Multiscale models for fluid mixing

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1. Introduction

Turbulence is a prototypical multiscale problem, with a cascade of length scales generally too broad to be modeled effectively by explicit numerical algorithms. The dimensionless Reynolds number \( Re = VL/m \) governs this process, where \( L \) is a characteristic length, \( V \) is a characteristic velocity, and \( m \) is the kinematic viscosity. Turbulent mixing couples turbulence to a concentration equation and introduces the Schmidt number \( Sc = vl/m \) as a new dimensionless parameter, where \( \mu \) is the coefficient of molecular mass diffusion. We consider flows which are compressible and which couple the concentration equation actively into the flow dynamics (due to a density contrast, measured by the dimensionless Atwood number \( A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1) \), with \( A > 0 \)). These two properties introduce features into the modeling not present in theories of passive scalar transport by a turbulent field [35,3].
RANS and LES call for closure models, to introduce the influence of the omitted scales upon those computed. LES are formulated in terms of an averaging procedure. When this average is replaced by the mesh block average over the computational grid, the LES method is called implicit (ILES). The closure models generally contain parameters which are set by comparison to a more exact computation. In this sense LES and DNS (and physical experiments to the extent available) are used to validate the parameters in RANS models and DNS is used to validate those in an LES model.

A major concern of the present paper is the convergence properties of the DNS simulations. Thus we consider a mixture of resolved and under resolved DNS simulations (with no explicit subgrid models). The motive of such a study is to determine parameters and verification tests for LES closure models.

Since we recognize at the outset that it is not possible to represent all details of a turbulent mixing flow in a feasible computation, we list here the types of observables we would hope to compute correctly. The most important macroscopic variables are those which define the mixing zone, that is the edge position for the mixing zone as a function of time, and the time dependent locations of the principal shock waves (if any) which play a role in defining it. Additional macroscopic variables which serve to define the flow include the dominant size of the bubbles (light fluid inclusions in the heavy fluid) and mean fluctuations of the mixing zone edge. From the point of view of turbulent combustion, the microscopic (atomic) properties of the mixture are important, to specify the stoichiometry needed for combustion. According to [36], the joint probability distribution of the species concentrations and of the temperature is a required input for LES combustion models.

In terms of numerical tools, our major contribution (joint with other authors) is a high quality treatment of fluid interfaces, embodied in the FronTier code, based on a front tracking algorithm. Recent improvements to this method are described in Sections 2.1 and 2.3. Not only does this code allow zero diffusion across an interface (\(Sc = \infty\)) but, through use of a subgrid algorithm, any finite \(Sc\) can be modeled efficiently [33]. Comparisons to other interface methods have shown the quality of this method.

In terms of modeling flows, a major accomplishment has been the agreement we have achieved among theory, simulation and experiment for primary macroscopic variables describing 3D RT flows, as summarized in Section 2.2. In Section 2.2 we also document sensitivity of these variables to details of physical and numerical modeling. Remaining issues in this context are the use of subgrid models to account for scales not resolved in an LES simulation and the modeling of experimental (as opposed to idealized) initial conditions for mixing experiments.

In Section 3 we study averaged equations, similar in spirit to the RANS ideas mentioned above. For the planar symmetric flow geometry that we consider here, the averaging is in the \(x, y\) plane and results in variables depending on \(x, t\). For the circularly symmetric 2D flows, we average over the symmetry variable (the angle) to obtain variables depending on \(r, t\). We study a complete first order closure of the primitive inviscid equations; extensions to include transport terms are studied in [4]. This closure is totally hyperbolic in its time propagation and satisfies all required boundary conditions. Even for shockless flow, the entropy is not conserved as averaging is not isentropic [26], but an entropy inequality is valid. Our main result is that by comparison to direct simulation data, the unknown parameters in the closure terms can all be set. All but one are insensitive and can be set to unity; the remaining parameter is sensitive for RT flows only and is directly related to the motion of the mixing zone edges. In this sense the averaged equation closure model introduces zero parameters for the description of the mixing zone interior. The comparison simulations did not employ a subgrid model, but a careful examination of the relevant term in a standard Smagorinsky subgrid model indicates that this term (for the momentum equation) is negligible for these simulations [4]. Subgrid models for mass diffusion are far from negligible, and the proper setting of parameters in such models and their assessment is a central concern of the present and following [28] papers.

