FULL TITLE
*ASP Conference Series, Vol. **VOLUME**, **YEAR OF PUBLICATION***
NAMES OF EDITORS

Subgrid models in turbulent mixing

H. Lim, Y. Yu, J. Glimm, X.-L. Li, D. H. Sharp

Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY 11794-3600, USA

Computational Science Center, Brookhaven National Laboratory, Upton, NY 11793-6000, USA

Los Alamos National Laboratory, Los Alamos, NM

Abstract. We are concerned with the chaotic flow fields of turbulent mixing. Chaotic flow is found in an extreme form in multiply shocked Richtmyer-Meshkov unstable flows. The goal of a converged simulation for this problem is to obtain converged solutions for such micro solution features as the joint probability distributions of the temperature and species concentration, as well as the macro features such as the edges of the mixing region. Here we introduce parameterized subgrid models of mass and thermal diffusion, to define LES that replicate the micro features observed in the DNS. The Schmidt numbers and Prandtl numbers are chosen to represent typical liquid and gas parameter values. The viscosity, and thus the Reynolds number, is allowed to vary through a range of values, to allow exploration of both DNS and LES regimes. Our main result is to explore the dependence of these solutions on mesh and Reynolds number.

1. Introduction

The turbulent mixing considered here is initiated by impulsive acceleration. It is produced by a shock wave passing through a layer separating two fluids of distinct densities. When the layer is perturbed (or not normal relative to the shock wave), vorticity is deposited on the interface by the shock passage. This vorticity causes the interface to roll up and become unstable. Upon a second shock wave passage, the interface enters an extremely chaotic regime. This problem is known as the Richtmyer-Meshkov (RM) instability. We consider a circular geometry, with a converging circular shock at the outer edge, and inside this, two fluids separated by a perturbed circular interface. The problem was previously described in detail (Yu 2006, Masser 2007, Lim 2007 AMAS, Lim 2007 CMAME). The chaotic aspects of the mixing following reshock challenge some convential ideas of computational science while supporting others. For this reason, the problem is of fundamental scientific interest, and may shed light on differing views for the computation of turbulent mixing flows.

A central issue in the modeling of turbulent mixing is to combine the somewhat distinct numerical methods which have evolved to deal separately with shocks (capturing) and with turbulence (high order algorithms with subgrid scale models). Our use of dynamic subgrid scale (SGS) models from the turbulence modeling community combined with a front tracking and shock capturing code is an original contribution to this goal. It is distinct from the common strategy of a filter to allow specialized algorithms tuned to either shocks or turbulence if they occur with spatial or temporal separation. Our strategy is to preserve the gradients of the capturing codes and even to sharpen them, as the tracking allows steeper gradients for the contact discontinuities or slightly smeared miscible boundaries between distinct fluids than can be obtained with an untracked shock capturing solution. The goal is to preserve (or enhance) the computational efficiency of the capturing codes in regard to a high density of geometrically complex solution gradients. Rather than try for more decades of Kolmogorov spectrum from the turbulence, we hope to have large eddy simulation (LES) convergence of critical observables of the flow, with a coarser grid description than would be accessible to turbulence style algorithms. However, rather than give up on detailed physical accuracy for the micro observables, as is more or less the strategy of the capturing codes, we hope to have converged simulations of finite Schmidt and Prandtl number effects. This is in contrast to statements made by authors of some capturing codes, that these codes contain a numerically determined effective viscosity, and presumably numerical Schmidt and Prandtl numbers which are otherwise not quantified, when run in a LES level of grid resolution.

The fluid interface, at late time, is volume filling. The Reynolds number and transport coefficients (viscosity, mass diffusion, and heat conductivity) are given dimensionlessly as $Re = UL/\nu_k$, the Schmidt number $Sc = \nu_k/D$, and the Prandtl number $Pr = \nu_k/\alpha$. Here ν_k is the kinematic viscosity, D the mass kinemaic diffusivity and $\alpha = \frac{\kappa}{\rho c_p}$ the kinematic thermal diffusion rate. κ is the heat conductivity, ρ the density and c_p the specific heat at constant pressure. U and L are characteristic velocity and length scales. We consider typical transport cases l, g from Table 1.

