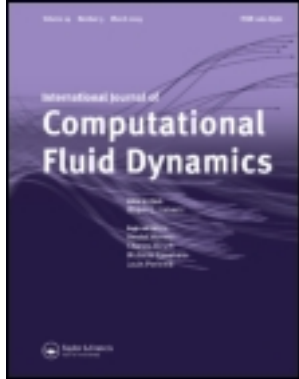


This article was downloaded by: [Washington University in St Louis], [Jonathan I. Katz]

On: 18 May 2012, At: 08:58

Publisher: Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



International Journal of Computational Fluid Dynamics

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gcfd20>

A von Neumann-Smagorinsky turbulent transport model for stratified shear flows

Bryan M. Johnson^a, Jonathan I. Katz^{a b c} & Oleg Schilling^a

^a Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA, 94551, USA

^b Department of Physics and McDonnell Center for the Space Sciences, Washington University, St. Louis, MO, 63130, USA

^c Los Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM, 87545, USA

Available online: 18 May 2012

To cite this article: Bryan M. Johnson, Jonathan I. Katz & Oleg Schilling (2012): A von Neumann-Smagorinsky turbulent transport model for stratified shear flows, International Journal of Computational Fluid Dynamics, 26:3, 173-179

To link to this article: <http://dx.doi.org/10.1080/10618562.2012.670226>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.tandfonline.com/page/terms-and-conditions>

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

A von Neumann–Smagorinsky turbulent transport model for stratified shear flows

Bryan M. Johnson^a, Jonathan I. Katz^{a,b,c,*} and Oleg Schilling^a

^aLawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551, USA; ^bDepartment of Physics and McDonnell Center for the Space Sciences, Washington University, St. Louis, MO 63130, USA; ^cLos Alamos National Laboratory, P. O. Box 1663, Los Alamos, NM 87545, USA

(Received 2 November 2011; final version received 18 February 2012)

A simple subgrid turbulent diffusion model based on an analogy to the von Neumann–Richtmyer artificial viscosity is explored for use in modelling mixing in turbulent stratified shear flow. The model may be more generally applicable to multicomponent turbulent hydrodynamics and to subgrid turbulent transport of momentum, composition and energy. As in the case of the von Neumann artificial viscosity and many subgrid-scale models for large-eddy simulation, the turbulent diffusivity explicitly depends on the grid size and is not based on a quantitative model of the unresolved turbulence. In order to address the issue that it is often not known *a priori* when and where a flow will become turbulent, the turbulent diffusivity is set to zero when the flow is expected to be stable on the basis of a Richardson/Rayleigh–Taylor stability criterion, in analogy to setting the von Neumann artificial viscosity to zero in expanding flows. One-dimensional predictions of this model applied to a simple shear flow configuration are compared to those obtained using a K – ε model. The density and velocity profiles predicted by both models are shown to be very similar.

Keywords: stratified flow; shear flow; turbulence modelling; transport coefficients; turbulent diffusion

1. Introduction

Turbulent diffusion in heterogeneous or multicomponent flows and turbulent heat transport in general is nearly ubiquitous and of great importance. Direct numerical simulation of these flows that resolves all spatiotemporal scales present is likely to long remain infeasible. The finer scales of heterogeneity are still large enough that microscopic transport processes (diffusion, viscosity and conductivity) do not smooth out the variations in the corresponding physical variables. It is then important to have a phenomenological, efficient and computationally robust algorithm that well describes the onset and effects of turbulence on the resolved flow.

When the composition of the fluid is heterogeneous the most important questions usually concern mixing of material of different compositions or in different phases (Dimotakis 2005), rather than turbulent momentum transfer. A number of two-equation Reynolds-averaged Navier–Stokes (RANS) turbulent transport models have been developed, including a K – ε model (Gauthier and Bonnet 1990) and a K – ℓ model (Dimonte and Tipton 2006), as well as extensions of such models such as the BHR model (Besnard *et al.* 1992) that account for all sources driving instability and turbulence (including shear) through their derivation from

the fluid dynamics equations and closure. These models can be complex to implement because they describe the evolution of turbulence with non-local and history-dependent functions of space and time. Alternatively, the success of the simple von Neumann artificial viscosity (von Neumann and Richtmyer 1950), still frequently used in Lagrangian numerical simulations of compressible flow, suggests that a similarly simple model of turbulent transport may be useful.

