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Uncertainty Quantification for Turbulent Mixing Simulations

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Abstract. We have achieved validation in the form of simulation-experiment agreement for Rayleigh-Taylor turbulent mixing rates (known as α) over the past decade. The problem was first posed sixty years ago. Recent improvements in our simulation technology allow sufficient precision to distinguish between mixing rates for different experiments. We explain the sensitivity and non-universality of the mixing rate. These play a role in the difficulties experienced by many others in efforts to compare experiment with simulation. We analyze the role of initial conditions, which were not recorded for the classical experiments of Youngs et al. Reconstructed initial conditions with error bars are given. The time evolution of the long and short wave length portions of the instability are analyzed. We show that long wave length perturbations are strong at $t = 0$, but are quickly overcome by the rapidly growing short wave length perturbations. These conclusions, based solely on experimental data analysis, are in agreement with results from theoretical bubble merger models and numerical simulation studies but disagree with models based on superposition of modes.

1. Introduction

Rayleigh-Taylor turbulent mixing is a classical fluid instability (Chandrasekhar 1961; Sharp 1984) in which a light fluid accelerates a heavy one. It has been a concern for 60 years, and subject to numerous controversies. We take an important step here towards resolving a currently active controversy regarding the role of initial conditions in observed experimental results.

Our simulation-experiment agreement (validation) (George et al. 2002; George & Glimm 2005; Liu et al. 2006), obtained over the past decade, was recently refined (Lim et al. 2010a,b,d,c), yielding definitive agreement with 14 experiments spanning immiscible and miscible cases (the latter with low, moderate and high Schmidt numbers). The agreement includes cases with measured initial data and one case simulated by others. The body of work, in total, is one of the most extensive validation/verification studies for Rayleigh-Taylor instability published. Most of the effort and that of other workers have focused on the overall growth rate of the mixing zone, defined as the coefficient α in the self similar scaling law

$$h = \alpha A g t^2 , \tag{1}$$

where h is the bubble penetration distance for light fluid entrainment into the heavy fluid, the Atwood number $A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$ is a dimensionless measure of the density difference, g is the acceleration body force, t is time and α is a dimensionless coefficient to be determined.

2. Validation Studies

As a summary of our previous validation studies, we show the experimental to simulation comparisons in Table 1, and also the sensitivities of α to changes in various parameters defining the problem. The sensitivities illustrate the lack of universality of α as does the difference between the first and third simulation-experiment, as these are nominally identical fluid systems.

Table 1. Validation (simulation/experiment comparison) for three experiments (above) and sensitivity of α to variation of experimental parameters for one of these.

Validation			
Exp. Ref.	Sim. Ref.	α_{exp}	α_{sim}
Smeeton & Youngs (1987) #112	Lim et al. (2010a)	0.052	0.055
Mueschke (2008) Hot/Cold	Glimm et al. (2011)	0.070± 0.011	0.070
Mueschke (2008) Salt/Fresh	Glimm et al. (2011)	0.085± 0.005	0.084
Sensitivities for Smeeton & Youngs (1987) #112			
parameter	variation	effect (α_{sym})	
Grashof No.	70%	≈ 10%	
Schmidt No.	500 ×	≈ 10%	
Init. Diff. Layer	2 ×, 0.5×	≈ 5%	
Domain	2×, 4×	≈ 2%	
Mesh	2×	No change	

3. Remaining Problems

Three issues remain in this validation/verification effort.

1. In some experiments, initial conditions were not measured.
2. Subgrid models are used, an issue we will address in the future. The comparative study of subgrid models, and of their accuracy and validity, deserves detained study by the numerical analysis community.
3. Some scientists assert that the experimental regime is not the right regime for the study of α.

We focus here on item #1. Item #2 will be considered in a future publication. Regarding item #3, many regimes, including the experimental ones, characterized by ranges of values for various dimensionless parameters, have their own rationale for further study.

Ultrahigh Reynolds numbers are relatively inaccessible to experiment and simulation, and although out of the scope of the present paper, remain an important focus for future investigations.

