \widetilde{u_i'' u_i''} = \overline{\rho} \, \widetilde{\mathcal{I}}. \tag{L46}$$

Set i = j in (L 44), performing a tensor contraction:

$$\frac{\partial}{\partial t} \left(\overline{\rho \, u_i'' u_i''} \right) + \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_i''} \, \widetilde{u}_k \right) = -2 \overline{\rho \, u_i'' u_k''} \frac{\partial \widetilde{u}_i}{\partial x_k} + 2 \overline{p' \, \frac{\partial u_i''}{\partial x_i}} \\ - \frac{\partial}{\partial x_k} \left(\overline{\rho \, u_i'' u_i'' u_k''} + 2 \, \delta_{ik} \, \overline{p' u_i''} - 2 \, \overline{\sigma_{ik}' u_i''} \right) + 2 \, \overline{u_i''} \left(\frac{\partial \overline{\sigma}_{ik}}{\partial x_k} - \frac{\partial \overline{p}}{\partial x_i} \right) - 2 \, \overline{\sigma_{ik}' \frac{\partial u_i''}{\partial x_k}}.$$

With (L 46), redefining indices yields an evolution equation for MDTKE (compare Chassaing *et al.* (2010, (10.52)) and Gatski & Bonnet (2013, (5.25) and (5.26))):

$$\frac{\partial}{\partial t} (\mathcal{K}) + \frac{\partial}{\partial x_j} (\mathcal{K} \,\widetilde{u}_j) = -\overline{\rho \, u_i'' u_j''} \frac{\partial \widetilde{u}_i}{\partial x_j} + \overline{u_i''} \left(\frac{\partial \overline{\sigma}_{ij}}{\partial x_j} - \frac{\partial \overline{p}}{\partial x_i} \right) + \overline{p' \, \frac{\partial u_i''}{\partial x_i}} \qquad (L\,47)$$

$$- \frac{\partial}{\partial x_j} \left[\frac{1}{2} \,\overline{\rho} \left(\widetilde{u_i'' u_i'' u_j''} \right) + \overline{p' u_j''} - \overline{\sigma_{ij}' u_i''} \right] - \overline{\sigma_{ij}' \, \frac{\partial u_i''}{\partial x_j}}.$$

L.10. Computational considerations for MDTKE

When analyzing terms on the right-hand side of (L 47) in the mixing layers of the present study, we find that numerical results are generally smoother when they are computed from Reynolds averages of gradients, instead of gradients of Reynolds averages, of the flow variables. (However, the two approaches do give comparable results, and they are analytically equivalent in the infinite-resolution limit.) For example, we compute the mean velocity gradient via

$$\frac{\partial \widetilde{u}_i}{\partial x_j} = \frac{1}{\bar{\rho}} \bigg(\overline{\rho \frac{\partial u_i}{\partial x_j}} + \overline{u_i \frac{\partial \rho}{\partial x_j}} - \widetilde{u}_i \, \overline{\frac{\partial \rho}{\partial x_j}} \bigg).$$

Also, for analysis of (L 47), it is convenient to express Reynolds and Favre averages of fluctuations in terms of Reynolds averages of flow variables computed directly in the simulation. The following identities are helpful:

