Verification and Validation for Turbulent Mixing Simulations

H. Lim, J. Iwerks, Y. Yu, J. Glimm and D. H. Sharp

Department of Applied Mathematics and Statistics Stony Brook University, Stony Brook NY 11794-3600; Los Alamos National Laboratory Los Alamos, NM

E-mail: hyulim@ams.sunysb.edu jiwerks@ams.sunysb.edu
yan2000@ams.sunysb.edu glimm@ams.sunysb.edu dcso@lanl.gov

Abstract. We present highlights from and supplementary material related to two recent studies giving verification and validation of a new approach to the simulation of turbulent mixing. The verification is based on (i) a mesh refinement study of a circular Richtmyer-Meshkov unstable flow, (ii) code comparison to a well documented code and (iii) comparison to a simple analytic model. The validation is based on simulation agreement with Rayleigh-Taylor unstable experiments of Smeeton-Youngs and of Mueschke-Andrews. The mesh refinement verification gives convergence for such molecular level variables as the probability density functions for the concentrations, temperatures and a chemical reaction rate. The validation study, beyond obtaining near perfect agreement with experiment, explores the various factors in the simulations that result in this agreement and in the differences between the two experiments. The significant variables are: fluid transport parameters, dimensionless groups (not widely recognized to be significant) to characterize the dominant short wavelength initial perturbations and experimentally measured (long wavelength) initial perturbations.

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1. Introduction: The nature of the problem for turbulent mixing

Turbulent mixing has been a challenge for at least a half century. It has attracted the talents of leading physicists and mathematicians over this time. However, successes in this area, in regard to verified and validated simulation codes, have been few. Here we build on two recent articles [8, 6]; we refer to these and to references cited therein for a further discussion of the history of turbulent mixing.

In these articles, we propose a new LES algorithm for turbulent mixing. This algorithm is based on control of numerical species concentration diffusion and numerical thermal diffusion. This goal is attained through use of front tracking, implemented in the code FronTier. FronTier itself has been verified and validated for turbulent mixing in a series of articles over the past several years [4, 5, 10]. The algorithm is also based on subgrid scale (SGS) models to capture the influence of the unresolved scales upon the resolved ones. We use dynamic SGS models [12], which have the advantage of being parameter free. This feature is achieved through the use of two levels of averaging, one to define the computational algorithm and a further averaging of the computed solution, as a kind of post processing operation carried out within each time step. The SGS for the doubly averaged solution can then be computed in two ways, either as a model for the doubly averaged solution or directly, using the singly averaged solution. Through this double determination, otherwise missing model coefficients are determined at the level of the doubly averaged equation. An asymptotic assumption and a known power law dependence of these coefficients on the mesh allows their transfer to the singly averaged level, that of the simulation itself. One determination of coefficients occurs for each of the momentum, concentration and energy equations, and in effect defines a turbulent viscosity, Schmidt number and Prandtl number. In other words the parameters of the model are set dynamically by reference to the simulation as it progresses. The dynamic SGS models have been in use for a number of years and have been subject to their own verification and validation studies.

Here we are concerned with the verification and validation of this union of two algorithms, each previously verified and validated. The new issue in the combination of the two algorithms is the use of the SGS models outside of their previously tested domains. We allow concentration and thermal gradients that are large at a grid level. We are concerned with processes that have a short time scale. Diffusion (concentration and thermal) play significant roles, but limited ones. The occurrence of the steep gradients in a range of application problems can be understood from the small time scales of supersonic flow or from a disparity of spatial scales, between a diffusion length scale and some macroscopic scale.

These tensions between SGS models and a sharp resolution of numerical flow features play out in the contrast between the methods of turbulence with SGS models and capturing methods, with their numerically steep gradients. The algorithm proposed here unites the best features of these separate ideas; it goes beyond many capturing codes, in the use of front tracking to eliminate numerical diffusion across a tracked
interface, while still allowing physical diffusion.

