Originally published in *Proceedings of the Fifth International Workshop on Compressible Turbulent Mixing*, ed. R. Young, J. Glimm & B. Boston. ISBN 9810229100, World Scientific (1996).

A Two–Phase Flow Formulation for the Rayleigh–Taylor Mixing Zone and its Renormalization Group Solution*

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Abstract. We present a two-phase flow formulation for the statistical evolution of fluid mixing *via* Rayleigh-Taylor instability. Our main results are a new first-order closure for the ensemble-averaged two-phase flow equations, its validation against computational data for compressible flows, and an exact renormalization-group fixed-point solution of this model in the incompressible limit. We do not fully solve the closure problem, as the boundary conditions at the most penetrating edges of the fluid mixing layer are left unresolved in our model.

1 Introduction

The Rayleigh-Taylor (RT) instability [14] of an interface separating fluids of distinct density is driven by an acceleration across the interface (typically gravity). Initial random disturbances at the interface lead to the formation of a chaotic mixing layer between the light and heavy fluids. Past studies of RT instability have focused on the rate of expansion of the mixing zone. In this paper, we present a model for the statistical evolution of physical quantities inside the mixing zone.

Ensemble averaging is a conventional and useful mathematical tool to determine the statistical behavior of chaotic fluid mixing. For nonlinear equations, ensemble averaging leads to a closure problem—namely, new unknowns emerge in the analysis. An

*This work was supported by the Applied Mathematics Subprogram of the U.S. Department of Energy, DE-FG02-90ER25084. Dr. Glimm was also supported by the Army Research Office, grant DAAL03-92-G-0185 and through the Mathematical Sciences Institute of Cornell University under subcontract to the University at Stony Brook, ARO contract number DAAL03-91-C-0027, and the National Science Foundation, grant DMS-9201581.

attempt to derive governing equations for these new variables leads to an endless hierarchy of equations for moments of increasing order. This hierarchy is usually broken at the level of first- or second-order moments by a closure hypothesis, which relates the higher-order moments occurring in the equations to products of lower-order moments. Here, we present a new way to resolve the closure problem for RT mixing. Our approach is a new first-order closure for compressible multiphase flow, which has been validated by comparison to full numerical simulations. In addition, we have obtained its renormalization group (RNG) fixed-point solution in the incompressible limit.

2 Analysis of Two-Phase Turbulence Moments

In this section, we propose a new two-phase closure hypothesis for RT mixing. To begin, we consider a two-phase flow in two space dimensions (x, z) at time t, with no microscopic mixing; *i.e.*, there is a well-defined characteristic function X_k for phase k,

$$X_k(x,z,t) = \begin{cases} 1 & \text{if } (x,z) \text{ is in phase } k \text{ at time } t, \\ 0 & \text{otherwise.} \end{cases}$$

Let the operation $\langle\cdot\rangle$ be a combined ensemble average and average over the transverse (x) direction. Then $\beta_k(z,t) \equiv \langle X_k \rangle$ is the volume fraction of phase k. The absolute volume, phase volume, and mass-weighted averages of a quantity $a(x,z,t)$ are

$$\overline{a} = \langle a \rangle, \qquad \overline{a}_k = \frac{\langle a X_k \rangle}{\langle X_k \rangle} = \frac{\langle a X_k \rangle}{\beta_k}, \qquad \widetilde{a}_k = \frac{\langle X_k \rho a \rangle}{\langle X_k \rho \rangle} = \frac{\overline{(\rho a)}_k}{\overline{\rho}_k},$$

respectively. We also define the absolute and phase volume fluctuations, $\delta a = a - \overline{a}$ and $\delta a_k = a - \overline{a}_k$.

To derive a closure model for the turbulent second-moments, we express second moments of the absolute fluctuating quantities in terms of second moments of the phase fluctuating quantities plus an expression involving only two-phase first moments, *i.e.*, phase volume averages. For a computational data set derived from RT mixing, we then show that the first contribution is small, and therefore that the absolute second moments are effectively given as functions of the two-phase first moments.

