

# Two-Phase Flow Properties of Turbulent Mixing by Rayleigh-Taylor Instability

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## Abstract

We discuss comparison with the familiar bubble/spike penetration law complicated by the lack of scale invariance, inability to carry the simulations to late time, the increasing Mach numbers of the bubble/spike tips, and sensitivity to the method of data analysis. We use the simulation data to assess the validity of recently proposed modelling assumptions characterizing the mixing process.

## 1 Introduction

We discuss comparison with the familiar bubble/spike penetration law  $h = \alpha A g t^2$  complicated by the lack of scale invariance, inability to carry the simulations to late time, the increasing Mach numbers of the bubble/spike tips, and sensitivity to the method of data analysis. The statistical evolution of a planar, randomly perturbed interface subject to Rayleigh-Taylor instability is explored through direct numerical simulation in two space dimensions. We use the simulation data to assess the validity of recently proposed modelling assumptions characterizing the mixing process.

An interface between two fluids is subject to the Rayleigh-Taylor (RT) instability when an external force is directed against the density gradient. This phenomenon is of importance in natural and technological problems encompassing a vast array of length scales, for example in supernova explosions, formation of salt diapirs, and laser implosion of inertial confinement fusion targets. See [17] for an overview of this problem, and [14] for further discussion.

As RT instability develops, small perturbations of a smooth contact surface rapidly grow into interpenetrating fingers of the distinct materials. This mixing process is non-linear and chaotic, in the sense of sensitive dependence on initial data. Furthermore,

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only the statistical properties of the initial interface perturbations are known. These features point to a stochastic approach as the appropriate method to develop a predictive model for the deterministic properties of an evolving mixing layer.

The most important quantity characterizing the mixing process is the mean concentration  $\beta_k(t, x)$  of fluid  $k$  at spatial position  $x$  and time  $t$ . In ICF, this function contains all of the information concerning the expected penetration of the instability. In astrophysics, it is a first order moment of the material interface geometry, a major ingredient of a statistical description of remnant formation (for example). The concentration profile is difficult to measure experimentally. In RT instability experiments, it is measurable only for fluids of similar density, where an index of refraction match is feasible [7].

A major motivation for construction of a stochastic model of the fluid mixing is therefore to predict  $\beta_k$ . Most such efforts [12, 18, 8, 5, 6, 20, 2, 10] can be more or less related to formal averages of the Euler or Navier-Stokes equations with a series of closure hypotheses for nonlinear terms and boundary conditions. This research goes in two directions, determined by whether the averaging is applied globally or within each distinct material. The former approach leads to the Reynolds-averaged equations of turbulence, while the latter leads to the equations of two-phase flow. In the two phase flow approach,  $\beta_k$  is a dependent variable, hence its prediction is accomplished by the closure and solution of the averaged equations. The recovery of  $\beta_k$  from a turbulence model is more difficult, unless there are only two fluids and they are both incompressible, in which case  $\beta_k$  is obtained from the mean density  $\bar{\rho}$  (a dependent variable) and known fluid densities  $\rho_1$  and  $\rho_2$ . For example, the fraction of fluid 1 is  $\beta_1 = (\bar{\rho} - \rho_2)/(\rho_1 - \rho_2)$ . See [3, 4].

We here discuss various aspects of the numerical solution of two-phase equations. Our concern is the bubble/spike penetration. There is a large amount of literature on this subject, and a comprehensive comparison of model, simulation, and experiment is given by Dimonte [7]. We report the proportionality coefficients  $\alpha_k$  in the bubble/spike penetration law  $Z_k = (-1)^k \alpha_k A g t^2$ , but we must point out that the mixing layers in our computations do not reach a scale-invariant regime, although they do develop to the same extent as reported in earlier *Frontier* simulations [2]. In fact, we find substantial evidence of single-mode behavior of both bubbles and spikes.

## 2 Growth Rate

The tracking of the contact surface allows use of the mathematical definitions of the bubble and spike penetrations as the limits of vanishing layer fraction. Furthermore, we directly compute an edge velocity as the fluid  $z$ -velocity evaluated at the position of the leading bubble/spike tip, not as the numerical time derivative of the edge position. This velocity is computed explicitly in the front-tracking method.