Table 1. Transport coefficients considered in this paper.

case	Schmidt	Prandtl
l (liquid)	10^3	50
g (gas)	1	1

2. Equations and Algorithms

We study the compressible Navier-Stokes equations with viscosity, mass diffusion and thermal conductivity, for two miscible species initially separated by a sharp interface. The primitive equations describe the DNS limit, in which transport effects are resolved. A measure of this limit, as applied to the momentum equation, is the criteria $\lambda_{K\mathrm{mesh}} \geq 1$ where $\lambda_{K\mathrm{mesh}} = \lambda_K/\Delta x$ and λ_K is the Kolmogorov length scale,

$$\lambda_K = (\nu_k^3/\epsilon)^{1/4} , \tag{1}$$

where

$$\epsilon = \nu_k|\mathbf{S}|^2 , \tag{2}$$

S is the strain rate tensor

$$S_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) \tag{3}$$

defined in terms of the velocity $\mathbf{v}$ and for any matrix $\mathbf{A} = A_{ij}$,

$$|\mathbf{A}|^2 = \sum 2A_{ij}^2 \ . \tag{4}$$

LES start from a filter, or averaging procedure applied to the primitive equations of compressible flow. We adopt what is known as an implicit filter, namely a grid block average. In this case the quantities in the defining equations are averaged over a grid block. New terms, arising from the average of the nonlinear terms, are introduced into the equations. We use a conventional definition of these terms, a dynamic definition following refs. (Germano 1991, Moin 1991, Ma 2006). The subgrid models are parameterized dynamically. For DNS, these terms have little effect.

We write the filtered continuity, momentum, energy and concentration equations of two miscible fluid species in an inertial frame. The filtered quantities are considered to be mesh block averages, and denoted with an overbar, while mass averaged quantities are denoted with a tilde.

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\overline{\rho}\widetilde{v}_i}{\partial x_i} = 0 \ , \tag{5}$$

$$\frac{\partial \overline{\rho}\widetilde{v}_j}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{v}_i\widetilde{v}_j + \overline{p}\delta_{ij})}{\partial x_i} = \frac{\partial \overline{d_{ij}}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_i} \ , \tag{6}$$

$$\frac{\partial \overline{E}}{\partial t} + \frac{\partial(\overline{E} + \overline{p})\widetilde{v}_i}{\partial x_i} = \frac{\partial \overline{d_{ij}}\widetilde{v}_j}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\overline{\kappa}\frac{\partial \widetilde{T}}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left((\widetilde{H}_h - \widetilde{H}_l)\overline{\rho}\widetilde{D}\frac{\partial \widetilde{\psi}}{\partial x_i}\right) \tag{7}$$

$$+ \left(\frac{1}{2}\frac{\partial \tau_{kk}\widetilde{v}_i}{\partial x_i} - \frac{\partial q_i^{(H)}}{\partial x_i} - \frac{\partial q_i^{(T)}}{\partial x_i} - \frac{\partial q_i^{(V)}}{\partial x_i}\right) \ , \tag{8}$$

$$\frac{\partial \overline{\rho}\widetilde{\psi}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{\psi}\widetilde{v}_i}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho}\widetilde{D}\frac{\partial \widetilde{\psi}}{\partial x_i}\right) - \frac{\partial q_i^{(\psi)}}{\partial x_i} \ , \tag{9}$$

where the subgrid scale (SGS) variables are the τ_{ij}, $q_i^{(H)}$, $q_i^{(T)}$, $q_i^{(V)}$ and $q_i^{(\psi)}$.

Detailed definitions of the closure terms are standard and are given in a subsequent publication.

The parabolic Navier-Stokes equations are solved via operator splitting, with separate solution steps for the hyperbolic and pure diffusion parts of the equations. The hyperbolic solutions are by the front tracking FronTier algorithm (Du 2005). The interface hyperbolic updates are split into normal and tangential operators defined at front points. The interior hyperbolic update uses a Godunov finite difference solver based on the MUSCL algorithm (Woodward 1984, Colella 1985). A sharp (tracked) interface in the hyperbolic update uses ghost cells (Glimm 1981) in the interior state update to eliminate (Liu 2007) transport related numerical mass and thermal diffusion across the interface.

An explicit solver, for both the interior and the front state parabolic solvers, with possible time step subcycling is sufficient to allow a stable computation for most of the transport parameter range considered. For some parameter values and for some variables, an implicit solver is used.