2. General considerations

The elementary Kolmogorov phenomenology (Tennekes and Lumley 1972) indicates an eddy turnover time $\tau_k \propto k^{-2/3}$ for eddy size $\sim 1/k$. Hence if the flow is turbulent, small eddies turn over much faster than larger ones. Assuming at least one turnover time for the largest driving eddies, there will be rapid mixing of a turbulent region down to its inner turbulence scale. Turbulent heat transport is analogous. If the Schmidt number

$$Sc \equiv \frac{\nu}{D}, \quad (1)$$

or Prandtl number

$$Pr \equiv \frac{\nu}{\alpha}, \quad (2)$$

*Corresponding author. Email: katz@wuphys.wustl.edu

(where ν is the kinematic viscosity, D is the diffusivity of composition and α is the diffusivity of temperature; the thermal diffusivity that couples these two scalar fields is customarily ignored) is of order unity or less, then diffusive mixing or heat transfer on scales smaller than the inner turbulence scale will be at least as rapid as the turnover of the smallest eddies, and much more rapid than that of the driving eddies. This is usually the case in dilute gases and weakly coupled liquids because momentum, thermal energy and composition are substantially carried by the same particles and $\text{Pr} = \mathcal{O}(1)$.

In a plasma, momentum is almost entirely carried by the ions and energy by the electrons; at high Reynolds number all of these quantities diffuse on the inner turbulence scale much faster than the turnover of the driving eddies. In liquid metals or ionised plasmas, rapid thermal conduction by electrons or rapid radiative transfer lead to $\text{Pr} \ll 1$ and this inequality holds even more strongly. Only in viscous liquids in which strong intermolecular forces carry momentum are $\text{Pr}, \text{Sc} \gg 1$ possible and the efficacy of diffusive heat transport and mixing on scales smaller than the inner turbulence scale is problematic.

In the classical Kolmogorov turbulent cascade, the inner scale of turbulence is approximated by the Kolmogorov dissipation scale $\ell_d \approx (\nu^3/\varepsilon)^{1/4}$, where ν is the kinematic viscosity and $\varepsilon \sim V^3/L$ is the kinetic energy dissipation per unit volume of a turbulent flow with characteristic velocity V at an outer scale L . This leads to an estimate of the timescale for microscopic diffusion to produce atomic-scale homogeneity

$$t_{\text{diff}} \approx \frac{\ell_d^2}{D} \approx \text{Sc} \sqrt{\frac{\nu L}{V^3}} \approx \frac{\text{Sc}}{\sqrt{\text{Re}}} \tau, \quad (3)$$

where the Reynolds number is $\text{Re} = VL/\nu$ and the turnover time is $\tau \equiv L/V$. In large Reynolds number flows, microscopic (diffusive) mixing on length scales from ℓ_d down to atomic dimensions is a very rapid process unless $\text{Sc} \gg 1$. An analogous result with Sc replaced by Pr holds for deviations from uniform temperature.

Only if $\text{Sc} \gg 1$ may diffusion down to the molecular or atomic scale be slower than the turbulent turnover timescale. For example, for ionic solutes in water typically $\text{Sc} = \mathcal{O}(300)$. In viscous liquids, such as pitch and the Earth's mantle, the Schmidt number may be orders of magnitude larger because strong intermolecular forces raise the viscosity and lower the diffusivity; momentum diffuses rapidly but chemical composition slowly. Viscous fluids may undergo turbulent large Reynolds number flows if driven strongly enough. In these cases the existence of turbulence is not sufficient to guarantee rapid mixing on the atomic scale, and the

atomic-scale mixing time, which determines rates of chemical reactions, must be evaluated for the parameters of interest.

3. Criterion for whether a flow is turbulent

In order to model subgrid diffusion in fluids with $\text{Sc} \lesssim 1$ when small-scale flow features cannot feasibly be resolved computationally, a criterion to determine where and when the flow are turbulent, as well as a model for turbulent mixing, are needed. It is often not possible to perform an instability analysis because of the complexity and non-stationary character of the large-scale flow. The automatic recognition within a numerical hydrodynamics code that a complex flow is turbulent and will support a turbulent cascade to large wave numbers and subgrid scales, much less the determination of its characteristics, is non-trivial. This limits the usefulness of even the most sophisticated turbulent transport models.