4. Reconstruction of Initial Conditions

In Kaman et al. (2010), we introduced a method for reconstruction of the time $t = 0$ data for RT instabilities. The idea is very simple; a more detailed explanation will be given in Glimm et al. (2011). Starting from an early time experimental plate showing the instability, we digitize all bubble minima, recorded as a series of heights, $h_j(t)$. We then take the Fourier transform of this data. The mode number $n = 0$ is the average bubble height. As is evident from the experimental plates, this mode is the dominant short wave length mode. The higher mode numbers provide fluctuations, which in the experiments being considered here are reduced in magnitude relative to the mean by an order of magnitude. For this reason, we plot the $n = 0$ mode at the location $n = n_{\max}(t)$. For Fourier analysis over $Z_{n_{\max}}$, this is justified, since $n_{\max} = 0$ modulo $n_{\max}$. The other modes are cut off at the Nyquist mode number $n_{\max}/2$. The amplitudes of all modes but $n = 0$ are small, not only at initial times but at all times, as a fraction of their wave length. Thus their dynamics can be described by Rayleigh-Taylor equations that are linearized about the perturbation amplitude. These linear equations are ODEs and their solution, called dispersion relations, yield an exponential growth law depending on the frequency or wave number. The most unstable mode, i.e. the most rapidly growing mode, is the dominant short wave length mode at the initial time.

In summary, the model mode dynamics is based upon:

A. single mode dynamics for each Fourier mode based upon the linear (dispersion relation theory) or the nonlinear theory or simulation of a single mode,

B. superposition, so that the individual Fourier modes can evolve independently of the other modes, except for the dominant short wave length mode,

C. special treatment for the dominant short wave length mode.

The number of modes decreases with time and accordingly, the wave length of the dominant short wave length mode increases with time. A model for RT mixing (Dimonte 2004) was proposed, which has these same basic features, but with a key difference from our treatment of item C. In Dimonte (2004), the short wave modes are removed from the ensemble when their amplitude is too large. Before that, they are given an extra velocity, about double that predicted by single mode theory or simulation. Such an extra velocity is required due to mode interactions, as has been noted earlier, see for example (Glimm & X.-Li 1988; Glimm & Sharp 1990; Cheng et al. 2002).

In place of this superposition model for the dominant short wave length mode (item C.), we employ the bubble merger model (Sharp & Wheeler 1961; Glimm & Sharp 1990; Cheng et al. 2002). The bubble merger model has very different dynamics for the dominant short wave length modes, with strong mode coupling in its dynamics. The bubble merger model assumes that at the shortest wave length, bubbles with mode number n, time t, do not originate from mode n bubbles at an earlier (discrete) time step, but from a combination of adjacent bubbles, i.e. smaller wave length modes (mode number $2n$, for example) at an earlier time. In 3D the merger of bubbles takes place in a planar array of bubbles and the geometry is more complex, see (Cheng et al. 2002). In any case, the analysis of experimental data (Smeeton & Youngs 1987) reveals that the superposition version of item C requires an unphysical velocity about two times the maximum velocity present in the bubble region, namely two times $2\alpha Agt$, whereas the bubble merger model uses velocities consistent with experimental data.

Using this methodology, we determined that the initial ($t = 0$) long wave length amplitudes $A(n)$ have a spectral energy $|A^2(n)|$ which satisfies a power law dependence $A^2(n) \sim n^{-3.3}$. Moreover, the long wave length fraction of the spectral energy (L_2 norm squared) was some 80% of the total spectral energy. Such phenomena has been postulated as leading to t^2 growth laws and contributing to α.

In Fig. 1 (left) we show the spectral amplitudes for $t = 0$ as reconstructed using the above methods. The $n = 0$ mode, which (as the average of all bubble minima) is the dominant short wave length mode, is plotted at the right, after the others given by Fourier analysis.

In the right frame, we consider only experiment #105 and show the spectral amplitudes for all $t = t_j$, the times of the j^{th} experimental plate. Note that the power law is largely missing at $t = t_j$, $j > 0$ and that the dominant short wave length mode has a markedly larger amplitude than all other modes at the same time, in contrast to Fig. 3 of Dimonte (2004). The inconsistency of the superposition model with experimental data can be read off of this figure, as indicated above. On this basis the conclusions regarding long wave initial data influencing the experimental α are also seen to be inconsistent with data.

