

# Scalar-energy spectra in simulations of $Sc \gg 1$ mixing by turbulent jets using the nonlinear large-eddy simulation method

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The nonlinear large-eddy simulation (nLES) method is applied to the first numerical study of passive-scalar mixing by a turbulent shear flow at a high Schmidt number ( $Sc \gg 1$ ). The work is intended to address inconsistencies between previous studies concerning the formation of power-law scaling in the scalar-energy spectra at viscous-convective scales. Results are reported for LES of a round turbulent jet at  $Sc=1024$  and  $Re_D=2000$ . The nLES method is first shown to recover the large-scale jet structure, including the self-similarity of far-field scalar moments. Scalar timeseries and spatial data produce the first power spectra from a LES shear-flow study that exhibits  $k^{-1}$  scaling at viscous-convective scales, consistent with the analysis of Batchelor [J. Fluid Mech. **5**, 113 (1959)] and recent direct numerical studies of simpler  $Sc \gg 1$  flows. © 2008 American Institute of Physics. [DOI: 10.1063/1.2921017]

High Schmidt-number mixing of passive scalars by turbulent jets, where  $Sc \equiv \nu/D \gg 1$  is the ratio of the kinematic viscosity to the scalar diffusivity, is important in many applications, such as the mixing of dyes in liquids, nutrient and heat transport in rivers and oceans, and pollutant dispersion.<sup>1,2</sup>

Such flows may give rise to a viscous-convective subrange, where mixing dynamics may depart from the  $Sc \approx 1$  case. Analytical work by Batchelor<sup>3</sup> and Kraichnan<sup>4</sup> famously predicted scalar-energy power-law scaling in the viscous-convective range as  $E_\phi(k) \sim \langle \chi \rangle \langle \gamma \rangle^{-1} k^{-1}$ , with  $\chi$  the total scalar-dissipation rate and  $\gamma$  the most compressive principal-strain rate. Attempts to verify such  $k^{-1}$  scaling, however, have produced conflicting results. Thus, an experimental study of mixing in a round turbulent jet at  $Sc \approx 2000$  reported no evidence of  $k^{-1}$  behavior at viscous-convective scales,<sup>5</sup> while recent direct numerical simulations (DNS) at  $Sc \leq 1024$  have produced  $k^{-1}$  scaling over a decade of scales.<sup>2</sup> However, the simpler flow configurations and lower  $Re_\lambda$  of the DNS studies make direct comparison with the experimental results somewhat problematic.

In this light, large-eddy simulation (LES), in which the larger turbulent scales are calculated explicitly while the smaller scales are modeled, may provide a more efficient alternative for studying  $Sc \gg 1$  mixing, if the LES can accurately reproduce the dynamics of scalar mixing at the scales of interest. Recently, nonlinear LES (nLES) has reproduced important characteristics of  $Sc \gg 1$  mixing by homogeneous turbulence, including the first scalar spectra from a LES exhibiting  $k^{-1}$  scaling in the viscous-convective range.<sup>6</sup> Here, the nLES method is extended to the first LES study of  $Sc \gg 1$  mixing by a turbulent free-shear flow, in this case an incompressible round jet, with the principal focus on evaluating scalar-energy spectral scalings at viscous-convective scales.

The hallmark of the nLES method is the direct calculation of the nonlinear stress  $u_i u_j$  in the filtered Navier–Stokes momentum equation,

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \bar{u}_i u_j + \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} - \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} = 0, \quad (1)$$

where

$$\bar{u}_i u_j \equiv \bar{u}_i \bar{u}_j + \overline{u_i u_j^{\text{sgs}}} + \overline{u_i^{\text{sgs}} u_j} + \overline{u_i^{\text{sgs}} u_j^{\text{sgs}}}, \quad (2)$$

and the direct calculation of the nonlinear scalar flux  $\overline{u_j \phi}$  in the filtered advection-diffusion equation,

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial}{\partial x_j} \bar{u}_j \bar{\phi} - D \frac{\partial^2 \bar{\phi}}{\partial x_j \partial x_j} = 0, \quad (3)$$

where

$$\bar{u}_j \bar{\phi} \equiv \bar{u}_j \bar{\phi} + \overline{u_j \phi^{\text{sgs}}} + \overline{u_j^{\text{sgs}} \bar{\phi}} + \overline{u_j^{\text{sgs}} \phi^{\text{sgs}}}, \quad (4)$$

using multifractal models for the subgrid fields  $u_j^{\text{sgs}}$  and  $\phi^{\text{sgs}}$ .<sup>7,6</sup> By calculating Eqs. (2) and (4) in their original forms as *nonlinear advective stresses*, the nLES method better models the nonlinear mechanism responsible for equilibrium-range mixing in actual hydrodynamic turbulence than many traditional LES approaches that rely upon *linear artificial-viscous or -diffusive* closures. Numerical errors are controlled by an adaptive-backscatter limiter developed in Refs. 6 and 8 that reduces the magnitude of selected inertial stresses and scalar fluxes in Eqs. (2) and (4) responsible for backscatter of kinetic and scalar energies.

The numerical scheme consists of a standard pressure-correction algorithm on a regular, staggered Cartesian mesh, where  $N=128^2 \times 384$ . Spatial derivatives are discretized us-

TABLE I. Centerline viscous and diffusive length scales  $\lambda_\nu$  and  $\lambda_D$ , respectively, from nLES simulation at  $Re_D=2000$  and  $Sc=1024$ , indicating that only the scalar field is under-resolved in the simulation.

$x/D$	$Re_\lambda$	$\lambda_\nu/\Delta$	$\lambda_D/\Delta$
15	33	13	0.07
20	27	17	0.09
25	23	20	0.10
30	20	22	0.11