While this idea has a natural appeal, the true test of its value lies in its performance, which is the subject of the present article. Briefly, we report (here and in [8, 6]):

1. The first validated high Schmidt number Rayleigh-Taylor simulation.
2. The first compressible LES/SGS validated Rayleigh-Taylor simulation.
3. The first Rayleigh-Taylor simulation to agree with all of the experimental data points, not just the late time asymptotics.
4. The first quantitative determination of the key factors affecting the Rayleigh-Taylor growth rate. (These are fluid transport parameters, dimensionless groups associated with the dominant short wavelength initial conditions and the long wavelength perturbation amplitudes and wavelengths.)
5. Identification of dimensionless groups to characterize short wavelength initial conditions, with a demonstration of their influence on $\alpha$.
6. Demonstration that no single explanation for the values observed experimentally for the Rayleigh-Taylor mixing rate parameter $\alpha$ (e.g. fluid transport or the nature of the dominant short wavelength perturbations or the long wavelength noise in initial conditions) will apply uniformly to all experiments.
7. The first apparently converged computation of the probability density functions for concentration, temperature and a chemical reaction rate in a typical turbulent mixing simulation (doubly shocked Richtmyer-Meshkov instability).
8. Strong evidence for a bimodal characterization of the joint concentration and temperature probability density functions, indicating incomplete mixing at a molecular level.
9. Dependence of the concentration and temperature probability density functions on the fluid transport parameters.

2. Verification

We use three methods of verification: mesh convergence, code comparison and comparison to a simple theoretical model. Because mesh convergence leads to a requirement for fine meshes and because we want to study the effect of modifying the fluid properties, we adopted a 2D model of the problem under study, namely a circular Richtmyer-Meshkov instability, with a reshock, after the original incoming shock wave has been reflected off of the origin.

We had previously observed mesh convergence and agreement under code comparison (with the LANL code RAGE) for such macroscopic variables as the time dependent edge of the mixing zone [17, 11], and in [8], the insensitivity of such variables to the fluid transport parameters. For this reason, we focus on the more difficult question of the microscopic observables, such as the joint temperature concentration probability density functions, or a chemical reaction rate probability density function.
For the microscopic variables, the code comparison produced a failure of verification. Two apparently converged simulations, using different codes gave strikingly different temperature distributions, for simulations that were not regularized through use of transport properties (i.e. ILES simulations). To address this issue, we have added finite values of transport and SGS models, leading to the present algorithm. We summarize the main verification results [8]:

1. Convergence under mesh refinement for the microscopic variable probability density functions,
2. Agreement of the converged solutions with a simple analytical model for these probability density functions,
3. Significant dependence of the probability density functions on the fluid transport properties.

2.1. Parameters for a 2D Richtmyer-Meshkov Simulation Study

The turbulent mixing considered here is initiated 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 passage of a second shock wave, the interface enters an extremely chaotic regime. This is an example of 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. This problem was previously described in detail [17, 11, 9, 7].

We study mesh refinement and mesh convergence with dependence on a range of Reynolds, Schmidt and Prandtl numbers, including some within the KDNS regime, in which turbulence properties are fully resolved. To avoid conflict with standard DNS terminology, we use the term KDNS to refer to a simulation which is resolved at the Kolmogorov scale, and which thus presumably resolves the fluid turbulence fully. Similarly we define as KBDNS a simulation resolved at both the Kolmogorov and Batchelor scales. KBDNS should resolve the turbulent mixing fully. The resolution requirements for KBDNS are much stricter than for KDNS at high Schmidt number. Simulations that are not KBDNS are LES and require SGS models.

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 $\nu_k$ is the kinematic viscosity, $D$ the kinematic mass diffusivity and $\alpha = \kappa/\rho c_p$ the kinematic thermal diffusion rate. $\kappa$ is the heat conductivity, $\rho$ the density and $c_p$ the specific heat at constant pressure. $U$ and $L$ are characteristic velocity and length scales. Gases typically have Schmidt and Prandtl numbers of the order of unity, while liquids typically have Schmidt numbers in the range $Sc \sim 4 \times 10^2$ to $10^4$ and Prandtl numbers in the range $Pr \sim 10$ to $10^2$ [1, 14]. Dense plasma transport coefficients have been estimated as $Sc \sim 0.6$ to $1.5$ [15] for a
Table 1. Transport coefficients considered, arranged in order of increasing diffusivity.

<table>
<thead>
<tr>
<th>case</th>
<th>Schmidt</th>
<th>Prandtl</th>
</tr>
</thead>
<tbody>
<tr>
<td>l (liquid)</td>
<td>$10^3$</td>
<td>50</td>
</tr>
<tr>
<td>g (gas)</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>p (plasma)</td>
<td>1</td>
<td>$10^{-4}$</td>
</tr>
</tbody>
</table>

range of plasma conditions relevant to NIF experiments. A representative plasma value $Pr \sim 10^{-4}$ can be inferred from [3]. We consider the transport cases l, g, p from Table 1.

