From *SIAM News*, Volume 39, Number 5, June 2006

Complex Fluid Mixing Flows: Simulation vs. Theory vs. Experiment

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It is an old saw that science has as its three pillars theory, experiment, and simulation. That we can believe simulation when the three do not agree is a testament to a newfound credence for simulations.

Our story concerns widely different simulation and experimental results in a problem of long standing: determination of the rates of chaotic mixing resulting from acceleration across a fluid density discontinuity, namely the classic Rayleigh–Taylor (RT) instability. RT and other interface instabilities [1,9] have long attracted the attention of leading applied mathematicians and physicists, not only Rayleigh and Taylor but also Kelvin, Chandrasekhar, Fermi, Garrett Birkhoff, and John Wheeler, among others. These instabilities occur in flows important both to basic science (supernova explosions) and to technology (inertial confinement fusion).

The simplest and most important variable used to describe the mixing rate of fluids of different densities is the dimensionless parameter α, which characterizes the penetration distance h of the lighter fluid (in structures called bubbles) into the heavier fluid: $h = \alpha\, Agt^2$. Here, g is the acceleration force, such as gravity; A is the Atwood number, a dimensionless measure of the contrast in the densities (ρ_1 and ρ_2) of the two fluids: $A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$; and t is time. In gravitational free fall, $\alpha = 1/2$; this value of α describes the penetration of the heavier fluid (in structures called spikes) in the case of an extreme density contrast, $A = 1$. The formula predicts constant acceleration for the mixing front, as explained below (Theory).

The Problem

Stated simply, the problem is that the values of the mixing rate α, as determined by experiment, theory, and (most) simulations, do not agree. Despite extensive efforts by large teams, working for years or in some cases decades, most simulations yield values of α much smaller (half or less) than the values determined experimentally.

Faced with this situation, some assert that the simulations and the experiments do not describe the same physical problem. A commonly favored view is that unobserved (because small in amplitude) long-wavelength noise in the initial state of experiments enhances the growth rate to a value about double that found in simulations. The simulations, being conducted under pure short-wavelength random initial conditions, should not, according to this view, agree with the experiments.

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Our view, in contrast, is that the discrepancy between experiment and simulation is caused by two systematic errors in the simulations. The first is excessive numerical diffusion and grid-related surface smoothing that occur with the solution algorithms commonly used for this problem. The second is omission of transport and other scale-breaking effects in the physical modeling. As explained below, results in excellent agreement with experiment are obtained, without the need to invoke hypothetical long-wavelength noise in the initial data, when *both* of these errors are corrected. Eliminating numerical diffusion and surface smoothing increases the computed growth rate by more than a factor of 2, scale-breaking effects reduce the growth rate somewhat, and a balance between the two gives a value close to that found experimentally.

Experiments

Experimental results have been remarkably consistent, with growth rates generally having the value $\alpha_{\text{experimental}} = 0.06 \pm 0.01$. At least four groups, using distinct experimental devices and a large range of distinct fluids, have found this value. From this we infer that the long-wavelength noise is not only too small to be observed initially, but also relatively universal or common across different apparatuses.

Theory

Theory supports the experimental values of α. We consider an ensemble of round-tipped cylindrical bubbles of a light fluid moving upward through a heavy fluid under the influence of gravity. We also assume a (correlated) statistical distribution of heights and radii for the bubbles in this ensemble. A simple statistical model of bubble interactions, leading to a prediction for the growth rate α that is consistent with experimental values, follows from three basic facts.

First, larger bubbles move faster than smaller bubbles, so that large bubbles will pull ahead of their smaller neighbors. Second, the smaller bubbles that are left behind drop out of the bubble penetration front. This allows the remaining bubbles at the front to grow larger, and move faster, endowing the mean position of the bubble front with an effective acceleration. Finally, interactions between pairs of bubbles at the front are observed to give the leading bubbles an additional velocity, which enhances the acceleration of the front.

