The nonlinear large-eddy simulation method applied to Sc≈1 and Sc≫1 passive-scalar mixing

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The nonlinear large-eddy simulation (nLES) method is extended here to simulations of $\mathrm{Sc}\approx 1$ and $\mathrm{Sc}\gg 1$ turbulent mixing of passive-scalar fields. These are the first LES studies to reproduce the instantaneous structure of the scalar-energy field $\bar{\phi}^2(\mathbf{x},t)$ at viscous-convective scales in the high Schmidt-number regime. The simulations employ a refinement of the nLES method with multifractal modeling first proposed by G. C. Burton and W. J. A. Dahm [Phys. Fluids **17**, 075111 (2005)]. In this approach, the nonlinear inertial stresses $\overline{u_i u_j}$ in the filtered Navier–Stokes equation and the nonlinear scalar fluxes $\overline{u_j \phi}$ in the filtered advection-diffusion equation are calculated directly, using multifractal models for the subgrid velocity and scalar fields, u_j^{sgs} and ϕ^{sgs}. Resolved energy levels are controlled by a new adaptive backscatter limiter that adjusts locally to changing flow conditions consistent with the mechanism governing energy transfer in actual hydrodynamic turbulence. No artificial viscosity or diffusivity closures are applied and no explicit de-aliasing is performed. The nLES approach is shown to simulate accurately $\mathrm{Sc}\approx 1$ mixing for flows between $\mathrm{Re}_\lambda \approx 35$ and 4100, the highest Re_λ tested. Characteristics of the resulting scalar field are examined, including the turbulence-to-scalar time-scale ratio and total scalar variance $\langle \phi'^2 \rangle$, indicating good agreement with prior studies. Simulations between $\mathrm{Sc}=8$ and 8192 produce the first scalar-energy spectra from an LES that exhibit k^{-1} scaling in the viscous-convective range, consistent with the analytical prediction of G. K. Batchelor [J. Fluid Mech. **5**, 113 (1959)]. The simulations indicate decreasing scalar anisotropy and increasing intermittency with increasing Schmidt number, also consistent with prior studies. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2840199]

I. INTRODUCTION

Passive-scalar mixing by turbulence is important to a wide range of engineering and scientific applications. Recent study has indicated that turbulent mixing is a complex process, differing in substantial respects from the underlying turbulence to which it is coupled. For example, scalar fields may become intermittent when mixed by weakly or nonturbulent flows,[1] as well as display persistent small-scale anisotropy when subjected to large-scale anisotropic forcing, contrary to the universality assumptions underlying Kolmogorov theory.[2,3] These and other differences may be particularly apparent at high Schmidt number, where the scalar diffusivity D is significantly smaller than the kinematic viscosity ν, i.e., where $\mathrm{Sc}\equiv \nu/D \gg 1$.[4,5] Sufficiently disparate viscosities and diffusivities give rise to a viscous-convective subrange, characterized by a wide separation between the viscous and diffusive scales, where $\lambda_\nu \gg \lambda \gg \lambda_D$. Since vorticity is essentially uniform in this scale range, further mixing occurs only through compressive straining of the turbulence, which tends to steepen scalar gradients, and the scalar diffusivity, which tends to reduce gradients. Such dynamics may give rise to unique characteristics of mixing in this scale range, including the possible scaling of the scalar-energy spectrum as $E_\phi(k) \sim k^{-1}$, as predicted by Batchelor.[6] Conclusive experimental and numerical support for such scaling, however, has remained elusive, and prior investigations have yielded inconsistent results.[7,8] Other characteristics, such as persistent scalar anisotropy and small-scale intermittency, appear to be functions of the Schmidt number,[8] although the exact nature of these dependencies remains unclear. Such factors make $\mathrm{Sc}\gg 1$ mixing a focus of current research.

Direct numerical simulation (DNS) has proven useful for studying passive-scalar mixing, but is limited in the case of $\mathrm{Sc}\gg 1$ flows by the need to resolve scales significantly smaller than λ_ν. A more efficient method for conducting such studies, therefore, may be through large-eddy simulation (LES), where only the larger turbulent scales are calculated explicitly, while the smaller scales are modeled. However, few LES studies of $\mathrm{Sc}\gg 1$ mixing have appeared in the literature,[9–11] and none has focused on the dynamics of scalar mixing at viscous-convective scales.

Recently, nonlinear LES (nLES) has been demonstrated as a physically-based method for conducting large-eddy simulations.[12,13] The hallmark of the nLES method is the direct calculation of the nonlinear term $\overline{u_i u_j}$ in the filtered Navier–Stokes momentum equation,

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

where

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

using a multifractal model for the subgrid velocities u_j^{sgs} that appear in Eq. (2). By modeling the unclosed term in its origi-