Other experiments and computations use a layer fraction criterion such as 1% – 99%; *i.e.*, the edges are defined to be where  $\beta_k$  attains the values 0.01 and 0.99. This practice is intended to remove uncertainty in the edge positions due to outliers and/or physical or numerical diffusion [8, 7], exhibited by "wings" in the layer fraction profile. The profiles computed by *FronTier* are noticeably discontinuous in slope near the edges; there is little tailing off or rounding of  $\beta_k$  in these regions. Consequently, the choice of cutoff is not important.

A  $\beta_k$  profile with "wings" has small  $|\partial\beta_k/\partial z|$  near the edges, hence large gaps between the corresponding 0%, 1%, and 5% contours, for example. The absence of this behavior in the present data can be attributed to the absence of diffusive processes, numerical or physical, in the simulations [16].

Since the computed flows are weakly compressible (final Mach number  $\sim 0.1$ ), we expect the edge trajectories to resemble the observed edge trajectories in experiments using incompressible fluids [15, 18, 7]. These experiments suggest the bubble side,  $\alpha_1$  is insensitive to the Atwood number  $A$  and observations fall within the range 0.05 to 0.07. On the spike side,  $\alpha_2 \approx \alpha_1$  at small  $A$  and increases with increasing  $A$ . The variation of  $\alpha_2/\alpha_1$  with  $A$  is well characterized in the linear electric motor (LEM) experiments of [7].

The  $gt^2$  asymptotic scaling of the edge trajectories is believed to correspond to a scale-invariant regime of incompressible RT mixing, where all lengths obey the same scaling law. Self-similar behavior is partially exhibited when volume fraction profiles taken at different times and horizontally scaled by the mixing zone width land nearly on the top of each other, as occurs in our simulations. However, stabilization of the profile shape may also occur for some time as a consequence of a stable mixing layer geometry. The edge displacements in our simulations do not closely follow the  $gt^2$  law.

Self-similarity of the velocity fields follows directly from integration of the two-phase continuity equations assuming a scale-invariant volume fraction, because these equations do not contain any closure assumptions. We are not aware of any experimental or computational evidence for the scale invariance of the pressure fields.

Our simulations, as well as previous front-tracking studies [11, 1, 9, 13], do not reach a sufficiently late stage to observe substantially self-similar behavior. Youngs [19] has also reported a similar observation. Therefore, the use of  $\alpha_k$  as a statistical summary of the edge  $k$  motion should be treated with caution. There are multiple ways to compute  $\alpha_k$ ; all of these methods should converge in the limit  $t \rightarrow \infty$ , but because this limit is approached to varying degrees in computation and experiment, the specific method of data analysis will likewise produce variations in  $\alpha_k$ . Here we present three methods to compute  $\alpha_k$  and the corresponding results for our numerical study.

Methods A and B are based on the single hypothesis that an edge attains a constant acceleration at late time,  $\dot{V}_k = 2(-1)^k \alpha_k Ag$ . It follows that (A)  $Z_k = (-1)^k \alpha_k Agt^2 + V_{k0}t + Z_{k0}$  and (B)  $V_k = 2(-1)^k \alpha_k Agt + V_{k0}$ . These expressions are fit to the edge velocity and position data by the least-squares method over a time interval that excludes the very early evolution.

Method (C) is a least-squares fit to the trajectory  $Z_k = (-1)^k \alpha_k Agt^2 + Z'_{k0}$  over an appropriate interval of time, which is similar to the method applied to experimental data [15, 18], and to simulation data [11]. Youngs [19] was careful to point out the possibility that the slope of  $|Z_k|$  vs.  $Ag t^2$  does not satisfactorily reach its limiting value.

We compute the  $\alpha_k$  on a run-by-run basis, by recording the paths of the global interface extrema within each realization. We could utilize the ensemble idea by analyzing only the global interface extrema for the entire ensemble. This approach would select the leading spike tip in run #5 and the leading bubble tip in run #6, which are respectively the leading spike and bubble tips for the entire ensemble at all times (for both  $A = 0.5$  and  $0.8$ ). There would then be no sampling involved and a leading bubble/spike tip would be local to one realization. Thus we sample the growth rate on a run-by-run basis in order to discern any statistical variation in  $\alpha_k$ .

Values of  $\alpha_k$  computed by Method C are systematically higher and less scattered than values computed by Method A. Methods A and C both use the position data, and have 3 and 2 fitting parameters, respectively. For given input data, the fewer parameters used in a least-squares fit, the more reproducible are the values of these parameters. The stable reproducible values of  $\alpha_k$  obtained from Method C may be aesthetically pleasing but they do not necessarily have a physical basis.