The following absolute second moments appear as additional dependent variables in the ensemble-averaged Euler equations (see, for example [1]),

$$B = \langle \delta\rho\delta\rho \rangle, \qquad A = \langle \delta\rho\delta\mathbf{v} \rangle, \qquad R = \langle \rho\mathbf{v}\mathbf{v} \rangle - \frac{\langle \rho\mathbf{v} \rangle \langle \rho\mathbf{v} \rangle}{\langle \rho \rangle},$$

$$S = \langle e\mathbf{v} \rangle - \frac{\langle e \rangle \langle \rho\mathbf{v} \rangle}{\langle \rho \rangle} = \langle \rho\epsilon\mathbf{v} \rangle - \overline{\rho}\widetilde{\epsilon}\widetilde{v}, \qquad G = \langle \delta\rho\delta\epsilon \rangle,$$

where ϵ is the specific internal energy and $e = \rho\epsilon$. One can show that [4]

$$F = \beta_1 F_1 + \beta_2 F_2 + F_{\text{two-phase}}, \tag{1}$$

where $F = B, A, R, S$, and G, F_k is the average of F over phase k, and

$$B_{\text{two-phase}} \equiv \beta_1\beta_2(\overline{\rho}_1 - \overline{\rho}_2)^2, \qquad A_{\text{two-phase}} \equiv \beta_1\beta_2(\overline{\rho}_1 - \overline{\rho}_2)(\overline{v}_1 - \overline{v}_2),$$

$$R_{\text{two-phase}} \equiv \beta_1\beta_2\frac{\overline{\rho}_1\overline{\rho}_2}{\overline{\rho}}(\widetilde{v}_1 - \widetilde{v}_2)^2, \qquad S_{\text{two-phase}} \equiv \frac{\beta_1\beta_2}{\overline{\rho}}(\overline{\rho}_2\overline{e}_1 - \overline{\rho}_1\overline{e}_2)(\widetilde{v}_1 - \widetilde{v}_2),$$

$$G_{\text{two-phase}} \equiv \beta_1\beta_2(\overline{\rho}_1 - \overline{\rho}_2)(\overline{\epsilon}_1 - \overline{\epsilon}_2).$$

For the RT two-phase mixing data that we have studied, we have found that the dominant contribution to the turbulent second moments comes from the two-phase first moments (the mean flow quantities). In this approximation, we have

$$F \approx F_{\text{two-phase}}. \tag{2}$$

As an example, we validate this two-phase approximation against an ensemble of five simulations. Each member of the ensemble has an initial randomly-perturbed interface with Atwood number $A_t = (\rho_2 - \rho_1)/(\rho_2 + \rho_1) = 2/3$ and dimensionless compressibility $M^2 = \lambda g/c_2^2 = 0.5$, where λ is the average perturbation wavelength, g is the gravitational acceleration, c is the sound speed, and the indices 1 and 2 refer to the light and heavy fluids, respectively. We assume that each fluid is a polytropic gas. In Figure 1, we see that the closure approximation (2) is nearly exact for B, A, and S (as it is also for G, not shown), and it captures most of the variation in R. A more detailed study, with systematic variation of both A_t and M^2, is included in [3].

Based on these comparison studies, we conclude that two-phase mean flow gives a good description of the turbulent second moments, and thus that the fluid mixing is dominated by two-phase behavior rather than by turbulence phenomena.

3 Effective Equations for RT Mixing

Equations for two-phase flow are derived in two steps. The first step is a mathematically exact averaging procedure which, due to the nonlinearity of the equations, introduces new unknowns. The second step is a modeling step, in which some of the unknowns are declared to be new dependent variables, for which new equations (not closing) are derived as above, while the remaining unknown quantities are approximated in terms of the original and new dependent variables. For incompressible flows, this process is described very elegantly by Drew [6]. Examples of compressible multiphase flow equations are given in [10] and [12]. We follow Drew's formalism, which was introduced, in part, in the previous section as well. A systematic description of the modeling of