In Section 4, we begin to develop the link between microscopic and macroscopic aspects of mixing. Specializing to a 2D circular RM flow, we find sensitivities to numerical and physical modeling for macroscopic variables (temperature) and microscopic variables (concentration probability distribution functions or pdfs). The link is through the interface between the fluids, defined as a 50% concentration isosurface. The interface length depends sensitively on the numerical and physical modeling. Consequently, interface sensitive quantities such as mass diffusion and atomic level mixing (concentration pdfs) have a similar dependence. Relevant to the discussion of the present simulations, we mention that macroscopic variables such as mixing zone edges and shock wave trajectories are insensitive to variation of physical and numerical modeling details [28,34] while the microscopic variables such as the concentration and temperature pdfs are highly sensitive. Again, our goal, starting with the present paper, and continuing with later papers in this series, is to establish converged definitions of the LES subgrid models, especially as they relate to the Schmidt number and to mass diffusion.

2. Numerical methods

2.1. Locally grid based tracking

In collaboration with coworkers, we have proposed Front Tracking as an algorithm to eliminate numerical mass diffusion across a fluid interface [16,13]. In this algorithm a front, i.e. a codimension one grid, specifies a fluid discontinuity location. This front moves freely through a regular rectangular grid. Riemann solutions constructed in a normal direction at the front provide the physics based dynamics to move the front at each time step. This algorithm is highly accurate, but it is not robust in the face of dynamically generated self intersections and topological bifurcations of the front. Locally in space and time, we reconstruct the front in a neighborhood of any such bifurcation. The reconstruction is based on the intersections of the front with the regular grid cell edges, and uses a small number of standard templates. With this modification, called locally grid based front tracking, the algorithm is both accurate and robust [13].

Our two main points regarding front tracking are the following: First, tests [29] of a mathematical nature, which have been used by others for comparison of interface codes, were extended [13] to include front tracking simulations. Within the context of these tests, the locally grid based tracking method is seen to be as accurate or better than particle methods, and better than all the others (level set, volume of fluid, untracked) included in this test. We did not include a timing comparison with our accuracy tests [13] as the only publicly available level set code we were aware of was coded in Matlab, and for this reason was judged to be an unfair (too slow) comparison to the FronTier code written in C, C++. We did not include comparison to the particle level set in this comparison as we were not aware of a publically available particle level set code suitable for such comparison. These tests assess capabilities at the time they were conducted and do not reflect possible future improvements to Front Tracking or other methods. Secondly, the tracking code, separated from physics implementations, is available for downloading at
The algorithm is conservative for interior cells, not cut by the front, but it is not conservative at the front. Under development is a totally conservative front tracking algorithm. In this case the front is tracked as a space time surface (three dimensions in the four-dimensional space time, for the case of three spatial dimensions). The space time cells cut by this surface are differenced using a finite volume approach [20,19,18,21,30,31].

2.2. Models with transport and scale-breaking phenomena

We improved the physics modeling for Rayleigh–Taylor mixing by adding scale-breaking physical phenomena: surface tension (for immiscible fluids) and physical mass diffusion (for miscible mixtures). For two fluid immiscible mixing, the interface is sharp and the numerical model of a tracked surface mimics the physics correctly. For miscible mixing, the tracked surface is a 50% isoconcentration surface. The equations solved in this section are the standard single fluid Euler equations [10], with the density jump introduced through a thermal discontinuity, and the equation of state a gamma law gas. To these equations, we have selectively added transport or surface tension terms, as discussed below. Mass flux through this isosurface, in accordance with Fick’s law, is modeled, so again the numerical modeling follows the physical model. The result of the improved models and the improved numerics was an impressive agreement between simulation and experiment for the overall growth of the mixing layer, defined dimensionlessly as $z$ below, for the bubble width to height ratio, for the fluctuations in the bubble heights, and for the measure $\theta$ of local averages of mixture [15,32,27]. For the case of physical mass diffusion, the amount of diffusion was so small in the experiments being modeled that a special modified tracking algorithm was needed to control and limit this diffusion [33].

For RT simulations, a primary macroscopic variable is the overall mixing rate $x$, defined as $x = h/Ag^2$, where $h$ is the penetration distance of the light fluid (bubbles) into the ambient heavy fluid. We have found this variable to be quite sensitive to details of physical modeling (transport coefficients, surface tension) and to their numerical analogues (numerical mass diffusion and numerical surface tension). For example, Fig. 1 shows (a) agreement of our simulation with the experimental results, (b) sensitivity of the simulation to the value of dimensionless surface tension $\sigma$ used in the numerical model, and (c) sensitivity to numerical mass diffusion in the untracked simulations. Compare the untracked simulation data points at the far left of the plot (for $\sigma = 0$) to the others.