As the turnover of eddies and microscopic diffusion on scales $\ll \ell_d$ are generally much faster than the lifetime of the flow, which is generally $\mathcal{O}(\tau)$, determining whether a flow is turbulent is much more important than a quantitative estimate of the turbulent diffusion coefficient itself. Criteria that require decision of *whether a flow is turbulent* are not useful in a numerical simulation in which the structure of the flow is not known in advance. A simple and automatic turbulence criterion is required. Without knowing if a flow is turbulent or not, it is not possible even to decide if a turbulence model should be used at all.

The model explored here uses a criterion for turbulent transport based on the Richardson stability criterion appropriate to large Reynolds number shear flow, tacitly assuming that instability leads to turbulence. If there is no shear it reverts to the Rayleigh–Taylor stability criterion for inviscid miscible fluids, $\vec{\nabla}\rho \cdot \vec{\nabla}p > 0$, generalising the criterion used in a K - ℓ model of turbulence produced by Rayleigh–Taylor and Richtmyer–Meshkov instability (Dimonte and Tipton 2006). An implicit criterion is present in the BHR model (Besnard *et al.* 1992) in which the mean velocity field drives or damps turbulence. While such a criterion for turbulence is not needed in simulations of flows (such as unstratified pipe flows) that are known to be unstable *a priori* at sufficiently high Reynolds numbers, it is essential in more complex heterogeneous flows containing both stable and unstable regions that are not predictable in advance. The criterion is analogous to setting the von Neumann artificial viscosity to zero in rarefying regions.

An analogous subgrid-scale (SGS) turbulence model was first proposed by Smagorinsky (1963) for use in large-eddy simulation (LES) of atmospheric

flows in which small-scale turbulence is numerically unresolved, and was further discussed elsewhere (Deardorff 1971, Ramshaw 1979). Many SGS models have subsequently been developed (Lesieur and Métais 1996, Pullin 2000, Kosović *et al.* 2002, Lesieur *et al.* 2005, Sagaut 2006, You and Moin 2007), but none appear to be universally applicable. The model considered here is similar in spirit to the von Neumann artificial viscosity model for dissipation in unresolved shocks (von Neumann and Richtmyer 1950). We renounce any attempt to model the SGS turbulence in detail or on the basis of fundamental principles, just as von Neumann and Richtmyer (1950) renounced any attempt to understand the microscopic dissipation mechanisms and structure of shocks (which also depend on the particular fluids involved, so that no single model can be generally valid). Any back-scatter of turbulent energy to larger scales has only a slight effect on the rapidity of turbulent mixing. Following their example, a model is constructed that instead depends explicitly on the numerical properties of the LES, while incorporating a criterion for instability and the *presence* of turbulence and turbulent diffusivity that depends on the resolved properties of the flow.

4. Turbulent diffusivity model

Modelling turbulent diffusivity has much in common with modelling shocks in compressible flows. In each case the difficulty is posed by subgrid dissipative processes that cannot be resolved computationally but are known to be present. The classic solution to the shock problem (von Neumann and Richtmyer 1950) is to define an ‘artificial viscosity’ that is explicitly dependent on the grid size (thus broadening a shock to a width of a few resolution elements) and introducing a nonlinear criterion for its presence, in essence a switch that turns it on when the fluid is being compressed and off when being rarefied (because in thermodynamically stable systems there are no rarefaction shocks). The resulting artificial viscosity is strongly nonlinear and has the unphysical property that it depends on the computational grid scale (as do most SGS models). It has been widely adopted because it accurately reproduces the shock jump conditions, at the expense of not reproducing the structure of the shock on the scale of the grid resolution or it’s (much finer and unresolved) microscopic structure.

An analogous heuristic artificial turbulent diffusivity for multicomponent flows explored here is

$$D_t = \begin{cases} 0 & \text{if } \text{Ri} \geq \frac{1}{4} \\ \frac{\Delta^2 |S_{ij}|}{3} & \text{if } \text{Ri} < \frac{1}{4} \end{cases}, \quad (4)$$

where the local Richardson number is

$$\text{Ri} = -\frac{\vec{a} \cdot \vec{\nabla} \rho'}{\rho' |S_{ij}|^2}, \quad (5)$$