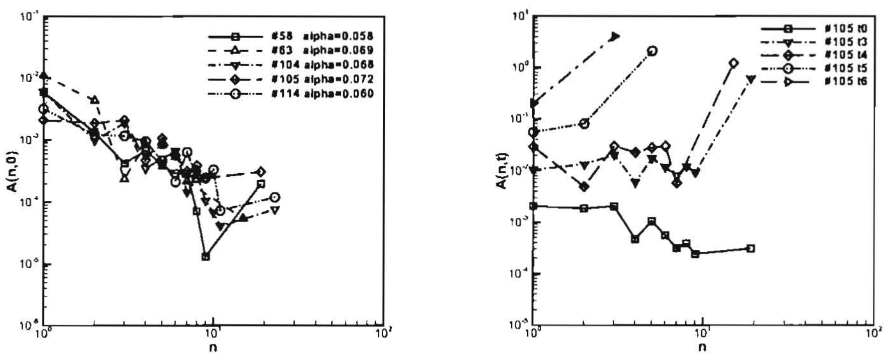

Figure 1. Spectral amplitudes $A(n, t)$ vs. wave number n derived from heights of bubble minima. The wave number $n = 0$, which represents the dominant short wave length mode, is plotted to the right, after all other n values. Left: $t = 0$ data as reconstructed by the method of backward in time propagation of early time observed spectral amplitudes. Right: All modes plotted for experiment #105, for all times, labeled as t_j for the j^{th} experimental plate. Data t_0 is the reconstructed initial conditions and the later t_j are as measured from experiment.

Thus we can say that the theory linking self similar initial long wavelength amplitudes with an influence by a factor of 2 or 3 on experimentally observed values of α has problems when compared with the Youngs et al. experimental data. Details will be provided in a subsequent publication. The hypothesis of self similar initial mode amplitudes is also inconsistent with measured initial data (Mueschke 2008).

In contrast, the dynamic bubble merger (Cheng et al. 2002), fully explains the experimentally observed self similar growth and predicts a value of α in agreement with experimental data. This theory also predicts correctly two other measures of the bubble dynamics: the height to width ratio for the bubbles and the fluctuations in the bubble heights about their mean value.

5. Uncertainty Quantification for Initial Conditions

We carry the uncertainty quantification analysis further by estimating uncertainties in the reconstruction of the unobserved initial data. We do this by assessing the accuracy of reconstruction for data that has been observed. We compare the observed data for the third experimental plate ($t = t_3$) as compared to the same data reconstructed from observations at the fourth plates, for five experiments (Burrows et al. 1984; Smeeton & Youngs 1987). We use an error model

$$\text{Error} = aA(n,t) + b \,. \tag{2}$$

Here, b results from uncertainty in reading data from the experimental plates themselves, approximately 50μ, and $a = 1$ corresponds to uncertainty in the propagation of observations from $t = t_k$ to inferences at $t = t_j$. The data leading to these numbers is displayed in Fig. 2, left. In Fig. 2, right, we show a scatter plot of predictions vs. means for two predictions (based on t_3 and t_4) of t_0 data, with plotted error model (2), $b = 2.5\mu$, $a = 1$. It follows that if $\mathcal{I}$ represents the long wave length contribution to the initial conditions, as reconstructed, we can bracket the uncertainty with simulations that use $0\mathcal{I}$ and $2\mathcal{I}$.

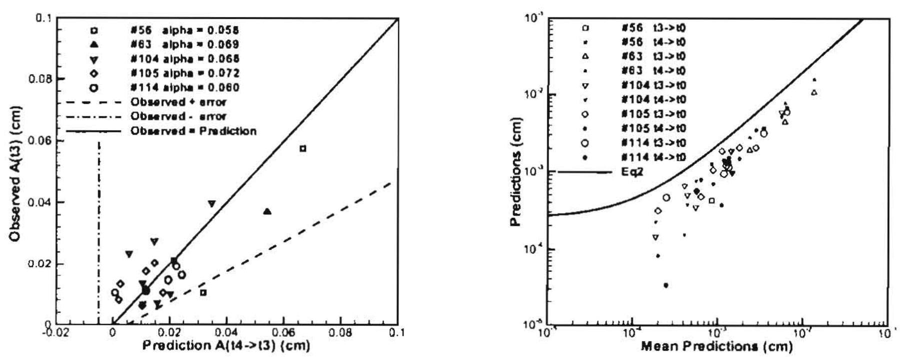

Figure 2. Scatter plot data from five experiments with error model bounds for $a = 1.0$ and (left) $b = 50$ microns. In the right plot, $b = 2.5$ microns, reduced by a typical propagation factor associated with the transfer of data to $t = t_0$. Left: observed vs. predicted modal amplitudes for $t = t_3$, with the prediction based on $t = t_4$ observations. Right: Prediction of $t = t_0$ data, based on $t = t_3$ and $t = t_4$ data, predictions vs. mean of $t = t_3$ and $t = t_4$ predictions.