The fact that all experiments have a common value of dimensionless surface tension was noted by us earlier [15]. The dimensionalization of the surface tension involves a length scale, as does the (presumed) initialization. The initial wave length, as determined by a theoretical dispersion analysis forces all experiments to have the same dimensionless surface tension. If this initial disturbance length scale is instead determined by observation of the data, a minor spread about the dimensionless surface tension values of Fig. 1 occurs. In this figure, the untracked alpha group simulation results are those of [11].

To further demonstrate the role of numerical mass diffusion, we define a time dependent Atwood number $A(t)$, based on the time dependent densities observed within the simulation. Specifically, for each $t$ and each $z$, we find the maximum and minimum density, and using these define a time and height dependent $A(t,z)$. This quantity is averaged over the upper half of the bubble portion of the mixing zone, roughly the upper quarter of the mixing zone, to define $A(t)$. This $A(t)$ contains all numerical effects of mass diffusion from the simulation. Using it, we define to a renormalized (mass diffusion corrected) mixing rate, $x_{ren} = h/2 \int (A) g ds$ (left frame) and $x_{ren}$ (right frame), for distinct simulations, tracked and untracked, and with and without physical mass diffusion. The left plots for $z$ do not coincide, indicating sensitivity of this variable to numerical methods and to physical modeling. With the standard definition of the mixing rate $x$ (i.e. the slope of the curves in this figure), the simulations differ by factors of two or more, so they are not at all the same. The right curves are identical, having nearly equal slopes, indicating that the numerical or physical mass diffusion (whose influence is removed in the right frame but not the left frame) is the primary factor differentiating these simulations. Here the physical mass diffusion is the molecular value taken from the experimental fluids, as described in the cited references. The phrase ideal refers to a simulation in which physical values of both surface tension and mass diffusion are set to zero.

We conclude that the differences among these simulations are due to mass diffusion (numerical or physical) and that once this difference is compensated for, the simulations behave in a similar manner. This sensitivity of the macro properties of the mixing (to the micro aspects of the flow (physical or numerical mass diffusion and surface tension) is a central theme of this paper, and will be developed more explicitly in Section 4.

2.3. Subgrid models

The subgrid model we used to represent molecular mass diffusion [33] is intended to express physical levels of mass diffusion, without adding numerical mass diffusion. Thus, its effect is to subtract (not add) diffusion relative to a more conventional (untracked) simulation method. Normally, subgrid models are introduced for a different purpose. Due to the amplification of small scale mixing at a subgrid level for turbulent flow, there is a physical basis for considering levels of diffusion beyond the value from molecular physics. The conventional subgrid model will introduce into the resolved scales (for an LES simulation), effects produced at a subgrid scale. In this sense the purpose of the subgrid model is to add diffusion. We reference [24], for example: the models are specific to 3D turbulence.

To assess the accuracy of these simulations in the absence of conventional subgrid models, we note that the DNS simulations of Section 4 do not require a subgrid model. The role of a viscosity subgrid model for the underresolved DNS simulation was assessed directly. In our 3D RT simulations we found this term to be three
orders magnitude smaller than the physical viscosity term, itself so small relative to the physical mass diffusion term [27] that we considered it as zero. For the 2D simulations of Section 4, we repeated some of these with a Smagorinsky term added. The effect was 8% to 10% in Fig. 6 and about 2% in Fig. 7. On this basis, we believe that our resolved DNS simulations are scientifically relevant.

Subgrid mass diffusion models are a different story. For the 3D RT simulations applied to macro observables, i.e. the motion of the mixing zone edges, we note the agreement with physical experiments and comments (already published and noted in Section 1) regarding possible limitations. We also note the consistency of our simulation results over a period of years, during which the meshes have become more refined. For surface tension (immiscible) simulations there is no mass diffusion and no subgrid mass diffusion model. For the 2D RM simulations our primary motivation is to obtain data to allow eventual parameterization of subgrid diffusion models. Only the resolved DNS simulations are judged to be scientifically relevant regarding concentration pdfs. The underresolved DNS simulations serve to illustrate the convergence process for the miscible case, for concentration pdfs. For this reason, we show only resolved DNS pdfs in Fig. 8 and correlation lengths in Table 1.

### Table 1

<table>
<thead>
<tr>
<th>Mass Diffusion</th>
<th>Sc = 10</th>
<th>Sc = 1.0</th>
<th>Sc = 0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion</td>
<td>0.06</td>
<td>0.28</td>
<td>0.63</td>
</tr>
<tr>
<td>Correlation</td>
<td>0.07</td>
<td>0.09</td>
<td>0.12*</td>
</tr>
<tr>
<td>Diffusion/Correlation</td>
<td>0.86</td>
<td>3.11</td>
<td>5.25*</td>
</tr>
</tbody>
</table>

*Representative value depending on setting of the transport coefficients. Further study is in progress.