\vec{a} is the local fluid acceleration,

$$S_{ij} \equiv \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{1}{3} \delta_{ij} \frac{\partial v_k}{\partial x_k}, \quad (6)$$

is the traceless symmetrised strain-rate tensor (Landau and Lifschitz 1959, Batchelor 2000), $|S_{ij}| \equiv \sqrt{2 S_{ij} S_{ij}}$, the gradient of potential density is defined (only $\vec{\nabla} \rho'$ is meaningful, not ρ' itself)

$$\vec{\nabla} \rho' \equiv \vec{\nabla} \rho - \frac{\partial \rho}{\partial p} \Big|_{\vec{\nabla} p}, \quad (7)$$

where the partial derivative is evaluated under thermodynamic conditions (isothermal, isentropic or intermediate, depending on rates of energy exchange) appropriate to matter displacements, and Δ is a characteristic (filter) length scale (often chosen in SGS modelling as $\sim 2\Delta x$, where Δx is the grid spacing); summation over repeated indices is implied. The correction (second) term in Equation (7) may be important when the scale of pressure variation is comparable to that of density, as in stratified geophysical and astrophysical flows in chemically homogeneous fluids (atmosphere, ocean, stars and fluid planets). In such fluids, large density gradients may not stabilise a shear flow because the fluid is nearly isentropic and the density gradient is offset by a pressure gradient; the troposphere is a familiar example.

This D_t is chosen in analogy to the Smagorinsky model of large-eddy simulation (see Galperin and Orszag 1993 for a review). The switch at $\text{Ri}=1/4$ is chosen because this is the usual Richardson criterion, here generalised (in accord with the equivalence principle of relativity) to allow for acceleration parallel to the density gradient in place of gravity. The form of D_t follows from dimensional considerations.

The factor of 1/3 allows for three spatial dimensions (in analogy with the factor 1/3 in the kinetic theory result $D = \nu \ell / 3$, where ℓ is the mean free path). If fitting data are available it may be appropriate to introduce an additional dimensionless multiplicative factor chosen to match those data. Such data may, for example, be obtained from a fine-scale but idealised three-dimensional numerical simulation of turbulent mixing in an unstratified isochoric (constant and uniform density) fluid.

The switch is adapted from the Richardson instability criterion (Turner 1973, Linden 1979, Drazin

and Reid 2004) in stratified fluids by using in Equation 5 the component of local acceleration $-\vec{a}$ along the gradient of potential density in place of the stratifying acceleration of gravity \vec{g} . If a flow is nearly adiabatic on displacement time scales, this is $\frac{\partial \rho}{\partial p}|_S$, while if it is nearly isothermal (as will be the case if conductive or radiative energy transfer to a heat bath is rapid) it is $\frac{\partial \rho}{\partial p}|_T$. Stratification can stabilise either the Rayleigh–Taylor or Kelvin–Helmholtz instability.

This criterion ignores the stabilising effect of viscosity, which is small at large Reynolds numbers and complicated when both shear and stratification affect stability. At smaller numerical Reynolds numbers (defined by the zone size), numerical viscosity is significant but is implicit in a numerical code. When this is the case, SGS turbulence is not manifested because the numerical viscosity rapidly smooths velocity gradients; provided $Sc = \mathcal{O}(1)$, molecular diffusivity is rapid and no turbulent diffusivity model is required. If $Sc \gg 1$ diffusion may be calculated explicitly and deterministically from the resolved flow field.

A number of heuristic prescriptions for Δ in Equation (4) have been used (Cabot and Moin 1993, Ferziger 1993, Piomelli 1993). Without detailed experimental data in complex and difficult to diagnose flows, it is difficult to decide which is most appropriate, and the best prescription may vary over space and time. We suggest that Δ be taken to be the smallest dimension of a two- or three-dimensional spatial zone. High aspect ratio zones are generally used only to resolve large gradients of composition or other variables in the direction of the smallest side of a zone; these smallest sides are likely to limit mixing lengths.

Alternative forms of the artificial turbulent diffusivity are possible. For example, a tensor D_{ij} could be defined by replacing $|S_{ij}|$ by S_{ij} in the expression for D_t . However, if the cascade isotropises the turbulence, as generally assumed in the absence of a more quantitative model, then D_t should be a scalar. When this model is applied in an Eulerian simulation, it is assumed that an interface-preserving algorithm is used to prevent rapid numerical diffusion of composition that may be spurious (for example, if the stratification is stable).

5. Comparison with the predictions of a Reynolds-averaged Navier–Stokes model

Ideally, the model would be compared with the results of DNS. Unfortunately, because turbulence is intrinsically three-dimensional, even if the flow giving rise to it is one-dimensional, DNS at Reynolds numbers large enough to make numerical viscosity negligible is not feasible. For this reason, the effects of turbulence are

modelled by comparing the predictions of the proposed new model to a well-known RANS model.