2.2. Convergence for Probability Density Functions

The probability density functions lie in an infinite dimensional space, and their convergence properties depend on the norm or metric used to define this space. The data is somewhat noisy, and for this reason we compare them using a regularizing norm. Distribution functions are defined as the indefinite integral of the probability density functions, and classical norms are used to compare differences of the distribution functions. In this subsection, we use the $L_\infty$ norm, also known as the Kolmogorov-Smirnov norm for the underlying probability density function, and in Sec. 2.3 we use the $L_1$ norm. To simplify the range of results reported in [8], we give here only the convergence for the specific chemical reaction rate. We observe that this is fully defined by the simulation, with its dynamic SGS model. Because we have mesh convergence of the temperature and concentrations, and because the specific chemical rate is a function of these temperatures and concentrations, no model (closure assumption) occurs in the evaluation of the chemical reaction rate probability density function. We take a very nonlinear function of the temperature, the chemical reaction rate, with an activation temperature in the middle of the observed temperature variables, to illustrate this point. See Table 2. The simulation, even after the averaging employed here (averaging over $\theta$ and $r$ within the mixing zone) is still subject to statistical fluctuations. To assess these fluctuations, we performed a small ensemble of simulations for the coarse grid, by varying statistically the initial perturbations. The results of the fluctuations over this ensemble are shown in columns 2 and 5 of Table 2. Here $\sigma$ is an ensemble standard deviation of the spatially averaged quantities, and $\langle \cdot \rangle$ is an ensemble mean. The statistical fluctuations are $3 \times$ to $15 \times$ larger than the mesh errors.

2.3. Comparison to a Simple Analytical Model

The analytical model has input from the simulation. It assumes the geometry defined by the simulation for the 50% isoconcentration interface between the two fluids. It also assumes the turbulent mass and thermal diffusion coefficients as defined by the SGS model.
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Table 2. Relative coarse grid ensemble fluctuations (±2σ) divided by ensemble mean, and mesh errors for the specific chemical production \( w \) for an activation temperature \( T_{AC} = 15,000^oK \) located in the middle of the observed range of temperatures. Comparison of the probability density function for the reaction rate is based on the Kolmogorov-Smirnov metric. Comparison is coarse mesh (c) to fine (f) and medium (m) to fine. Cases l and g denote fluid parameters representative of a liquid and a gas.

<table>
<thead>
<tr>
<th></th>
<th>l</th>
<th></th>
<th></th>
<th>g</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>2σ/ ⟨w⟩</td>
<td>c to f</td>
<td>m to f</td>
<td>2σ/ ⟨w⟩</td>
<td>c to f</td>
<td>m to f</td>
</tr>
<tr>
<td>≈ 300</td>
<td>0.24</td>
<td>0.04</td>
<td>0.03</td>
<td>0.29</td>
<td>0.03</td>
<td>0.02</td>
</tr>
<tr>
<td>≈ 6000</td>
<td>0.49</td>
<td>0.04</td>
<td>0.04</td>
<td>0.45</td>
<td>0.03</td>
<td>0.04</td>
</tr>
<tr>
<td>≈ 600K</td>
<td>0.25</td>
<td>0.09</td>
<td>0.03</td>
<td>0.25</td>
<td>0.09</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Using this input, the model first computes an exit distance, which is the distance to exit the current phase, computed as the minimum distance to exit taken along all rays in arbitrary directions emanating from the point in question. The exit distance follows an exponential distribution, which is fully characterized by its mean. The mean is a function of \( t \) and \( r \), with a statistical average over the angular variable \( \theta \). However, to improve the quality of the statistics, we enlarge the ensemble and average over \( r \) also, for \( r \) values within the mixing zone. This analysis is applied at a specific time \( t \), shortly after the time \( t_0 \) of reshock.