3. Multiscale modeling of macro phenomena

3.1. Two fluid equations

Turbulent mixing gives rise to chaotic flow behavior and an absence of pointwise convergence for numerical simulations. We interpret convergence statistically, and study convergence in terms of averages. In a systematic study of a RM unstable flow [44], we used the following steps to achieve convergence in this sense. First we separated the flow into homogeneous regions defined by the principal waves (incoming, reflected outgoing shock waves, edges of the mixing zone). Position errors in the location of these waves were analyzed and convergence properties established. In the relatively smooth regions between these waves, mean convergence rates were determined. We found different convergence properties for different regimes: singly vs. double shocked material, single vs. mixed phase regions and heavy vs. light fluids. The benefit of the error analysis carried out separately in these distinct homogeneous flow regimes was a large decrease in the variance of the error and a more accurate description of the convergence properties.

3.2. Averaged equations

For many purposes, the mean flow properties of each fluid phase or species is sufficient information and the detailed flow description provided by a finely resolved simulation is more than is required. It is for this reason that the derivation of averaged equations is a popular study. In [25,26] and earlier papers in this series, we have proposed averaged equations for the interior of the mixing zone, coupled to the buoyancy drag equations for the motion of the edges of the mixing zone. The equations for the interior have a functional form derived from a mathematical analysis of the averaged, unclosed, equations. Closure comes from assigning values to unknown parameters in these functional forms. We then observe that all but one of the parameters are insensitive and conveniently set to one, while the single remaining parameter is specified by the mixing zone edge motion. The buoyancy drag equations [7,8] for the motion of the edges of the mixing zone fit all available RT and RM data using a single (light fluid) drag coefficient (and for large A, a second parameter to model the A dependence of the heavy fluid drag coefficient). No additional parameters are needed for the averaged equations. In other words, the modeling of the interior of the mixing zone is parameter free.

We obtain closure models which have a 10% average error in residuals for the closure terms, measured in comparison to two fluid direct RT and RM simulations. Models from other authors [40,41,1] have errors, similarly measured, that were two times larger or more. Here error is defined as

$$\frac{\sum |\text{closure} - \text{exact}| dz}{\sum |\text{exact}| dz},$$

where the sum extends over the closure terms (i.e. over the $v'$, $p'$, and $(pv')'$ closure terms) and over time steps within a time period of mixing [4] and the integral extends over the mixing zone. The terms exact are defined by (6) applied to the unaveraged simulation data. A more detailed discussion of related issues can be found in [4].

Applying the ensemble average to the Euler equations for fluid flow, we obtain the one-dimensional two-pressure two-phase flow averaged equations. We follow [12,5,6,39] to obtain...
for the volume fraction \( \beta_k = \langle \chi_k \rangle \), velocity \( \mathbf{v}_k \), density \( \rho_k \), pressure \( \rho v \), and total energy \( E_k \) of phase \( k \). Here \( g = g(t) > 0 \) is the gravity and \( \langle \cdot \rangle \) is an average over the \( x, y \) symmetry plane and an in principle an ensemble average. Also \( X_k \) is the indicator function of phase \( k \). Generalizations of these equations, not shown here in the interest of simplicity, allow for circular or spherical averages in a cylindrical or spherical geometry.

The equations differ from the primitive Euler equations through inclusion of an Eq. (2) for the transport of the volume fraction. They contain volume fraction factors \( \beta_k \) not present in the primitive equations. They differ through the unclosed expectations in the momentum and energy equations. These expressions will be closed below. The equations are in one space and one time variable, in contrast to the primitive equations, in three space and one time variable. Also the discontinuous interface is removed from the (smooth) initial conditions.

Three interfacial terms are defined by

\[
\langle \mathbf{v} \cdot \nabla X_k \rangle = v^* \frac{\partial \beta_k}{\partial t} + \left( p \frac{\partial X_k}{\partial x} \right) = p \frac{\partial \beta_k}{\partial t}, \quad \langle \mathbf{v} \cdot \nabla X_k \rangle = \langle \mathbf{v} \rangle \frac{\partial \beta_k}{\partial t}. 
\]

We have thus defined

\[
v^* \mathbf{v} = \mathbf{v} \frac{\partial \beta_k}{\partial t} + \mathbf{v} \mathbf{q}_k, \quad q = v, p, pv, \text{ represent averages of microscopic quantities.}
\]