Here, the predictions of the simplified subgrid model are compared to those from a standard K – ε model in a one-dimensional simulation of a stratified shear flow (Johnson and Schilling 2011a,b). The code used to evolve both models was an implementation of the ZEUS algorithm (Stone and Norman 1992) widely used in the astrophysical community. It evolves the one-dimensional Euler equations using a time explicit finite-difference method with Van Leer advection, along with additional terms appropriate to each model. The fluid quantities vary in the x -direction, with y being the direction of the shear velocity. An equation for both the density

$$\frac{d\rho}{dt} = \frac{\partial}{\partial x} \left(D_t \frac{\partial \rho}{\partial x} \right), \quad (8)$$

and the velocity

$$\rho \frac{dv_y}{dt} = \frac{\partial}{\partial x} \left(\rho D_t \frac{\partial v_y}{\partial x} \right) \quad (9)$$

is solved in the simplified model, where $d/dt = \partial/\partial t + v_x \partial/\partial x$, D_t is given in Equation (4) with $\Delta = \Delta x = L/N$ (L is the size of the computational domain and N is the number of grid cells in this one-dimensional calculation), and the magnitude of the one-component strain-rate tensor is $|S_{ij}| = |\partial v_y/\partial x|$.

The equations solved in the K – ε model are (Gauthier and Bonnet 1990)

$$\bar{\rho} \frac{d\bar{v}_y}{dt} = \frac{\partial}{\partial x} \left(\mu_t \frac{\partial \bar{v}_y}{\partial x} \right), \quad (10)$$

$$\begin{aligned} \frac{dK}{dt} = & \left[\left(\frac{\partial \bar{v}_y}{\partial x} \right)^2 - \frac{1}{\sigma_\rho \bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial x} \frac{\partial \bar{p}}{\partial x} + \frac{4}{3} \left(\frac{\partial \bar{v}_x}{\partial x} \right)^2 \right] v_t \\ & - \frac{2}{3} \frac{\partial \bar{v}_x}{\partial x} K - \varepsilon + \frac{1}{\bar{\rho}} \frac{\partial}{\partial x} \left(\mu_t \frac{\partial K}{\partial x} \right), \end{aligned} \quad (11)$$

$$\begin{aligned} \frac{d\varepsilon}{dt} = & \frac{\varepsilon}{K} \left[C_{\varepsilon 1} \left(\frac{\partial \bar{v}_y}{\partial x} \right)^2 - \frac{C_{\varepsilon 0}}{\sigma_\rho \bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial x} \frac{\partial \bar{p}}{\partial x} + \frac{4}{3} \left(\frac{\partial \bar{v}_x}{\partial x} \right)^2 \right] v_t \\ & - \frac{2}{3} \frac{\partial \bar{v}_x}{\partial x} \varepsilon - C_{\varepsilon 2} \frac{\varepsilon^2}{K} + \frac{1}{\bar{\rho}} \frac{\partial}{\partial x} \left(\mu_t \frac{\partial \varepsilon}{\partial x} \right), \end{aligned} \quad (12)$$

where

$$v_t = \frac{\mu_t}{\bar{\rho}} = C_\mu \frac{K^2}{\varepsilon} \quad (13)$$

is the turbulent viscosity, K is the turbulent kinetic energy, ε is the turbulent kinetic energy dissipation

rate, $\bar{p} = \bar{\rho}R\tilde{T}$ is the mean pressure (R is the universal gas constant), \tilde{T} is the mean temperature, and σ_ρ , σ_K , σ_ε , $C_{\varepsilon 1}$ and C_μ are positive dimensionless coefficients. An overbar denotes a Reynolds average and a tilde denotes a Favre average (density-weighted Reynolds average $\tilde{\phi} = \overline{\rho\phi}/\bar{\rho}$), each over the turbulent region.