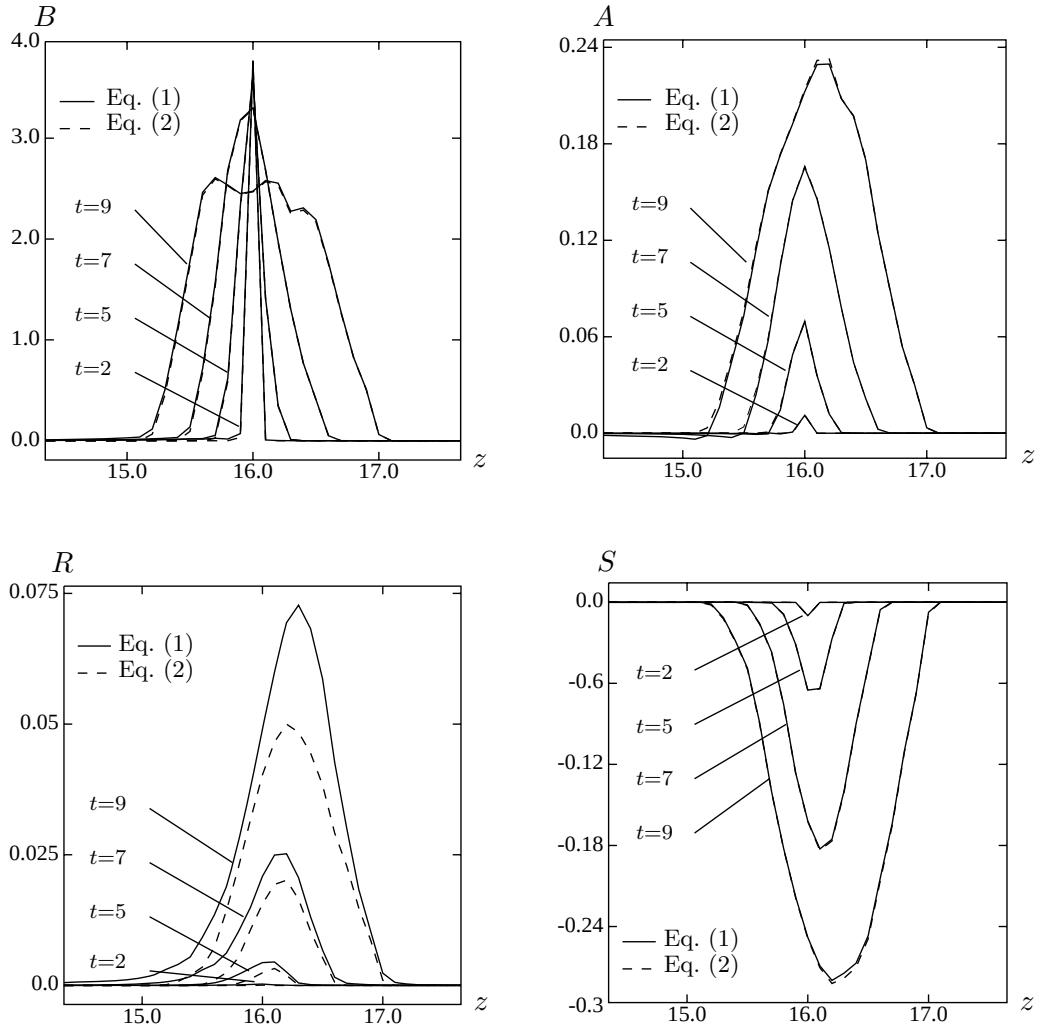

Figure 1: A comparison between Eq. (1) and its approximation, Eq. (2), for $F = B$, A, R, and S. In these simulations, $A_t = 2/3$ and $M^2 = 0.5$.

multiphase fluid equations can been found in [7], which presents a detailed discussion of local balance, averaging, jump conditions at interfaces, and constitutive equations. Other examples of turbulence and multiphase flow models that have been proposed to describe interfacial fluid mixing are given in [11, 2, 5], and [15].

The averaged Lagrangian interface satisfies the equation $\partial\beta_k/\partial t + \langle \mathbf{v}_{\text{int}} \cdot \nabla X_k \rangle = 0$, where $\mathbf{v}_{\text{int}}$ is the velocity of the interface. Contained in this equation as well as in the averaged Euler equations are terms which are proportional to ∇X_k, namely $\langle \mathbf{v}_{\text{int}} \cdot \nabla X_k \rangle$, $\langle p \nabla X_k \rangle$, and $\langle p\mathbf{v} \cdot \nabla X_k \rangle$. Since ∇X_k is a δ function in the direction normal to the material interface, these terms represent the coupling between the phases. They are intrinsically defined in higher dimensions only, and therefore cannot be determined exactly in the effective one-dimensional dynamical equations without knowing the exact solution in higher dimensions. To complete our closure for the effective dynamical equations, we now model the interfacial terms.