We have derived a functional form for each \( q^* \) and identified in them the free parameters. Thus the closure, given the mixing zone edge motion, is a zero parameter model. We assume a closure which represents \( q^* \) as a convex sum of the primitive variables \( q_k \) for \( q = v, p, pv \)

\[
q^* = \mu^q_1 q_1 + \mu^q_2 q_2, \quad q = v, p
\]

and a related bilinear expression

\[
\langle pv^* \rangle = p^* (\mu^p_1 v_1 + \mu^p_2 v_2) + v^* (\mu^p_1 p_2 + \mu^p_2 p_1) - (\mu^p_1 p_2 v_2 + \mu^p_2 p_1 v_1)
\]

for \( pv^* \). The convex coefficients \( \mu^q_1 \) are assumed to have a fractional linear form, based on a mathematically exact reformulation of the original (unclosed) equations. Namely

\[
\mu^q_1 = \frac{\beta_k}{\beta_k + d_k^p q_k}, \quad q = v, p, pv
\]

here \( k' \) is the complementary index to \( k \). We determined [4] that the parameters \( d_k^v \) and \( d_k^p \) are insensitive in our comparison to RT and RM data and so we set

\[
d_k^v = 1 = d_k^p.
\]

Also \( d_k^v \) is insensitive for the RM data and in this case we set it to 1; for the RT data, it is determined from the edge motion data [22,23]. In this sense, the model for the mixing zone interior has no adjustable parameters and the full mixing model has only one or two. Accuracy of the closure is obtained by comparing values from (6) to those obtained from using (8)–(11).

These equations differ from conventional equations for multiphase flow in the form of the closures, especially for the pressure, in the assumption of distinct phase pressures, and in their totally hyperbolic property (absence of complex eigenvalues for time propagation) in the inviscid case.

4. Multiscale modeling of micro phenomena

We return to the two fluid flow models of Section 3.1. In other words we next consider the full two fluid flow with no averaging. We are concerned here with the 2D Richtmyer–Meshkov instability referenced above. 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 [44]. Initial and late time simulation density plots are shown in Fig. 3.

This problem was the subject of a code comparison study (RAGE and FronTier) [34], which showed general agreement in most of the macroscopic variables, but differences in a few. In this sense the study raised fundamental issues. The fluid interface (measured in the FronTier simulation only), at late time, is volume filling. In its mesh dependence, it has a chaotic nature, both terms referring to the fact that the late time interface length occupies a statistically constant fraction compared to the edge length of each mesh block within the mixing zone. The transport coefficients (viscosity and mass and thermal diffusion) are small and, as is a common practice, were set to zero in the original study. Our main conclusion is that the modeling assumption \( \nu = 0 = \mu \) leaves the problem underspecified; we show that the solution, in its macroscopic behavior, depends on the Schmidt number; it similarly depends on the Prandtl number. With no physical transport mechanism, the numerical analogues (numerical mass and thermal diffusion and numerical or artificial viscosity) and their ratios, the numerical Schmidt and Prandtl numbers, play the role of the missing physical variables, and select the solution. A computer code may then converge to the nonunique solution defined by its own numerical Schmidt and Prandtl numbers.

In order to explore grid convergence effects on simulated turbulence and mixing in high Schmidt number flows, we artificially specify a range of values for viscosity and mass diffusivity. In this way we explore a range of resolved and underresolved DNS studies for a single problem.

We start with the primitive Navier–Stokes equations with transport for a mixture of two compressible species

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0, \quad (12)
\]

\[
\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \mathbf{d}, \quad (13)
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (E + \rho) \mathbf{v} = \nabla \cdot \kappa \nabla T + \nabla \cdot \mathbf{d} \cdot \mathbf{v}, \quad (14)
\]

\[
\frac{\partial \rho \psi}{\partial t} + \nabla \cdot \rho \psi \mathbf{v} = \nabla \cdot \rho \psi \nabla T, \quad \psi = \mu, n
\]

The dependent variables \( \rho, \psi, \mathbf{v}, \rho, p, E \) denote, respectively, the total mass density, the species mass fraction, the velocity, pressure, total energy, \( \kappa \), the coefficient of heat conductivity, is set to zero in the present work.

The equation of state (EOS) is defined for each of the species as a stiffened gamma law gas, and according to [2], the mixture EOS is a stiffened gamma law gas also. The viscous stress \( \mathbf{d} = 2\nu(S - \frac{1}{2} \text{tr} \mathbf{S}) \mathbf{I} \) and \( S_h \) is strain rate tensor

\[
S_h = \frac{1}{2} \left( \frac{\partial \mathbf{v}}{\partial x} + \frac{\partial \mathbf{v}}{\partial y} \right).
\]

A more fundamental theory of multifluid viscosity is described in the book of Williams [43], to which the present theory is an approximation.