The density and shear velocity were initialised with smoothly-varying profiles that transition between high and low constant values at the boundaries of the computational domain:

$$\rho(x) = \rho_L + (\rho_H - \rho_L)\sigma\left(\frac{x - L/2}{x_0}\right), \quad (14)$$

$$v_y(x) = -\frac{Mc_L}{2} + Mc_L\sigma\left(\frac{x - L/2}{x_0}\right), \quad (15)$$

where the light and heavy fluids have density ρ_L and ρ_H , respectively, the function

$$\sigma(z) \equiv \frac{1}{1 + e^{-z}} \quad (16)$$

smoothly interpolates between zero and one, c_L is the sound speed in the low-density fluid, and M is the Mach number in the low-density fluid. The pressure was initialised to hydrostatic equilibrium with a body force $g\rho$:

$$p(x) = p_L + g\left[\rho_L\left(x - \frac{L}{2}\right) + (\rho_H - \rho_L)x_0 \times \ln\left(1 + e^{\frac{x-L/2}{x_0}}\right)\right], \quad (17)$$

where $p_L = c_L^2\rho_L/\gamma$. The particular values chosen for the calculations were $\rho_L = 1$, $\rho_H = 2$, $C_L = 10$, $\gamma = 5/3$, $M = 0.1$ (so that the flow was nearly incompressible), $L = 1$, $x_0 = 0.5L$, and $N = 100$. Based on the Richardson criterion, this profile is unstable for $0.434L \lesssim x \lesssim 0.6L$. The coefficients of the $K-\varepsilon$ model were set to $C_\mu = 0.09$, $C_{\varepsilon 0} = 1.1$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$ and $\sigma_K = \sigma_\varepsilon = \sigma_U = 0.7$. Most of these coefficient values are standard and based upon comparison to experiment (Chen and Jaw 1998, Pope 2000, Durbin and Petterson Reif 2001). A value of $\sigma_\rho = 0.427$ was used to obtain growth for a Richardson number less than 0.25, and the initial conditions were set to $K_0 = 10^{-4}$ and $\varepsilon_0 = 10^{-5}$.

Figures 1 and 2 show profiles from evolving the initial profiles described above until the density and shear velocity have diffused by approximately the same amount. The times of comparison are arbitrary because the time at which diffusion becomes important in a $K-\varepsilon$ model is dependent upon the assumed initial turbulence level, and the diffusion time scale in the

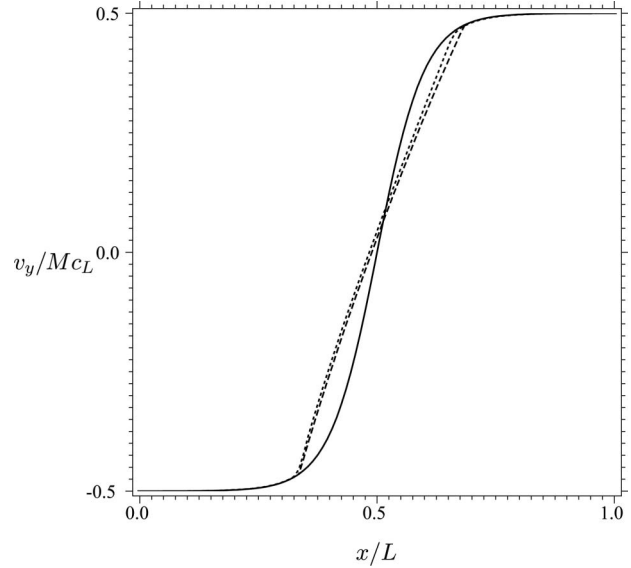


Figure 1. Profiles of v_y for the unstable profile described in the text normalised by Mc_L . The solid line is the initial profile, the dashed line is the final result from the von Neumann–Smagorinsky transport model and the dotted line is the final result from the $K-\varepsilon$ model.

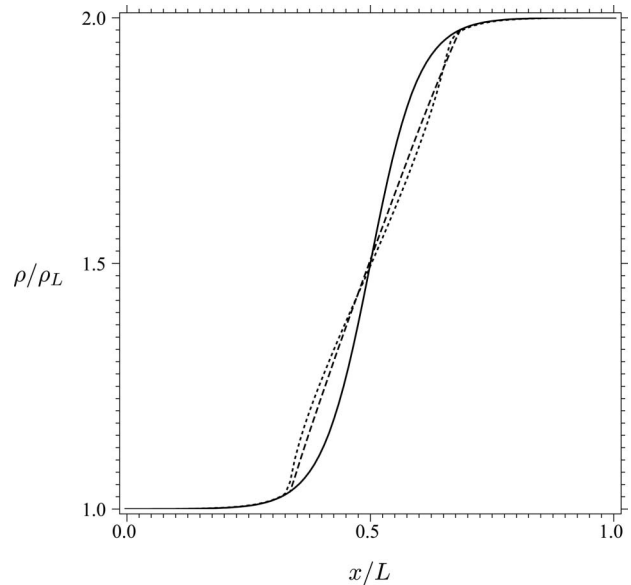


Figure 2. Profiles of ρ for the unstable profile described in the text normalised by ρ_L . The solid line is the initial profile, the dashed line is the final result from the von Neumann–Smagorinsky transport model and the dotted line is the final result from the $K-\varepsilon$ model.

simple von Neumann–Smagorinsky model is a function of the numerical resolution.