A second input to the theoretical model is the laminar and turbulent concentration and thermal diffusion coefficients, with the turbulent coefficients determined dynamically from the SGS model. Because of the rapid increase in the interface length (2D) following reshock, we assume that all diffusion takes place over the time period \( [t_0, t] \) between reshock and the current time. From the one dimensional diffusion equation, with its analytic solution applied over the above defined exit distance and over the time \( t - t_0 \), we compute the diffused species mass and the temperature at any point in the mixing zone. These predicted concentrations and temperatures are assembled into a joint concentration, temperature probability density function, as predicted by the model, and these predictions are compared to the corresponding probability densities, as computed directly from the simulation. Comparison of the probability density functions is via the \( L_1 \) norm of the difference of the associated distribution functions. The data has been binned in a 10 × 10 set of concentration temperature bins for the purpose of this computation. The results are summarized in Table 3. We consider typical fluid, gas and plasma fluid parameters, see Table 1, and we consider three Reynolds numbers, \( Re = 300, 6000, 600K \). The reported errors are dimensionless, with a maximum possible value of 2.
Table 3. Errors in the model compared to the simulation, for the joint temperature concentration probability density function. The error is measured as the $L_1$ norm of the difference in the distribution functions for the two probability density functions, with the total measure in the $L_1$ norm normalized to 1. The model somewhat underpredicts mixing, due to the assumed absence of diffusive transport in the model prior to the time of reshock. Results for the finest grid are shown. The error is not grid related, and similar results obtain for coarser grids.

<table>
<thead>
<tr>
<th>$Re$</th>
<th>l</th>
<th>g</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>≈ 300</td>
<td>0.06</td>
<td>0.06</td>
<td>0.05</td>
</tr>
<tr>
<td>≈ 6000</td>
<td>0.07</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>≈ 600K</td>
<td>0.07</td>
<td>0.08</td>
<td>0.06</td>
</tr>
</tbody>
</table>

3. Validation: From Smeeton-Youngs to Mueschke-Andrews in 6 Degrees of Separation

3.1. Main Validation Results

We study validation in the context of Rayleigh-Taylor mixing, wherein a heavy fluid is accelerated by a light one. Denoting the penetration distance $h$ of the light fluid (the “bubbles”) into the heavy, the macroscale description of the mixing process is summarized in the equation

$$h = \alpha Ag t^2,$$

which defines the dimensionless bubble side Rayleigh-Taylor mixing rate $\alpha$. Here $g$ is the accelerating force, $t$ is time and the Atwood number $A$ is defined as

$$A = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1},$$

with $\rho_i$ the density of fluid $i$. The combination $Ag$, an effective or renormalized gravity, also enters into the dimensionless Grashof number

$$Gr_\lambda = \frac{2Ag\lambda^3}{\nu_k^2}.$$  

Here $\lambda$ is a characteristic length scale. $Gr$ is the ratio of accelerating to viscous damping forces. If $\lambda = \lambda_{th}$ is defined by a viscous based dispersion analysis as the wavelength of the Rayleigh-Taylor mode with the most rapid growth rate, then $Gr$ is a pure number,

$$Gr_{\lambda_{th}} = 2(4\pi)^3 \approx 3900.$$  

We are concerned with experiment #112 of Smeeton-Youngs [16] for the miscible mixing of NaI solution and fresh water. We also study the hot-cold water channel experiments and related fresh-salt water channel experiments of Mueschke [13]. Our simulations are in near perfect agreement with experiment #112, agree with the value for $\alpha$ for the hot-cold water experiment, and are close but not perfect for the Mueschke fresh-salt water experiment. In Figs. 1-7 we compare the simulation with the experimental
plates. See also Table 4. Due to a small time dependence of the acceleration, we introduce the scaled acceleration distance for variable acceleration as used in [16],

\[
X = A \left[ \int_0^t (g(t'))^{1/2} dt' \right]^2 .
\]  

Note that the difference between the $\alpha$ based on $X$ and that based on a time independent $\bar{g}$ is 0.001, which is 1/3 of the difference between the experimental and simulation values of $\alpha$.

Our analysis indicates significant differences between the Smeeton-Youngs and the Mueschke experiments. The Smeeton-Youngs experiments have no appreciable long wavelength noise (according to our analysis), less viscous dissipation, and more initial mass diffusion. The dominant short wavelength perturbations are driven at a wavelength $\lambda = \lambda_{\text{exp}} = \lambda_{\text{th}}$ where the dispersion theory used to define $\lambda_{\text{th}}$ is based upon
Figure 3. As above, third experimental plate. Right: (c) British Crown Copyright 2010/MOD.

Figure 4. As above, fourth experimental plate. Right: (c) British Crown Copyright 2010/MOD.

Figure 5. As above, fifth experimental plate. Right: (c) British Crown Copyright 2010/MOD.
viscosity, initial mass diffusion and time dependent mass diffusivity. The Mueschke experiments are the opposite, with significant long wavelength perturbations, more viscous dissipation, less initial mass diffusion and $\lambda_{\text{exp}} > \lambda_{\text{th}}$. We identify two new dimensionless groups for the characterization of experiments or simulations; these appear to have an influence on $\alpha$. Let $\lambda_{\text{IMD}}$ be the width of the initial mass diffusion layer between the two (miscible) fluids. The dimensionless ratios $\lambda/\lambda_{\text{th}}$ and $\lambda/\lambda_{\text{IMD}}$ are observed to be significant in the determination of $\alpha$.