To these equations, we apply a filter, or local average, to derive the the filtered continuity, momentum, energy and concentration

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \right) = 0, \quad (15)
\]

\[
\frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \mathbf{v} \right) = \nabla \cdot \mathbf{d} + \nabla \cdot \kappa \nabla T, \quad (16)
\]
The equations of two miscible fluid species in an inertial frame [24]. The filtered quantities are considered to be mesh block averages, and denoted with an overbar, while mass averaged quantities are denoted with a tilde. We obtain

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{17}
\]

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nabla \cdot \tau + \nabla \cdot \mathbf{d} - \nabla \cdot \mathbf{\tilde{q}}, \tag{18}
\]

\[
\frac{\partial E}{\partial t} + \mathbf{v} \cdot \nabla E = \nabla \cdot \mathbf{\tilde{q}} + \nabla \cdot \mathbf{\tilde{d}} - \nabla \cdot \mathbf{\tilde{q}}^T, \tag{19}
\]

\[
\frac{\partial \rho \mathbf{e}}{\partial t} + \nabla \cdot (\rho \mathbf{e} \mathbf{v}) = \nabla \cdot \rho \mathbf{\tilde{q}} \mathbf{v} - \nabla \cdot \mathbf{\tilde{q}}^T. \tag{20}
\]

Also

\[
E = \rho \mathbf{e} + \rho \mathbf{v}^2 / 2 + \tau_{\text{vis}} / 2 \tag{21}
\]

and $e$ is the internal energy.

The Reynolds stress $\tau$ is given by

\[
\tau = \rho(\mathbf{v} \mathbf{v} - \mathbf{\bar{v}} \mathbf{\bar{v}}). \tag{22}
\]

The closure terms $\tau$, $q^T$ and $q^w$ are set to zero, consistent with our objective to solve the DNS limit and obtain data to allow parameterization of these terms. In this sense, we solve the primitive equations, which result from dropping the closure terms, and not the filtered equations. For this purpose, the bars and tildes in (17)–(21) can be omitted. However, for comparision, we have done sample simulations with a standard Smagorinsky definition for $\tau$ and observed effects less than 10% in the DNS limit.

We have already observed [27] that the interface for the problem under study has a length proportional to $\Delta x^{-1}$, with respect to its mesh (non) convergence (i.e. rate of divergence) properties. Here we re plot this data [27] in Fig. 4, left frame. The interface length divided by the mixing zone area is plotted vs. time, with both the length and the area measured in mesh units. The mixing
area is defined as $\pi \times (r_{max} - r_{min})$, where $r_{max}$ and $r_{min}$ are the radii which encompass the 5% and 95% volume fraction contours after a radial average of the data. This area is then converted into grid block units. A related study, for a single mode RT instability in 3D is shown in Fig. 4, right frame. The flow morphology of a single mode RT disturbance is far less chaotic than a multimode RT flow, but there is still vortex shedding from the mushroom caps at the spike tip, and at late time, resulting patches of chaotic and turbulent flow.

From Fig. 4, left, we observe that somewhat after reshock, the interface fills a constant fraction of the mesh area of the mixing zone. The mesh level surface fraction is time independent, after a relaxation period following the second shock passage. This mesh level surface fraction is about 30% relative to the mixing zone itself. In this sense the interface is mesh volume filling, cutoff by the mesh, and has a chaotic nature in relation to mesh refinement.

The divergent nature of the interface raises questions for the convergence of the numerical procedure, in the absence of regularizing physics. As a simple, prototypical error analysis, we propose the formula:

$$\text{Error} = C_1 \times \Delta x \times (\text{Interface Length or Area}) = C_1 C_2$$

for the error measured in $L_1$ in space at a fixed time, thus raising questions regarding convergence for the unregularized problem. This formula is suggested by Fig. 4, in which the perturbation wave length of the initial data is fixed, and for fine grids, is exceedingly well resolved. Here the $C_i$ are $1(1)$ constants, apparently independent of $\Delta x$ over the grids explored here. $C_1$ is related to numerical mass diffusion, and might take on values in the range of 3.0 for typical codes; for FronTier, we typically see values four to eight times smaller [14]. $C_2$ for the present problem and grid levels, has a value in the range 0.2 to 0.3.