Made quantitative, these ideas lead to the theoretical prediction $\alpha_{\text{theory}} = 0.06$. This prediction is not based on any long-wavelength initial noise and thus should, although it does not, agree with (most) simulations. The theory predicts not only α, but also a number of other features of the flow, which we have confirmed quantitatively in analyses of our "front-tracking" simulations, as described below. Agreement be-tween theory and experiment, even for these expanded flow features, was derived as part of the original presentation of the theory; see [2].

Simulations

It is well known within the computational science community that use of (Eulerian) finite-difference methods in the solution of fluid equations with density discontinuities leads to substantial numerical mass diffusion. Mass diffusion is particularly important in chaotic RT simulations for three reasons. First, density differences drive the instability, and mass diffusion thus masks the driving force of the instability. Second, the interface between the two fluids is unstable, and its area increases very significantly throughout the simulation, thereby allowing for enhanced numerical (or physical) mass diffusion in a 3D mixing context.

Third, the solution methods are expensive; representing a balance between conflicting objectives, they lead to gross under-resolution and, consequently, substantial numerical mass diffusion. The two conflicting objectives are (1) statistical inclusion of a sufficient number of modes to give randomized mode–mode interactions a chance to develop and (2) numerical resolution per mode sufficient to allow accurate simulations. In a typical 3D simulation, the bubbles grow in the z direction and are arranged in a roughly planar array, with some 50×50 modes initially present in an x, y plane, each resolved with about 5×5 mesh cells. It is known that the numerical diffusion of a density jump will quickly spread to a width of three cells; under such conditions, it is clear that much of the density contrast is obliterated in the numerical integration of the equations.

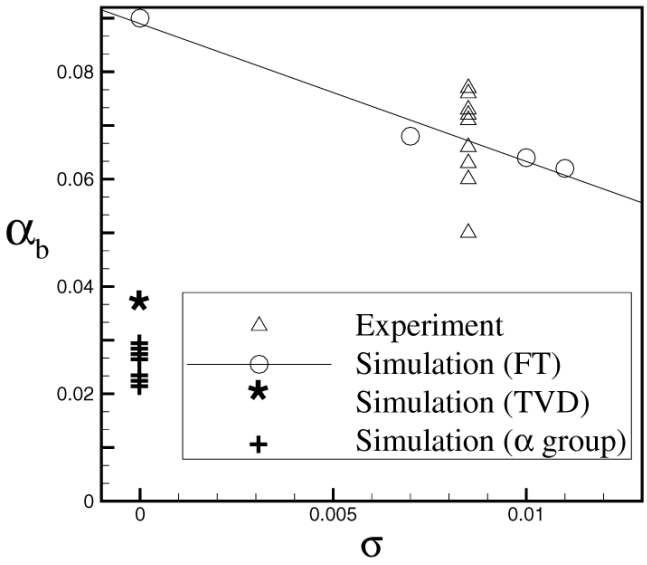

Figure 1. *Plot of growth rate α vs. dimensionless surface tension as determined experimentally and in various tracked and untracked simulations. Front-tracking simulations and plot courtesy of Xinfeng Liu.*

In an analysis of such a simulation, performed with a typical numerical method, Xiaolin Li [6] quantitatively confirmed this unpleasant picture. The numerical mass diffusion reduced the density contrast (the value of the Atwood number A, computed on a time-dependent basis) by 50%, just about the amount by which the simulation underpredicted experimental values; see [4].

Over the years, working with several colleagues, we have developed high-resolution numerical methods specifically designed to avoid numerical mass diffusion. Our front-tracking method uses two grid systems: One, a regular grid, stores the normal fluid variables throughout space. The other, a surface grid, is defined on a moving surface (the "front") that follows (tracks) the moving discontinuity.

Conventionally, difference operators are defined using stencils that may cross the tracked interface. When this occurs, these difference stencils and operators are replaced. The state values on the remote side of the interface are replaced with extrapolated ghost-cell state values. In this way the state values associated with the stencil are all taken from a single side of the tracked interface. This ghost-cell algorithm, introduced by Glimm, Marchesin, and McBryan in 1980, has been used in many other interface algorithms.