The three interfacial terms can be expressed as $\langle f \nabla X_k \rangle$, where $f = \mathbf{v}_{\text{int}}$, p, and $p\mathbf{v}$. We define an effective interfacial quantity f_{eff} as

$$\langle f \nabla X_k \rangle = \langle f_{\text{int}} \nabla X_k \rangle \equiv f_{\text{eff}} \nabla \langle X_k \rangle , \tag{3}$$

where f_{int} is f evaluated at the interface, due to the δ function property of ∇X_k.

As fluid of phase 1 (2) penetrates phase 2 (1), the frontier portion of that fluid occupies a small volume and is near the interface. Therefore, in that region $\overline{f}_1$ ($\overline{f}_2$) is a good approximation for f_{eff}. Interpolating with the volume fraction, we obtain

$$f_{\text{eff}} \approx \beta_1 f_2 + \beta_2 f_1 \equiv f_* . \tag{4}$$

Therefore the interfacial terms are approximated as follows,

$$\langle f \nabla X_k \rangle \approx (\beta_1 \overline{f}_2 + \beta_2 \overline{f}_1) \frac{\partial \beta_k}{\partial z} \equiv f_* \frac{\partial \beta_k}{\partial z} . \tag{5}$$

This equation, written for $f = \mathbf{v}_{\text{int}}$, p, and $p\mathbf{v}$, represents the interchange of volume, momentum, and energy, respectively, between the two phases. In Figure 2, we validate the approximations $v_{\text{eff}} \approx v_*$ and $p_{\text{eff}} \approx p_*$ using the results of numerical simulations with $A_t = 2/3$ and $M^2 = 0.5$ (the approximation for $(pv)_{\text{eff}}$ is as good as that for v_{eff}). In these figures, as well as in the more detailed study [3], we see that the approximations agree very well with their corresponding exact expressions.

Our derivation of the averaged Euler equations follows [6], with the following approximations. As in Sec. 2, we set $R_k = S_k = 0$. We also set $\widetilde{v}_k = \overline{v}_k$ and drop a small truncated correlation term in the conservation of energy equation, approximations which have been tested and demonstrated to be highly accurate [3, 4]. Using our model for the interfacial terms, Eq. (5), we obtain the following effective equations,

$$\frac{\partial \beta_k}{\partial t} + v_* \frac{\partial \beta_k}{\partial z} = 0, \tag{6}$$