We pass from the NaI solution-fresh water experiments of Smeeton-Youngs to fresh-salt water of Mueschke in six steps, varying one significant parameter at a time. For all steps, an effect on $\alpha$ is observed. The effect on $\alpha$ is generally well above the observed differences between the simulations and experiments, but often within the (larger) reported error bars in the Mueschke experiments. See Fig. 8. A number of different factors have an influence on $\alpha$. Proceeding from left to right in this figure, the
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Table 4. Relative errors in the bubble penetration of the experiment compared to the simulation. All units are in cm. The first column is a variable acceleration scaled acceleration distance. The second column, using the time averaged acceleration \( \overline{g} \), is an effective scaled acceleration distance. The simulation is compared to the experiment with a time offset \( t_0 \), with \( t_0 \) chosen by least squares to minimize the simulation-experiment differences. The simulation values for the penetration distance \( h \) are reported at the offset time. The first and third columns are used to determine the experimental \( \alpha \). Experimental data courtesy of D. Youngs.

<table>
<thead>
<tr>
<th>( X )</th>
<th>( A\overline{g}(t - t_0)^2 )</th>
<th>( h_{\text{exp}} )</th>
<th>( h_{\text{sim}} )</th>
<th>( \Delta h_{\text{rel}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>29.8</td>
<td>30.7</td>
<td>1.03</td>
<td>1.03</td>
<td>0.00</td>
</tr>
<tr>
<td>35.7</td>
<td>36.6</td>
<td>1.43</td>
<td>1.39</td>
<td>-0.03</td>
</tr>
<tr>
<td>42.1</td>
<td>43.1</td>
<td>1.78</td>
<td>1.76</td>
<td>-0.01</td>
</tr>
<tr>
<td>49.1</td>
<td>50.1</td>
<td>2.19</td>
<td>2.14</td>
<td>-0.02</td>
</tr>
<tr>
<td>56.7</td>
<td>57.9</td>
<td>2.56</td>
<td>2.52</td>
<td>-0.02</td>
</tr>
<tr>
<td>64.6</td>
<td>65.9</td>
<td>2.90</td>
<td>2.93</td>
<td>+0.01</td>
</tr>
<tr>
<td>73.1</td>
<td>74.6</td>
<td>3.18</td>
<td>3.34</td>
<td>+0.05</td>
</tr>
</tbody>
</table>

steps are:

1. Modify the Schmidt number \( Sc = \text{viscosity}/(\text{mass diffusivity}) \),
2. Modify the Grashof number \( Gr = 2Ag\lambda^3/\nu^2 \) (where \( \nu \) is the kinematic viscosity),
3. Modify the dominant short wavelength in the initial conditions and the initial mass diffusion layer to the Mueschke experimental values,
4. Modify the short wavelength initial conditions to have amplitudes measured experimentally by Mueschke,
5. Add experimentally measured long wavelength initial amplitudes, as measured by Mueschke,
6. Modify the Schmidt number (back) to fresh-salt water values.

In each step, the variables not mentioned are held fixed. In Step 3, modifying the short wavelength parameters with a fixed Grashof number, leads to a significant modification of the viscosity (as this occurs in the definition of \( Gr \)), and thus of the mass diffusivity (as this occurs in \( Sc \)). As we see from the Fig. 8, Step 4 produces the smaller effect. This is the change from short wavelength initial conditions as given by two dimensionless parameters to the experimental short wavelength initial conditions. Not only are the other changes all significant, but they have different signs. No single factor can explain the passage from [16] to [13] or even the direction of the change. The changes and parameters can be grouped under three headings, each with its own affect on \( \alpha \):

\(|\Delta \alpha| \approx 0.005 - 0.015 \) Fluid transport parameters
\(|\Delta \alpha| \approx 0.009 \) Short wavelength initial condition parameters
\(|\Delta \alpha| \approx 0.0 - 0.028 \) Long wavelength initial conditions
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3.2. Parameters for Simulation of Experiment #112 and Related Simulations