The simplified model provides reasonable results that are quite similar to those from the more complex,

well-established $K-\varepsilon$ model. The effects of the turbulence switch in the simplified model are apparent in its linear (within the previously turbulent region) density profile in Figure 2 that is determined by the instability criterion and the velocity profile. It does not show the curvature of the density profile found by the $K-\varepsilon$ model that is a consequence of the overshoot of turbulence (and more effective mixing) beyond nominal stability in the region of steepest initial velocity gradient and strongest instability. Our local and instantaneous model cannot include these non-local and non-instantaneous effects, but they make only small differences in the final result.

6. Discussion

Turbulent mixing is a long-standing problem and many models have been introduced. Typically they involve several adjustable coefficients, and these may be chosen to give excellent fits in regions of parameter space for which appropriate data are available. For example, the BHR model (Besnard *et al.* 1992, Ulitsky *et al.* 2001) contains 10 coefficients chosen to fit a classic shock tube experiment. With so many parameters available the fit is excellent, but that does not establish its validity when extrapolated outside the range of conditions to which they were fitted. For many important problems no data exist in the parameter range of interest, and a simple model may be more robust than a sophisticated one. It is also likely to be simpler to implement and to run faster.

Subgrid turbulent viscosity and heat transport present problems analogous to that of subgrid turbulent mixing. Sophisticated models exist, but also contain several coefficients in the closures of the moment equations. If Sc is not too large, it may be a reasonable approximation to use the model proposed here for D_t and to take $v_t = Sc_t D_t$, estimating Sc_t from numerical simulations like those used to test the model for D_t , or simply taking the widely adopted value $Sc_t = 0.7$ in the absence of such information. Similarly, it may be reasonable to take $\alpha_t = D_t$.

If atomic-scale diffusion of composition is important and $Sc \gg \sqrt{Re}$, then it is necessary to introduce a more complete description than uniform mixing to describe the state of the fluid because turbulence effects a uniform (on an atomic scale) distribution of momentum faster than diffusion effects a uniform distribution of composition. For example, each fluid element in the turbulently mixed region may be described as containing fractions f_i , proportional to their contribution to the mass mixed by the turbulence, of each of the compositions contributing to the turbulently mixed region. The composition β_1, \dots, β_n of each fraction f_i , where the β_j denote individual

elements or chemical species, would relax towards uniform mixing with a characteristic time given by t_{diff} from Equation 3. In general, t_{diff} would depend on the β_j and be different for each j because distinct species have different microscopic D and Sc .

Acknowledgements

We thank G. Dimonte, P. E. Dimotakis, R. A. Gore, L. G. Margolin, D. I. Meiron and G. B. Zimmerman for useful discussions. JIK thanks the Los Alamos National Laboratory and the Lawrence Livermore National Laboratory for hospitality. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and by Los Alamos National Laboratory under contract DE-AC52-06NA25396.