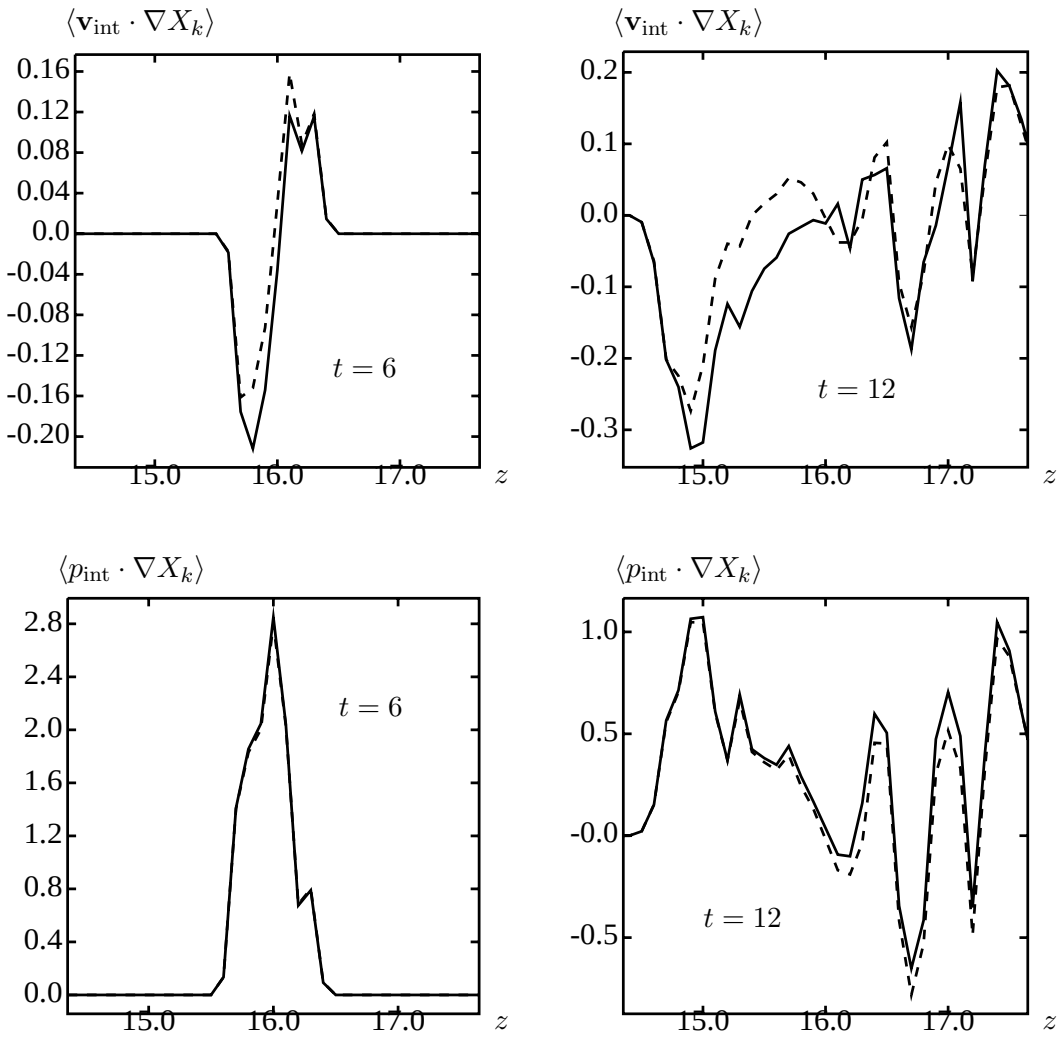

Figure 2: A comparison between the interfacial terms $\langle \mathbf{v}_{\rm int} \cdot \nabla X_k \rangle$ and $\langle p \nabla X_k \rangle$ (solid curves) and their respective approximations as $(\beta_1 \overline{v}_2 + \beta_2 \overline{v}_1)(\partial \beta_k / \partial z)$ and $(\beta_1 \overline{p}_2 + \beta_2 \overline{p}_1)(\partial \beta_k / \partial z)$ (dashed curves). In these simulations, $A_t = 2/3$ and $M^2 = 0.5$.

$$\frac{\partial \beta_k \overline{\rho}_k}{\partial t} + \frac{\partial \beta_k \overline{\rho}_k \overline{v}_k}{\partial z} = 0, \tag{7}$$

$$\frac{\partial \beta_k \overline{\rho}_k \overline{v}_k}{\partial t} + \frac{\partial \beta_k \overline{\rho}_k \overline{v}_k \overline{v}_k}{\partial z} = -\frac{\partial \beta_k \overline{p}_k}{\partial z} + \beta_k \overline{\rho}_k g + p_* \frac{\partial \beta_k}{\partial z}, \tag{8}$$

$$\frac{\partial \beta_k \overline{\rho}_k \widetilde{\epsilon}_k}{\partial t} + \frac{\partial \beta_k \overline{\rho}_k \widetilde{\epsilon}_k \overline{v}_k}{\partial z} = -\overline{p}_k \frac{\partial \beta_k \overline{v}_k}{\partial z} + (pv)^* \frac{\partial \beta_k}{\partial z}, \tag{9}$$

for $k = 1, 2$, and

$$\beta_1 + \beta_2 = 1. \tag{10}$$

To complete the system of equations, we need an effective equation of state for each phase, but not for the mixture. Considering the internal energy ϵ_k as a function of density ρ_k and pressure p_k, we approximate the single-phase equation of state from the microscopic (pre-averaged) equation of state as follows,

$$\epsilon_k = \epsilon_k(\rho_k, p_k) \qquad \longrightarrow \qquad \widetilde{\epsilon}_k \approx \epsilon_k(\overline{\rho}_k, \overline{p}_k). \tag{11}$$

In this approximation, we assume that pressure and density variations within a phase are small relative to variations in these quantities between phases. This simplification avoids the difficulties commonly associated with composing equations of state for mixtures.