The FronTier numerical Schmidt and Prandtl numbers are ∞, and the code allows efficient simulation of any desired (physical) Schmidt or Prandtl number.

3. The Joint Probability Distributions for Concentration and Temperature

The joint pdf for the temperature and species mass concentrations of the fluid mixture is defined as a function of time and radius, assuming that the probability data is collected from the angular variation in space. To create the pdfs from the simulation data, we collect the temperature and concentration variables along a band of constant radii within the mixing zone. Mixed cells are not averaged, but each cell fraction contributes its own concentration fraction and temperature with its own probabilities (proportional to area). The concentration fractions and temperatures are then binned.

The liquid joint pdfs are bimodal, with peaked mass fractions of nearly pure fluid, highly correlated with temperature, so that the heavy material is hotter. The gas pdfs are concentrated near a curve in concentration-temperature space, joining the light to the heavy fluid concentrations. The origin of this shape could be explained by the following process: First the shock heats the heavy fluid, so it is hotter. Then portions of the heavy and light fluid diffuse into one another, so that the temperature pdf at fixed concentration is determined from the temperature pdf of the pure fluids before mixture through diffusion. We display typical plots of the pdfs representative of these types.

Acknowledgments. This work was supported in part by U.S. Department of Energy grants DE-AC02-98CH10886 and DE-FG52-06NA26208, and the Army Research Office grant W911NF0510413. The simulations reported here were performed in part on the Galaxy linux cluster in the Department of Applied Mathematics and Statistics, Stony Brook University, and in part on New York Blue, the BG/L computer operated jointly by Stony Brook University and BNL. Los Alamos National Laboratory Preprint LA-UR-XX-YYY.

References

P. Colella. A direct Eulerian MUSCL scheme for gas dynamics. *SIAM journal on scientific computing*, 6(1):104–117, 1985.

Jian Du, Brian Fix, James Glimm, Xicheng Jia, Xiaolin Li, Yunhua Li, and Lingling Wu. A simple package for front tracking. *J. Comput. Phys.*, 213:613–628, 2006. Stony Brook University preprint SUNYSB-AMS-05-02.

M. Germano, U. Piomelli, P. Moin, and W. H. Cabot. A dynamic subgrid scale eddy viscosity model. *Phys Fluids A*, 3:1760–1765, 1991.

J. Glimm, D. Marchesin, and O. McBryan. A numerical method for two phase flow with an unstable interface. *J. Comput. Phys.*, 39:179–200, 1981.

H. Lim, Y. Yu, J. Glimm, X.-L. Li, and D. H. Sharp. Chaos, transport, and mesh convergence for fluid mixing. *Acta Mathematicae Applicatae Sinica*, 2007. Submit-