This method has been (and continues to be) improved, through extensions to 3D and robust treatment of topology bifurcations. In a feature that is still experimental (and was not used, for example, in the simulation results reported here), the differencing of the front is completely conservative, and replaces the ghost-cell algorithm.

This algorithm has been tested extensively on purely mathematical surface deformation problems of interest to the computational interface community. In comparisons, it has outperformed other methods (including level-set and volume-of-fluids methods); see [3,8] and references cited there.

As we worked to improve the strictly numerical aspects of the front-tracking algorithm, it became clear that the value obtained for the RT mixing rate α was too high, and increasingly so with each front-tracking improvement. At this point, we improved the physical modeling, solving equations that better represent physical reality.

The simulations are generally conducted with idealized physics, omitting surface tension (for immiscible fluids), physical mass diffusion (for miscible fluids), viscosity, and compressibility. These are generally small effects and, except for the last one, have the effect of lowering the mixing rate. The first three have provided the leading order correction for idealized physics in most experiments. We included all four, and the result was a striking success: The simulations, now having *both* better physics and better numerics, finally agree with experiments. See [5,7] and references cited there, as well as Figure 1 and Table 1.

Initial Conditions

For comparisons of simulation and experiment, the physical parameters, especially surface tension, diffusivity, and viscosity, need to be expressed in dimensionless terms. Most of the parameters involved have been tabulated in physics tables or measured experimentally. But there is a length scale defined by the wavelength that dominates the initial conditions, and this is part of the non-dimensionalization. What we need is to characterize a typical length present in the interface perturbations.

Experimentally, the initial surface is taken to be as smooth (flat) as possible, after which initial disturbances emerge with characteristic lengths. A theory of small-amplitude (linearized) solutions can be derived and solved either analytically or with the help of simple numerics to predict growth rates for disturbances in unstable flows [1]. The growth rates depend on the wavelength, and there is typically a wavelength for which the disturbance grows most rapidly. It is this most rapidly growing wavelength that is generally expected to be observed initially in the growing mixing layer. Usually, this is (approximately) the case, but for one series of experiments (the splitter plate experiments of Andrews et al.), it is not. In such cases, the observed rather than theoretically predicted initial wavelength must be used.

Simulation Results

Most simulations underpredict α relative to experiments, and they do so without in-cluding scale-breaking mechanisms, which (with the exception of compressibility) would further decrease the simulated value of the mixing rate α. In other words, the disagreement with experiment is even worse than the often mentioned factor of 2. Our ideal fluid simulations predict an elevated mixing rate, $\alpha = 0.09$, which the inclusion of scale-breaking physics (for example, surface tension or mass diffusion with experimental values for the coefficients of the scale-breaking terms) reduces by some 20% to 30%. Compared with our idealized physics mixing rate, most simulations underpredict α by a factor of 3 rather than 2. Table 1 shows the scope of the new, and systematic, agreement of simulation with experiment.

Significance

Direct numerical simulation (DNS) (validated against experiment) is needed to validate averaged equations, also called "mix model equations." Mix is a first cousin of turbulence, and as with turbulence, practical computations are needed to reproduce average and macroscopic behavior, while glossing over (averaging) the highly complex microphysics of the detailed flow behavior. The derivations, generally through averaging of the DNS equations, introduce averages of nonlinear terms as new terms in the equations.

A definition of these averaged nonlinear terms involves closure and, usually, scientific disagreement as to possible competing closures. The experimental data are usually too sparse to serve as a solid guide for distinguishing between alternative closures, but validated direct numerical simulations are much more detailed in terms of the variables recorded (and then averaged) for the purpose of comparison between alternative closures and closed averaged equations. Thus, the direct numerical simulations (once validated), are a link in the validation chain of other, more commonly used equations.

Caveats and Controversies

Controversial aspects of the ideas discussed here include:

- whether front tracking is a leading method for the computation of unstable interfaces,
- whether transport and other scale-breaking physical characteristics significantly affect the experimentally observed mixing rate, and
- whether improved numerics and improved physics, as proposed here, rather than unobserved long-wavelength initial perturbations, are the way to resolve the discrepancy between experiment and simulation.