On the other hand, the high variation in Method A values of  $\alpha_k$  is largely attenuated by the large sample size ( $N = 20$ ). Even though Method B uses one fewer parameter than Method A, there is no attenuating effect on the  $\alpha_k$  variation because the advantage of having one less parameter is cancelled by the extra noise in the edge velocity data

(compared to the position data). One might expect Methods A and B to be approximately equivalent, as one expression is the time derivative of the other, but the nonlinear operation of least-squares fitting does not commute with differentiation. Method A and B values of  $\alpha_k$  are similar to the extent that the velocity is linear in time. Also, the edge velocity may have a discontinuity due to the leading structure tip being overtaken by another tip, but the edge position is always continuous in  $t$ .

If there is a substantial time interval of scale-invariant growth, then all three methods should yield approximately the same  $\alpha_k$ . They do not. For this reason, we prefer Method B, because under its assumptions  $2\alpha_k Ag$  has physical meaning as the average acceleration of edge  $k$ . Methods A and C yield "effective accelerations" that are perhaps suitable for comparison of simulations and experiments, provided that the method is applied consistently, but do not by themselves have much physical significance.

Another consequence of the lack of self-similarity is that the value of  $\alpha_k$  is sensitive to the choice of time interval for curve fitting. We present our computed values of  $\alpha_k$  for a few setting of the lower and upper cutoff times  $t_{lo}$  and  $t_{hi}$ , values  $\alpha_1$  and  $\alpha_2$  are computed for each realization, and by each method. A value of  $\alpha_k$  is reported as the sample mean for 20 realizations, and it is accompanied by the sample standard deviation. Attempts to measure the variation of  $\alpha_k$  within a single realization, for example by systematic variation of the cutoff times, were inconclusive. Results are displayed in Table 1, along with the corresponding experimental values due to Dimonte and Schneider [7].

Method C values of  $\alpha_1$  are directly comparable to previous front-tracking results [1] for coarser grids (approximately 13 cells/ $\lambda$ ). Our fine grid calculations (80 cells/ $\lambda$ ) give a value of  $\alpha_1$  roughly 15% larger than before.

The data displayed in Table 1 reveals the sensitivity of  $\alpha_k$  to the method of data analysis and the variation of  $\alpha_k$  from run to run. Note that the LEM values of  $\alpha_k$  are smaller than the values obtained in rocket-rigged experiments [15, 18], for which  $\alpha_1$  is in the range 0.06 – 0.07.

Comparing Method B values of  $\alpha_k$  to experimental values is meaningful, as the numbers represent the average acceleration of the bubble/spike tips during the mixing zone expansion. Our  $\alpha_1$  data is in good agreement with but systematically under the LEM data. Our  $\alpha_2$  data is over the LEM data at  $A = 0.5$  and under it at  $A = 0.8$ . Because our simulations do not reach a scale-invariant regime, it is important to consider how the value of  $\alpha_k$  varies if the flow computation is carried to a later time.

The lack of  $gt^2$  scaling in the bubble and spike trajectories is most apparent in graphs of tip velocity *vs.* time, which should be linear during the time that the scaling law holds.

The nonlinear growth of isolated RT bubbles and spikes has been studied in detail by Zhang [21]. Discarding the very brief initial state of small amplitude (exponential) growth, the bubble/spike tip velocity undergoes a linear variation in time (constant acceleration), gradually flattening out toward a terminal value. The study was not carried to a sufficiently late time to determine whether the terminal velocity persists indefinitely.

The two distinct regimes of nonlinear RT bubble/spike growth characterized by Zhang are seen prominently in fine-grid computations with randomly perturbed interfaces. In fact, our grid resolution on a per wavelength basis is comparable to the resolution in Zhang's simulations. There is a noticeable tendency for single-mode features in random surface simulations to be less prominent on coarser grids, with the result that the bubble velocities are more nearly linear in  $t$  for their entire evolution. We suggest that a coarse grid artificially induces at earlier time the coarse-graining or inverse cascade associated with a self-similar flow.

We see that the 40-cell trajectories are underresolved. It implies that a coarse-grid effect may be misinterpreted as a true physical phenomenon. Because the mixing zone expands more slowly on coarser grids, the 40-cell run was carried to a later time, late enough so that the 40-cell zone width attains a final value roughly equal to the final 80-cell zone width. The values of  $\alpha_1$  are 0.078 (40 cells/ $\lambda$ ) and 0.045 (80 cells/ $\lambda$ ) for  $A = 0.5$ , and 0.083 (40 cells/ $\lambda$ ) and 0.047 (80 cells/ $\lambda$ ) for  $A = 0.8$ . We also find evidence of single-mode behavior in the spike trajectory, but at 40 cells/ $\lambda$  the spike trajectories are too underresolved to draw similarly strong conclusions.