Here we give the parameters for the simulation of experiment #112, and also for the first three intermediate steps in Fig. 8. For the simulation of experiment #112, ie, the left most entry in Fig. 8, we use the experimental parameters. The experimental domain is 2.5 cm × 15 cm × 15 cm. According to dispersion theory, based on (i) viscosity, (ii) mass diffusion, and (iii) initial mass diffusion, the wavelength of maximum growth rate is \( \lambda = \lambda_{th} = 0.21 \text{ cm} \). Accordingly, the initial perturbations were initialized in the range \([0.157,0.315]\) cm, centered about \( \lambda = 0.21 \text{ cm} \). This choice of \( \lambda \) was confirmed by examination of the experimental plates. In the second and subsequent frames of #112, a bubble size can be determined approximately by counting, yielding (for the second frame) a wavelength about \( 0.38 \text{ cm} \approx 2\lambda_{th} \), consistent with the wavelength of the
simulation at the same time.

We chose a mesh size 0.026 cm, sufficient to give about 8 cells per initial wavelength. The experiment was simulated four times, to test both statistical and mesh resolution. We simulated the full size domain, a domain reduced by a factor of 2 in the $x$ and $y$ directions, and a domain reduced by a factor of 4. For the quarter sized domain, we also simulated with a refined mesh, about 16 cells per initial wavelength. For the full-sized simulation, the mesh was $96 \times 576 \times 576$. The results of these 4 simulations showed a spread of $\pm 0.001$ in the values for $\alpha$, and a deviation (for the full sized simulation) of 0.001 from the experimental value, after a redetermination of $\alpha$ from the raw data points, but using the methodology (least squares with a $t$ offset) of the present study, for consistency of comparison.

The simulations were compressible, with a gamma law gas EOS, with $\gamma = 1.67$. The experimental value of acceleration $g = 39g_0$, with $g_0$ earth gravity, $g_0 = 0.000981$ cm/ms$^2$, was used. The experimental Atwood number, $A = 0.308$, was used. The kinematic viscosity was set at $\nu = 1.01E-5$ cm$^2$/ms, according to the Handbook of Physics and Chemistry. The kinematic diffusivity is $1.80E-8$ cm$^2$/ms and the Schmidt number is 560. The thickness of the initial mass diffusion layer is 0.35 cm. The amplitude of the initial perturbations was chosen roughly at the end of the period of validity of the linear Rayleigh-Taylor theory, namely 0.002 cm = 0.010 $\lambda$. As this value is unrelated to the time of initiation of the experiment, an offset in the height was allowed in the comparison to the experimental data.

The next three data points, proceeding left to right in Fig. 8, modify the foregoing by change of the Schmidt number, the Grashof number, and the parameters which characterize the short wavelength perturbations. To modify the Schmidt number, we increase the diffusivity. This changes the value of $\lambda$ and $\lambda_{th}$, while we keep $\lambda/\lambda_{IMD}$ and $\lambda/\lambda_{th} = 1$ fixed. The change in $\lambda$, in order to keep a constant value for $Gr$, requires a change in viscosity and thus further changes in diffusivity. The mesh is fixed at 8 cells per mode, and the domain dimensions in the $x$ and $y$ directions are modified to preserve the number of modes. To accomplish the mutually dependent parameter changes, an iterative method was used. See Table 5.

The next two data points use a similar method for the choice of parameters. When modifying the Grashof number, other dimensionless parameters are held fixed, as above. See Table 5.

Similarly when modifying the two dimensionless parameters characterizing the short wavelength perturbations, $Sc$ and $Gr$ are held fixed, but due to the interdependencies, the viscosity and diffusivity must be modified. Changing the wavelength $\lambda$ of the dominant short wavelength perturbation relative to $\lambda_{tm}$, far from being an innocent change, increases considerably the viscous and diffusive transport parameters and produces a significant decrease in $\alpha$. See Table 5.
Table 5. Input parameters for the first four simulations from Fig. 8.