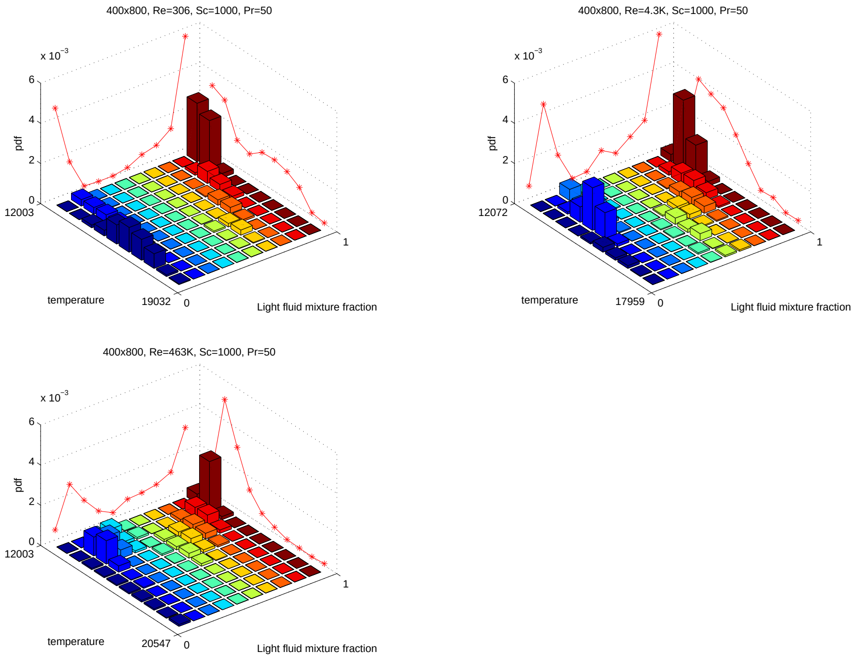

Figure 1. Case l: Reynolds number dependence of the joint pdfs of light species and temperature at time $t = 90$. The data has been collected into 10×10 bins. Left to right: $Re \approx 300,\ 6000,\ 600,000$. The mesh is 400×800 in all cases.

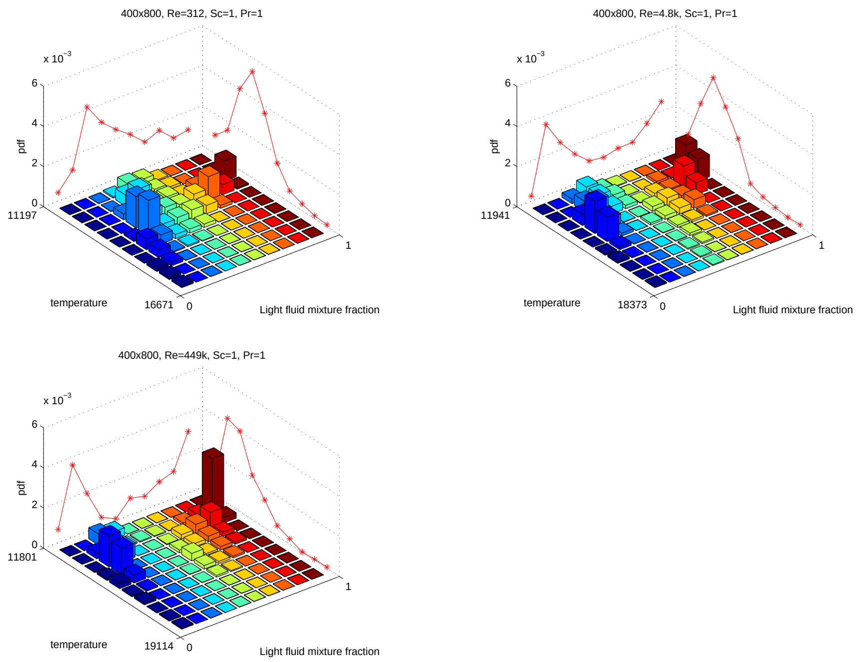

Figure 2. Case g: As is Fig. 1.

ted. Stony Brook University Preprint SUNYSB-AMS-07-09 Los Alamos National Laboratory preprint number LA-UR-08-0068.

H. Lim, Y. Yu, H. Jin, D. Kim, H. Lee, J. Glimm, X.-L. Li, and D. H. Sharp. Multi scale models for fluid mixing. *Special issue CMAME*, 2007. Accepted for publication. Stony Brook University Preprint SUNYSB-AMS-07-05.

X. F. Liu, Y. H. Li, J. Glimm, and X. L. Li. A front tracking algorithm for limited mass diffusion. *J. of Comp. Phys.*, 222:644–653, 2007. Stony Brook University preprint number SUNYSB-AMS-06-01.

T. Ma. *Large eddy simulation of variable density flows.* Ph.d. thesis, University of Maryland, 2006.

T. O. Masser. *Breaking Temperature Equilibrium in Mixed Cell Hydrodynamics.* Ph.d. thesis, State University of New York at Stony Brook, 2007.

P. Moin, K. Squires, W. Cabot, and S. Lee. A dynamic subgrid-scale model for compressible turbulence and scalar transport. *Phys. Fluids*, A3:2746–2757, 1991.

P. Woodward and P. Colella. Numerical simulation of two-dimensional fluid flows with strong shocks. *J. Comput. Phys.*, 54:115, 1984.

Y. Yu, M. Zhao, T. Lee, N. Pestieau, W. Bo, J. Glimm, and J. W. Grove. Uncertainty quantification for chaotic computational fluid dynamics. *J. Comput. Phys.*, 217:200–216, 2006. Stony Brook Preprint number SB-AMS-05-16 and LANL preprint number LA-UR-05-6212.