Due to the turbulent cascade of active length scales, new (smaller) instability length scales are introduced dynamically, unless some physical or numerically based regularization prevents this. In the absence of regularization, it is ultimately the grid which cuts off the development of the finest scale, and the smaller of those remaining will, of necessity, be under resolved, as (23) suggests, independently of mesh refinement. As observed in Section 2.2, convergence depends on the variables under study. Thus we expect the pessimistic conclusion of (23) to apply only to those macro flow variables which depend sensitively on the micro structure of the mixing.

4.1. Convergence revisited: finite $Re$, $Sc$

We define $Re = VL/\nu$ as follows. $\nu$ is the kinematic viscosity, and $\langle \cdot \rangle$ is an angular average (and in principle an ensemble average). $V$ is the turbulent fluid velocity, $V = \sqrt{\langle \delta V^2 \rangle}$. Here $\delta V_r = V_r - \langle V_r \rangle$ is the fluctuating part of the radial velocity, $\delta V_{ir} = V_{ir}$ is the fluctuating part of the rotational velocity, and $\delta V^2 = \delta V_r^2 + \delta V_{ir}^2$. $L$ is the radial width ($r_{max} - r_{min}$) of the mixing zone. A constant dynamic viscosity is used directly in the simulations, so the kinematic viscosity, needed for the determination of $Re$, is density dependent, and computed as an angular average. To minimize the mesh dependence of various computed quantities, we also introduce the mesh Reynolds number $Re_{mesh} = \frac{V L}{\nu}$ and $Re_{mesh}$ is defined as $\frac{V L}{\nu}$, where $V$ is the turbulent fluid velocity, and $\nu$ is the dynamic viscosity. The Kolmogorov length scale $l_k = \langle \delta V^2 \rangle^{1/4}$ or the viscous inner scale, approximately $50 \lambda_k$, is a measure of the lengths at which viscosity plays a role, and this is related to the level of mesh refinement needed for a DNS simulation. For comparison, $\Delta x$ for the finest grid and smallest Reynolds number considered here is comparable to $\lambda_k$ and well below the inner viscous scale, indicating that the calculation is in the DNS range. Here $\epsilon$ is the dissipation rate

$$\epsilon = \frac{\nu}{2} \langle S_{ij}^2 \rangle.$$

Plots relating $Re$ and $\lambda_k$ to $Re_{mesh}$ are given in Fig. 5. Many of our plots refer to a specific time $t = 90$, a time corresponding to the beginning of the fully developed chaotic regime, after reshock.

Our first result concerns the mesh length fraction, as plotted in Fig. 4. It is largely independent of the Schmidt number and is also mainly independent of Reynolds number for $Re_{mesh} \geq 8$. Below these values, the chaotic development of the interface appears to be cut off, in that mesh refinement with no other change of parameters (which will decrease $Re_{mesh}$ but not $Re$) also decreases the mesh length fraction. The cutoff is notably sharper for the smaller $Sc = 0.1$ than for $Sc = 1.0$. The cutoff region is the region in which the solution appears to be “fully resolved”, i.e. DNS in regard to the interface length. See Fig. 6.

We propose two quantities for which there is at least some evidence to suggest a possible dependence on the chaotic structure of the interface: the probability distribution of (light and heavy fluid) concentrations, and the temperature, both at late times.

The identification of temperature as a sensitive quantity originated in a careful study [34], comparing RAGE and FronTier simulations. Continuing this investigation, we observe a dependence of the maximum temperature on $Re_{mesh}$ in the same parameter region. See Fig. 7. According to [34], we expect approximate convergence for $T_{max}$ with a mesh of $800 \times 1600$, so the mesh dependence in Fig. 7 is expected. This is most pronounced in the under resolved range of simulations. We also observe roughly a factor of 10 change in the values of $Re_{mesh}$ for the location of the drop in $T_{max}$ between $Sc = 0.1$ and $Sc = 1.0$. All data points of Fig. 7 lie below the ideal (Re $= \infty$, Sc $= \infty$) values of FronTier and virtually all are above the ideal values reported for RAGE [34]. On the basis of the evidence reported, we believe that $T_{max}$ is sensitive to various details of numerical and physical modeling.