<table>
<thead>
<tr>
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<th>#1</th>
<th>#2</th>
<th>#3</th>
<th>#4</th>
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<td>Dimensionless physical parameters</td>
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<td></td>
</tr>
<tr>
<td>$g/g_0$</td>
<td>39</td>
<td>39</td>
<td>39</td>
<td>39</td>
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<tr>
<td>$A$</td>
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<td>0.308</td>
<td>0.308</td>
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<tr>
<td>$Gr$</td>
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<td>2.1E6</td>
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<td>6.9E5</td>
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<tr>
<td>$Sc$</td>
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<td>7</td>
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<tr>
<td>$\nu$ (cm$^2$/ms)</td>
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<td>1.01E-5</td>
<td>3.91E-5</td>
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<td>$D$ (cm$^2$/ms)</td>
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<td>5.60E-6</td>
<td>3.01E-4</td>
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<tr>
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<tr>
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<td>1</td>
<td>1</td>
<td>2.62</td>
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<td>$\lambda/\lambda_{IMD}$</td>
<td>0.6</td>
<td>0.66</td>
<td>1</td>
<td>12</td>
</tr>
<tr>
<td>Initialization parameters</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda$ (cm)</td>
<td>0.21</td>
<td>0.23</td>
<td>0.34</td>
<td>3.6</td>
</tr>
<tr>
<td>$\lambda_{th}$ (cm)</td>
<td>0.21</td>
<td>0.23</td>
<td>0.34</td>
<td>1.37</td>
</tr>
<tr>
<td>$\lambda_{IMD}$ (cm)</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
<td>0.3</td>
</tr>
<tr>
<td>Domain and mesh parameters</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mesh</td>
<td>$96 \times 576 \times 576$</td>
<td>$24 \times 144 \times 576$</td>
<td>$24 \times 144 \times 576$</td>
<td>$96 \times 144 \times 120$</td>
</tr>
<tr>
<td>Domain (cm$^3$)</td>
<td>$2.5 \times 15 \times 15$</td>
<td>$0.69 \times 4.14 \times 16.56$</td>
<td>$1.02 \times 6.12 \times 24.5$</td>
<td>$43.2 \times 64.8 \times 54$</td>
</tr>
<tr>
<td>$\Delta x$ (cm)</td>
<td>0.026</td>
<td>0.029</td>
<td>0.043</td>
<td>0.45</td>
</tr>
</tbody>
</table>

3.3. Parameters for Simulation of Mueschke’s Experiments

Here we give the parameters for the simulation of the hot-cold water and fresh-salt water experiments of Mueschke and also for the simulation (after Step 4) with all long wavelength initial perturbations removed from the hot-cold water experiment.

We employ the same computational domain size as Mueschke used in his simulation: 28.8 cm × 18 cm × 24 cm. The resolution of $288 \times 180 \times 240$ gives $\Delta x = \Delta y = \Delta z = 0.1$ cm, which under resolves the Kolmogorov length scale $\eta_K \approx hRe_h^{-3/4} \approx 0.055$ cm by about a factor of 2. Since this is no longer a DNS and still further from the Batchelor scale, we use SGS terms.

The experimental Grashof number is preserved as we specify other simulation parameters below. It is

$$Gr_{\lambda_{exp}} \approx 6.87 \times 10^5,$$  \hspace{1cm} (6)

defined with $\lambda_{exp} = 3.6$ cm, the experimental wavelength of maximum amplitude. We modify, however, $A$, $g$ and $\nu$ from their experimental values. The modified values are $A = \frac{1}{3}$, $g = 100 \times g_0 = 0.0981$ cm/ms$^2$, with $g_0$ earth’s gravity and $\nu = 0.0221$ cm/ms$^2$ the simulation kinematic viscosity. The purpose of these changes is to increase
the compressibility to a larger but still small value, thereby increasing the compressible
time steps (a CFL limitation), and obtain a feasible simulation problem with an identical
value for $Gr_{\text{exp}}$. In order to maintain the experimental Schmidt number, $Sc = \frac{\nu}{D} = 7$,
it was also necessary to modify the kinematic mass diffusion $D$, so that $D = 0.0003014$
cm/ms$^2$. These changes do not affect pure length scales, so that the initial mass
diffusion layer width between the two fluids remains at the value of 0.3 cm determined
by Mueschke. The change in timescales necessitates a scaling of the initial velocity
perturbation amplitudes.

Perturbation data is taken from plots found in [13] that gave experimental density
spectra along the $x$ and $y$ directions and experimental $z$ direction velocity spectrum
along the $x$-axis. Random phases are uniformly selected from $[-\pi, \pi]$ for each density
mode. Velocity modes use the same phases as the density modes in the $x$-direction.

The Navier Stokes equations are solved with a multiple component polytropic
gamma law gas EOS with $\gamma = 1.67$. The boundary conditions in the $x$ and $y$
directions are periodic, while in the $z$ direction we have Neumann boundaries. The ambient
pressure was set to 52.87 g/cm ms$^2$ in order to keep the compressibility, $M^2 = \frac{2}{c_h^2}$ where
$c_h$ is the sound speed of the heavy fluid, low (0.008).