$$\begin{split} \widetilde{u}_{i} &= \frac{\overline{\rho \, u_{i}}}{\overline{\rho}} , \qquad \overline{u_{i}''} = \overline{u_{i} - \widetilde{u}_{i}} = \overline{u}_{i} - \widetilde{u}_{i} , \\ \overline{\rho \, u_{i}'' u_{j}''} &= \overline{\rho \, (u_{i} - \widetilde{u}_{i}) \, (u_{j} - \widetilde{u}_{j})} = \overline{\rho \, u_{i} u_{j}} - \overline{\rho \, u_{i}} \, \frac{\overline{\rho \, u_{j}}}{\overline{\rho}} - \overline{\rho \, u_{j}} \, \frac{\overline{\rho \, u_{i}}}{\overline{\rho}} + \overline{\rho} \, \frac{\overline{\rho \, u_{i}}}{\overline{\rho}} \, \frac{\overline{\rho \, u_{j}}}{\overline{\rho}} \\ &= \overline{\rho \, u_{i} u_{j}} - \frac{(\overline{\rho \, u_{i}}) \, (\overline{\rho \, u_{j}})}{\overline{\rho}} , \qquad \mathcal{K} = \frac{1}{2} \left[\overline{\rho \, u_{i} u_{i}} - \frac{(\overline{\rho \, u_{i}}) \, (\overline{\rho \, u_{i}})}{\overline{\rho}} \right] , \\ \overline{\rho} \, (\widetilde{u_{i}'' u_{i}'' u_{j}''}) &= \frac{1}{2} \, \overline{\rho \, u_{i}' u_{i}'' u_{j}''} = \frac{1}{2} \, \overline{\rho \, (u_{i} - \widetilde{u}_{i}) \, (u_{i} - \widetilde{u}_{i}) \, (u_{j} - \widetilde{u}_{j})} \\ &= \frac{1}{2} \left(\overline{\rho \, u_{i} u_{i} u_{j}} - \widetilde{u}_{j} \, \overline{\rho \, u_{i} u_{i}} - \widetilde{u}_{i} \, \overline{\rho \, u_{i} u_{j}} + \widetilde{u}_{i} \widetilde{u}_{i} \, \overline{\rho \, u_{i}} \\ &- \widetilde{u}_{i} \, \overline{\rho \, u_{i} u_{j}} + \widetilde{u}_{i} \widetilde{u}_{j} \, \overline{\rho \, u_{i}} + \widetilde{u}_{i} \widetilde{u}_{i} \, \overline{\rho \, u_{j}} - \overline{\rho} \, \widetilde{u}_{i} \widetilde{u}_{i} \widetilde{u}_{j} \right) \\ &= \frac{1}{2} \, \overline{\rho \, u_{i} u_{i} u_{j}} - \frac{1}{2} \, \widetilde{u}_{j} \, \overline{\rho \, u_{i} u_{i}} - \widetilde{u}_{i} \, \overline{\rho \, u_{i} u_{j}} + \overline{\rho} \, \widetilde{u}_{i} \widetilde{u}_{i} \widetilde{u}_{j} \, , \end{split}$$

 $\frac{1}{2}$

$$\overline{p'u_j''} = \overline{p'(u_j - \tilde{u}_j)} = \overline{(p - \bar{p})u_j} - \overline{p'\tilde{u}_j} = \overline{pu_j} - \bar{p}\overline{u}_j,$$

$$\overline{p'\frac{\partial u_i''}{\partial x_i}} = \overline{(p - \bar{p})\frac{\partial}{\partial x_i}(u_i - \tilde{u}_i)} = \overline{p\frac{\partial u_i}{\partial x_i}} - \overline{p}\frac{\partial \tilde{u}_i}{\partial x_i} - \overline{p}\frac{\partial \overline{u}_i}{\partial x_i} + \overline{p}\frac{\partial \tilde{u}_i}{\partial x_i}$$

$$= \overline{p\frac{\partial u_i}{\partial x_i}} - \overline{p}\frac{\partial \overline{u}_i}{\partial x_i},$$

$$\overline{\sigma'_{ij}u_i''} = \overline{(\sigma_{ij} - \bar{\sigma}_{ij})(u_i - \tilde{u}_i)} = \overline{\sigma_{ij}u_i} - \overline{\sigma}_{ij}\tilde{u}_i - \overline{\sigma}_{ij}\overline{u}_i + \overline{\sigma}_{ij}\tilde{u}_i = \overline{\sigma_{ij}u_i} - \overline{\sigma}_{ij}\overline{u}_i,$$

$$\overline{\sigma'_{ij}\frac{\partial u_i''}{\partial x_j}} = \overline{(\sigma_{ij} - \bar{\sigma}_{ij})\frac{\partial}{\partial x_j}(u_i - \tilde{u}_i)} = \overline{\sigma_{ij}\frac{\partial u_i}{\partial x_j}} - \overline{\sigma}_{ij}\frac{\partial \tilde{u}_i}{\partial x_j} - \overline{\sigma}_{ij}\frac{\partial \overline{u}_i}{\partial x_j} + \overline{\sigma}_{ij}\frac{\partial \tilde{u}_i}{\partial x_j}$$

$$= \overline{\sigma_{ij}\frac{\partial u_i}{\partial x_j}} - \overline{\sigma}_{ij}\frac{\partial \overline{u}_i}{\partial x_j}.$$

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