The main evidence for simulation sensitivity of the density distribution is our earlier analysis relating the simulated RT mixing

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**Fig. 5.** Left: $Re$ vs. $Re_{mesh}$ at $t = 90$ for several mesh levels. Right: a similar plot for the mesh Kolmogorov scale $\lambda_{k,mesh} = \lambda_{k}/\Delta x$ vs. $Re_{mesh}$. Both plots are virtually independent of $Sc$ for the range of $Sc$ considered. For each grid level, some of the simulations are resolved below the Kolmogorov scale, and are thus DNS.
rate $\alpha$ to numerical mass diffusion, discussed in Section 2.2. See also Fig. 2. It was a pleasant discovery of the code comparison study [34] that the RM mixing growth rates and the edges of the RM mixing zone are similar (but not identical) in this comparison. We are not aware of many studies of pdfs for mixture fractions in RT and RM chaotic mixing. In the 3D RM planar gamma law gas simulations of [24], at a time significantly after reshock, the mixture fraction pdf shows a weakly bimodal character and is fit to a smooth curve. We find only a few types of histograms from the many different simulation patterns. Most are strongly bimodal, with narrow peaks at mixture fractions perhaps 0.1 and 0.9. For a few, the light fluid peak (at 0.9) is considerably diffused or even missing completely. We display a typical plot of the pdf for each of these types. All of the simulations in the under resolved region ($Re_{\text{mesh}} \geq 10$) are bimodal. In the DNS regime ($Re_{\text{mesh}} \leq 10$), the highly diffusive simulations ($Sc = 0.1$) have a partially or highly diffused light fluid component, while the less diffusive simulations ($Sc > 1$ and especially $Sc = 10$) tend to be bimodal. See Fig. 8. The data presented is from the time $t = 90$, which is the beginning of highly chaotic stage of interface development. We also examined the light fluid mixture fraction pdf at $t = 110$, in order to allow more time for diffusion, and did not observe a striking change in the pdfs.

We emphasize that all frames of Fig. 8 are in the DNS regime, with $Re_{\text{mesh}} = \mathcal{O}(1)$ and some degree of convergence (or reduced resolution $\Delta$).
divergence) for the interface length. Thus the progression of increased diffusion observed in Fig. 8 reflects a change in the physical formulation of the problem, namely an approximate 10-fold increase in mass diffusion with each successive frame, and is not related to mesh convergence or subgrid model issues.

To understand these results, we first realize that the result of diffusing heavy fluid into a region of light fluid can easily make a large change in the mixture fraction, while the diffusion of the same fraction of light fluid into a region of heavy fluid will have a relatively smaller effect. This appears to be the reason that we only observe extensive diffusion of the light fluid regions.

To differentiate among the cases showing more or less diffusion within the light fluid regions, we need to introduce two length scales and their dimensionless ratio. The first is a diffusion length scale, set to \( \sqrt{4D(t - t_0)} \). Here \( D \) is the diffusion constant, and \( t_0 \) is a time for the beginning of the diffusion. The value for \( t_0 \) depends on the location within the mixing zone and on the species type. For example, majority phase at the edge of the mixing zone has just entered the mixing zone, and for such a fluid parcel, \( t_0 \approx t \). An analysis of this issue was conducted in [9], but for the present purposes, and with the midline of the mixing zone used for data collection, we assume that \( t_0 \) is the time of the reshock passage through the interface, \( t_0 \approx 70 \).

The second length scale is a kind of minimum radius for the fluid component, or mean distance to the complementary phase, introduced in [37,38] for models of opacity, and studied in [17] as a measure of fine scale mixing length, in an RT context. For the three simulations studied in Fig. 8, we plot the probability of a minimum distance for change of fluid component, starting at a random point in the light fluid at the mid radius (being analyzed). The results are shown in Fig. 9, for angular (tangential) direction correlations. The results are fit to an exponential and the correlation length is determined. The results are summarized in Table 1. The results in the table are clear: for \( \lambda_{\text{diffusion}} < \lambda_{\text{correlation}} \), the mixture fraction is strongly bimodal. For \( \lambda_{\text{diffusion}} > \lambda_{\text{correlation}} \), the mixture fraction is weakly bimodal or even unimodal.

5. Conclusions

In this paper, we have formulated goals for turbulent mixing. The goals are observables of the solution to be computed; they include macroscopic observables such as the trajectories of the principal mixing zone edges and shock waves (if any) of the solutions. They also include microscopic variables such as the joint temperature and concentration probability distribution function of the mixture. We survey recent results of the authors and co-workers on turbulent mixing, and present new results.

We have observed that some of these observables are sensitive to details of physical and numerical modeling.

For these cases, it is our observation that numerical mass diffusion is a serious concern, and without regularizing physics, will remain so even in the presence of large amounts of mesh refinement. Examples of simulations which achieve agreement in macroscopic variables with physical experiment while controlling numerical mass diffusion are presented.

Because of this simulation sensitivity, we have examined the process of convergence to the fully resolved DNS limit. We regard this convergence study as a step towards our future goal to define diffusion sub scale models and their parameterizations, to allow practical converged solutions.

References