When simulating the fresh/salt water channel experiment, the Schmidt number is
$Sc = 620$ as specified by Mueschke. Keeping viscosity unchanged from the simulation
value given above, we need only modify $D$ to be $D = 0.0000034$ cm/ms$^2$. All other
input parameters are identical to the hot/cold water simulation.

For the simulation with all long wavelength initial perturbations are removed we
ignore input amplitudes with $k_x \leq 0.87$ cm$^{-1}$ and $k_y \leq 2.09$ cm$^{-1}$. This omits the first
dominant amplitude peak in each direction for density and the first dominant amplitude
peak in the $x$-direction for velocity. See also Table 6.

4. Conclusions

The algorithm proposed here has passed verification and validation tests in a manner
that appears to be unique and to go beyond the capabilities of other codes. Such tests
are in some sense never complete, and will no doubt be revisited in the future. Important
progress in turbulent mixing simulation has been achieved through use of this algorithm,
both in terms of agreement with experimental data, and in terms of resolution of long
standing issues, such as the relative importance of different factors contributing to the
values of $\alpha$, and their different importance in differing experimental apparatus.

Resolution of problems typically opens up new problems, and the present case is
no exception. We propose the following as important issues for the future of turbulent
mixing.

1 Deeper analysis of the modeling of initial conditions in the rocket rig experiments.

Specifically, the apparent lack of influence of long wavelength perturbations for
(most of) these experiments.
Table 6. Input parameters for the final three simulations from Fig. 8.

<table>
<thead>
<tr>
<th>#5</th>
<th>#6</th>
<th>#7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensionless physical parameters</td>
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<td></td>
</tr>
<tr>
<td>$g/g_0$</td>
<td>100</td>
<td>100</td>
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<tr>
<td>$A$</td>
<td>0.333</td>
<td>0.333</td>
</tr>
<tr>
<td>$Gr$</td>
<td>6.9E5</td>
<td>6.9E5</td>
</tr>
<tr>
<td>$Sc$</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>Dimensional physical parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\nu$ (cm$^2$/ms)</td>
<td>2.21E-2</td>
<td>2.21E-2</td>
</tr>
<tr>
<td>$D$ (cm$^2$/ms)</td>
<td>3.01E-4</td>
<td>3.01E-4</td>
</tr>
<tr>
<td>Initialization parameters, dimensionless</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda/\lambda_{th}$</td>
<td>2.62</td>
<td>2.62</td>
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<tr>
<td>$\lambda/\lambda_{IMD}$</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>Initialization parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda$ (cm)</td>
<td>3.6</td>
<td>3.6</td>
</tr>
<tr>
<td>$\lambda_{th}$ (cm)</td>
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<td>1.37</td>
</tr>
<tr>
<td>$\lambda_{IMD}$ (cm)</td>
<td>0.3</td>
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<tr>
<td>Domain and mesh parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mesh</td>
<td>$288 \times 180 \times 240$</td>
<td>$288 \times 180 \times 240$</td>
</tr>
<tr>
<td>Domain (cm$^3$)</td>
<td>$28.8 \times 18 \times 24$</td>
<td>$28.8 \times 18 \times 24$</td>
</tr>
<tr>
<td>$\Delta x$ (cm)</td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>

2 Explanation of the spread in experimental values for $\alpha$ through detailed simulation analysis of the individual experiments. Beyond the experiments referenced above, we mention the successful modeling [10] of the air-helium experiments [2].

3 Experimental validation of the temperature-concentration probability density functions. This will presumably require chemical reactions to indicate concentrations experimentally.

4 Analysis of the relative merits of various SGS models. Just as numerical algorithms come in various flavors, so do SGS models. What are the strengths and limits of each? Especially for test problems, such as those studied here, typical of turbulent mixing.

5 Blending the LES/SGS technology developed here into multiphysics studies, for example for high speed turbulent combustion, or astrophysical studies.

6 Which SGS models, if any, remain valid as the length separation between the resolved scales and the Batchelor or Kolmogorov scales increases? This question can be stated as the validity of SGS models in the high $Re$ limit, with the mesh held constant. This question is important to oceanographers and astrophysicists, among others.
Acknowledgments

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We thank David Youngs for the high quality scanned images from Figs. 1-6, the experimental data from Table 4, the permission to use them, and for helpful comments. [1] K. Asano. Mass Transfer: From Fundamentals to Modern Industrial Applications. Wiley-VCH, 2006.