In graphs of tip velocity *vs.*  $t$ , we see to varying degrees a constant acceleration inflecting to a constant velocity turning upward to a constant but different acceleration. Perhaps only the latter acceleration should be considered in computing  $\alpha_k$ , but this regime is not clearly distinguished in many of the realizations. One might expect to see single-mode behavior more strongly attenuated in the bubble tip trajectory, due to the onset of bubble competition, but we see little evidence of this behavior in our data.

Zhang [21] provided formulas for the terminal and inflection velocities for single-mode RT bubbles and spikes. Evaluating his formulas using the average perturbation wavelength  $\lambda$ , we obtain values of the terminal velocity that land in the neighborhood of the plateaus in the edge velocity curves and values of the single-mode inflection velocity that are close to the multimode data. These observations indicate a substantial degree of single-mode behavior in the trajectories of the leading bubble and spike tips.

In realizations having a prominent constant bubble/spike acceleration following the

constant velocity regime, it is worthwhile to compute the associated value of  $\alpha_k$ , as this value may be a more realistic indication of the late time mixing zone growth rate. For the trajectories, we see straight-line fit to the late time constant acceleration portion. The values of  $\alpha_k$  implied by these lines are  $\alpha_1 = 0.066$ , close to experimental data, and  $\alpha_2 = 0.238$ , drastically higher than experimental data.

The reader may note another possible explanation for the noticeably single-mode character of the bubble and spike trajectories; a high degree of regularity in the initial data. Multimode behavior, especially bubble competition, is present to the extent that the fingers are disparate in size and shape. Such disparities increase over time due to the steady external acceleration, but the onset of multimode behavior is delayed if the fingers are highly uniform at early time. The explanation may be valid, but it is incomplete, as it requires a further explanation for the stronger multimode character of the edge trajectories on coarse grids.

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$\alpha_1, A = 0.5$ ( $0.05 \pm 0.01$ )	$[t_{lo}, t_{hi}]$	Method A	D.S.	Method B	D.S.	Method C	D.S.
	[0.24, 1.32]	0.039	0.009	0.043	0.008	0.079	0.006
	[0.24, 1.42]	0.049	0.008	0.048	0.009	0.075	0.006
	[0.36, 1.32]	0.033	0.010	0.044	0.009	0.077	0.006
$\alpha_2, A = 0.5$ ( $0.07 \pm 0.02$ )	$[t_{lo}, t_{hi}]$	Method A	D.S.	Method B	D.S.	Method C	D.S.
	[0.24, 1.32]	0.091	0.014	0.096	0.017	0.121	0.010
	[0.24, 1.42]	0.092	0.014	0.102	0.016	0.119	0.010
	[0.36, 1.32]	0.082	0.009	0.088	0.013	0.120	0.009
$\alpha_1, A = 0.8$ ( $0.05 \pm 0.01$ )	$[t_{lo}, t_{hi}]$	Method A	D.S.	Method B	D.S.	Method C	D.S.
	[0.24, 1.14]	0.049	0.012	0.047	0.013	0.078	0.007
	[0.24, 1.02]	0.048	0.011	0.049	0.013	0.082	0.006
	[0.36, 1.14]	0.042	0.014	0.043	0.013	0.077	0.006
$\alpha_2, A = 0.8$ ( $0.19 \pm 0.03$ )	$[t_{lo}, t_{hi}]$	Method A	D.S.	Method B	D.S.	Method C	D.S.
	[0.24, 1.14]	0.157	0.020	0.171	0.021	0.171	0.012
	[0.24, 1.02]	0.150	0.020	0.155	0.018	0.171	0.012
	[0.36, 1.14]	0.153	0.026	0.167	0.026	0.170	0.013

Table 1: The asymptotic bubble and spike penetration coefficients  $\alpha_k$  computed by three different least-squares fits on three different time intervals  $t \in [t_{lo}, t_{hi}]$ . The data shown is the average of  $\alpha_k$  over 20 runs and the standard deviation based on its run-to-run variation. The experimental value due to Dimonte and Schneider [7] is indicated on the left hand side of each table.