6. Conclusions

The long standing controversy in simulation values for the overall mixing rate α for Rayleigh-Taylor instabilities is revisited. Recent simulations, based on a compressible multiphysics code, show excellent agreement between simulation and experiment. The key to this agreement is the use of subgrid scale models in an LES simulation and use of Front Tracking to control (or, as in the present immiscible case, eliminate) numerical mass diffusion across a tracked front. Among the several issues widely discussed as important to this problem, we focus here on the initial data, often not measured experimentally. To this end, we propose a method of reconstruction of the initial data, based on the observations of the early time data. This reconstruction, of course, contains uncertainties, and on this basis uncertainty quantification RT simulations are also proposed. Arguments linking self similar power law initial spectrum with a changes in α by factors of 2 or 3 are found to be inconsistent with experimental data.

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References

Burrows, K. D., Smeeton, V. S., & Youngs, D. L. 1984, Experimental investigation of turbulent mixing by Rayleigh-Taylor instability, II, AWE Report Number 0 22/84

Chandrasekhar, S. 1961, Hydrodynamic and Hydromagnetic Stability (Oxford: Oxford University Press)

Cheng, B., Glimm, J., & Sharp, D. H. 2002, Chaos, 12, 267

Dimonte, G. 2004, Phys. Rev. E, 69, 056305

George, E., & Glimm, J. 2005, Phys. Fluids, 17, 1. Stony Brook University Preprint number SUNYSB-AMS-04-05

George, E., Glimm, J., Li, X. L., Marchese, A., & Xu, Z. L. 2002, Proc. National Academy of Sci., 99, 2587

Glimm, J., & Sharp, D. H. 1990, Phys. Rev. Lett., 64, 2137

Glimm, J., Sharp, D. H., Kaman, T., & Lim, H. 2011, Philosophical Transactions of The Royal Society A: Turbulent mixing and beyond. Submitted for publication

Glimm, J., & X.-Li 1988, Phys. Fluids, 31, 2077

Kaman, T., Glimm, J., & Sharp, D. H. 2010, Condensed Matter Physics, 13, 43401. Stony Brook University Preprint number SUNYSB-AMS-10-03 and Los Alamos National Laboratory Preprint number LA-UR 10-03424

Lim, H., Iwerks, J., Glimm, J., & Sharp, D. H. 2010a, PNAS. Stony Brook Preprint SUNYSB-AMS-09-05 and Los Alamos National Laboratory preprint number LA-UR 09-06333

Lim, H., Iwerks, J., Yu, Y., Glimm, J., & Sharp, D. H. 2010b, Physica Scripta. Stony Brook Preprint SUNYSB-AMS-09-07 and Los Alamos National Laboratory preprint number LA-UR 09-07240

Lim, H., Yu, Y., Glimm, J., & Sharp, D. H. 2010c, IMA Volumes in Mathematics and its Applications. Nonlinear Conservation Laws and Applications, 153, 405. Stony Brook University Preprint SUNYSB-AMS-09-08 and Los Alamos National Laboratory preprint number LA-UR-09-008281

— 2010d, High Energy Density Physics, 6, 223. Stony Brook University Preprint SUNYSB-AMS-09-02 and Los Alamos National Laboratory preprint number LA-UR-09-01364

Liu, X. F., George, E., Bo, W., & Glimm, J. 2006, Phys. Rev. E, 73, 056301

Mueschke, N. J. 2008, Ph.D. thesis, Texas A and M University

Sharp, D. H. 1984, Physica D, 12, 3

Sharp, D. H., & Wheeler, J. A. 1961, Late Stage of Rayleigh-Taylor Instability, Tech. rep., Institute of Defense Analyses. Unpublished Technical Report

Smeeton, V. S., & Youngs, D. L. 1987, Experimental investigation of turbulent mixing by Rayleigh-Taylor instability (Part 3), AWE Report Number 0 35/87