These questions will be resolved within the scientific communities affected. Our own views are yes, yes, and yes.

Certainly, answers to the first question have the potential to change over time as various methods are improved and new ones are proposed. The question, however, refers not to competitive pressures in the numerical analysis community, but rather to the intellectual question of what is needed to achieve an RT simulation that agrees with experimental data. Several others have achieved credible values for α, although not necessarily with systematic control of all relevant physical parameters, as is the case with the simulations reported here. One such simulation is based on a molecular dynamics method, and others were performed in Israel, Russia, and at Lawrence Livermore National Laboratory. The latter, based on a spectral element algorithm developed at Brown University, has been discussed in conference presentations. There is no doubt that solutions to the RT problem are extremely sensitive to variations in the numerical algorithm used for the solution. Our view is that this fact should inspire a sense of caution in the interpretation of the simulations and inspire a new generation of research in numerical algorithms and their validation.

Regarding the final bullet, we plot in Figure 1 the growth rate α vs. dimensionless surface tension for experiments, several front-tracking simulations, and other (untracked) simulations.

Experimental data not included in our validation concern immiscible fluids with surfactants, which require more specialized modeling, not yet carried out. In the future, we hope to consider the experiments with an initially diffused layer (Smeeton–Youngs). Also omitted from our validation studies are experiments of Linden et al., and Russian and Israeli experiments. Compressibility and Richtmyer–Meshkov instabilities

Scale-breaking physical effects	$\alpha_{experiment}$	$\alpha_{simulation}$	Experiments	Fluids
Surface tension	0.050–0.077	0.067	Reed-Youngs; Smeeton-Youngs	liquid–liquid; liquid–gas
Surface tension with surfactant	0.051–0.061	TBD	Smeeton-Youngs; Dimonte-Snider	liquid–liquid
Mass diffusion	0.070	0.069	Banerjee-Andrews	gas–gas
Initial mass diffusion	0.062	TBD	Smeeton-Youngs	liquid–liquid
Viscosity	0.070	0.070*	Snider-Andrews	liquid–liquid
Compressibility	TBD	up to 0.2	lasers	plasma–plasma

Table 1. *Comparison of experiments and simulations. *Preliminary result, courtesy of W. Bo and X. Liu.*

(shock-induced mixing) are typical of laser acceleration experiments.

Whether the mixing flows undergo a turbulent transition and, if so, the effects on mixing continue to be investigated. Chaotic mixing, often called turbulent mixing, is not necessarily turbulent. Chaotic mixing involves density discontinuity structures across a spectrum of length scales, whereas turbulence involves chaotic vortex structures across a spectrum of length scales. The possible role of turbulence in some chaotic mixing flows is only one of many questions regarding the internal structure of the mixing layer that have received less attention than the mixing rate itself.

Conclusions

In view of the validation success for the direct numerical mix simulations described here, we believe that it is time to declare a milestone, if not a victory, and for chaotic mixing to follow the conventional path of science, with agreement among experiment, theory, and simulation replacing explanations for disagreements. We see this agreement being achieved through adjustment of scale-breaking physical parameters to experimental values. Also needed are experiments that test a wider range of the dimensionless scale-breaking parameter values.

We want to emphasize the role of experiment in this chain of logic, especially in view of the fact that most readers of *SIAM News* are closer to simulation than to experiment. Of course, the experiments start the validation chain, providing data for DNS validation. But this is to significantly understate the role actually played by experiment. We live in a simulation-driven environment. The experiments played a key role in defining the problem and energizing the effort that led to an improved simulation algorithm. The experiments were instrumental in convincing us, and we hope others, of the correctness of the results obtained with improved physical models and improved algorithms, notwithstanding a consensus that a set of simulation results that disagree with experiment must, given the consensus, somehow be correct.

Acknowledgments

It is a pleasure to thank our many colleagues at Stony Brook University, Los Alamos National Laboratory, and Brookhaven National Laboratory who contributed to the work reported here, as well as our many colleagues in the turbulence modeling community whose ideas and thinking have contributed to our own.

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