References

- Batchelor, G.K., 2000. *An introduction to fluid dynamics*. Cambridge: Cambridge University Press.
- Besnard, D.C., *et al.*, 1992. *Turbulence transport equations for variable-density turbulence and their relationship to two-field models*. Los Alamos National Laboratory Report LA-12303-MS. Los Alamos, NM: Los Alamos National Laboratory.
- Cabot, W. and Moin, P., 1993. *Large eddy simulation of scalar transport with the dynamic sub-grid scale model*. In: B. Galperin and S.A. Orszag, eds. *Large eddy simulations of complex engineering and geophysical flows*. Cambridge: Cambridge University Press, 141–158.
- Chen, C.-J. and Jaw S.-Y., 1998. *Combustion: an international series. Fundamentals of turbulence modeling*. London: Taylor and Francis.
- Deardorff, J.W., 1971. On the magnitude of the subgrid scale eddy coefficient. *Journal of Computational Physics*, 7, 120–133.
- Dimonte, G. and Tipton, R., 2006. $K-L$ turbulence model for the self-similar growth of the Rayleigh-Taylor and Richtmyer-Meshkov instabilities. *Physics of Fluids*, 18, 085101.
- Dimotakis, P.E., 2005. Turbulent mixing. *Annual Review of Fluid Mechanics*, 37, 329–356.
- Drazin, P.G. and Reid, W.H., 2004. *Hydrodynamic stability*. 2nd ed. Cambridge: Cambridge University Press.
- Durbin, P.A. and Petterson Reif, B.A., 2001. *Statistical theory and modeling for turbulent flows*. New York: Wiley.
- Ferziger, J.H., 1993. *Sub-grid scale modeling*. In: Galperin, B. and Orszag, S. A., eds. *Large eddy simulations of complex engineering and geophysical flows*. Cambridge: Cambridge University Press, 37–54.
- Galperin, B. and Orszag, S.A., eds. 1993. *Large eddy simulations of complex engineering and geophysical flows*. Cambridge: Cambridge University Press.
- Gauthier, S. and Bonnet, M., 1990. A $k-\varepsilon$ model for turbulent mixing in shock-tube flows induced by Rayleigh-Taylor instability. *Physics of Fluids A* 2, 1685–1694.
- Johnson, B.M. and Schilling, O., 2011a. Reynolds-averaged Navier-Stokes model predictions of linear instability. I. Buoyancy- and shear-driven flows. *Journal of Turbulence*, 12, 36-1–36-38.

- Johnson, B.M. and Schilling, O., 2011b. Reynolds-averaged Navier–Stokes model predictions of linear instability. II. Shock-driven flows. *Journal of Turbulence*, 12, 37-1–37-31.
- Kosović, B., Pullin, D.I., and Samtaney, R., 2002. Subgrid-scale modeling for large-eddy simulations of compressible turbulence. *Physics of Fluids*, 14, 1511–1522.
- Landau, L.D. and Lifschitz, E.M., 1959. *Fluid mechanics*. Oxford: Pergamon Press.
- Lesieur, M. and Métais, O., 1996. New trends in large-eddy simulations of turbulence. *Annual Review of Fluid Mechanics*, 28, 45–82.
- Lesieur, M., Métais, O., and Comte, P., 2005. *Large-eddy simulations of turbulence*. Cambridge: Cambridge University Press.
- Linden, P.F., 1979. Mixing in stratified fluids. *Geophysical and Astrophysical Fluid Dynamics*, 13, 3–23.
- Piomelli, U., 1993. In: B. Galperin and S.A. Orszag, eds. *Large eddy simulations of complex engineering and geophysical flows*. Cambridge: Cambridge University Press, 119–137.
- Pope, S.B., 2000. *Turbulent flows*. Cambridge: Cambridge University Press.
- Pullin, D.I., 2000. A vortex-based model for the subgrid flux of a passive scalar. *Physics of Fluids*, 12, 2311–2319.
- Ramshaw, J.D., 1979. *Alternate interpretation of the subgrid scale eddy viscosity*. Los Alamos National Laboratory Report LA-7955-MS. Los Alamos, NM: Los Alamos National Laboratory.
- Sagaut, P., 2006. *Large eddy simulation for incompressible flows: an introduction*. New York: Springer-Verlag.
- Smagorinsky, J., 1963. General circulation experiments with the primitive equations. *Monthly Weather Review*, 91, 99–164.
- Stone, J.M. and Norman, M.L., 1992. ZEUS-2D: a radiation magnetohydrodynamics code for astrophysical flows in two space dimensions. I – The hydrodynamic algorithms and tests. *Astrophysical Journal Supplement* 80, 753–790.
- Tennekes, H. and Lumley, J.L., 1972. *A first course in turbulence*. Cambridge, MA: MIT Press.
- Turner, J.S., 1973. *Buoyancy effects in fluids*. Cambridge: Cambridge University Press.
- Ulitsky, M., et al., 2001. *A guide to the BHR turbulence mix model in CHAD*. Los Alamos National Laboratory Report LA-UR-01-0980. Los Alamos, NM: Los Alamos National Laboratory.
- von Neumann, J. and Richtmyer, R.D., 1950. A method for the numerical calculation of hydrodynamic shocks. *Journal of Applied Physics*, 21, 232–237.
- You, D. and Moin, P., 2007. A dynamic global-coefficient subgrid-scale eddy-viscosity model for large-eddy simulation in complex geometries. *Physics of Fluids*, 19, 065110.