Altogether there are ten equations, Eqs. (7)–(9) and (11) for $k = 1, 2$, Eq. (6) for one of the phases, and Eq. (10), and ten unknowns, β_k, $\overline{v}_k$, $\overline{\rho}_k$, $\overline{p}_k$, and $\widetilde{\epsilon}_k$ for $k = 1, 2$. For $0 < \beta_k < 1$, our system of equations is closed, with no free parameters.

Equations (6)–(10) are hyperbolic, with characteristic speeds $\overline{v}_k$ and $\overline{v}_k \pm c_k$ for each phase and $\beta_1 \overline{v}_2 + \beta_2 \overline{v}_1$ for the volume fraction mode. Therefore, the number of independent modes of the system changes across any surface on which one of the volume fractions vanishes, as there is no incoming sound wave for the phase of vanishing volume fraction. In this sense, our closure model is incomplete, but it has reduced the closure problem from a volume to a surface condition, and has given it an improved physical basis.

4 RNG Fixed Point Solution

We now present the RNG fixed-point solution of the two-phase model for RT mixing in the incompressible limit [8]. Introducing the new variables $z' = z/A_t g t^2$, $t' = \ln(t)$, $v' = v/A_t g t$, $p' = p/(A_t g t)^2$, and $\epsilon' = \epsilon (A_t g t)^2$, we re-write Eqs. (6)–(8) in terms of these scaled variables, let ρ_k = const., and take the fixed-point limit by setting all t'-derivatives equal to zero, resulting in (after dropping the primes)

$$(v_* - 2z)\frac{\partial \beta_k}{\partial z} = 0, \qquad 2z\frac{\partial \beta_k}{\partial z} - \frac{\partial \beta_k \overline{v}_k}{\partial z} = 0, \tag{12}$$

$$2z\frac{\partial\beta_k\overline{v}_k}{\partial z} - \frac{\partial\beta_k\overline{v}_k^2}{\partial z} - \beta_k\overline{v}_k = \frac{1}{\rho_k}\frac{\partial\beta_k\overline{p}_k}{\partial z} - \frac{p_*}{\rho_k}\frac{\partial\beta_k}{\partial z} - \frac{\beta_k}{A_t}. \tag{13}$$

We can first solve for the volume fraction and velocity independent of the pressure. According to accepted scaling relations for the mixing layer, the distance from the original undisturbed interface position to the edge of the mixing layer has the form $\alpha A_t g t^2$, where $\alpha = \alpha_B$ at the bubble (penetration of the light fluid) edge, and $\alpha = \alpha_S$ at the spike (penetration of the heavy fluid) edge of the mixing zone. In the present scaled variables, these positions are independent of time, and are $z = -\alpha_B$ (bubble edge) and $z = \alpha_S$ (spike edge), at which $\beta_1 = 0$ and $\beta_1 = 1$, respectively. Using these boundary conditions and Eq. (10), Eqs. (12) have the following exact solution in the interior of the mixing region,

$$\beta_1 = \frac{z+\alpha_B}{\alpha_B+\alpha_S}, \qquad \beta_2 = \frac{-z+\alpha_S}{\alpha_B+\alpha_S}, \qquad \overline{v}_1 = z - \alpha_B, \qquad \overline{v}_2 = z + \alpha_S. \tag{14}$$

Next, we assume a force balance involving form drag and buoyancy to relate the density and velocity differences at the spike and bubble edges through the introduction of new dimensionless (drag) coefficients, C_B and C_S. This information, which is a closure hypothesis for the boundaries of the mixing region, completes the fixed-point solution for β and v by providing the functional relations $\alpha_B = \alpha_B(C_B, C_S)$ and $\alpha_S = \alpha_S(C_B, C_S)$. These relations will be studied in more detail in a forthcoming paper [9]. We emphasize that without information about the drag coefficients, our model makes no prediction of α_B and α_S.

From this solution and Eq. (13), we derive simple ODEs for the pressure difference and sum in the stationary limit,

$$\frac{\partial(\overline{p}_2 - \overline{p}_1)}{\partial z} = 2(\alpha_S\rho_2 + \alpha_B\rho_1) + \rho_2 + \rho_1, \tag{15}$$

$$\frac{\partial(\overline{p}_2 + \overline{p}_1)}{\partial z} = \frac{2(\overline{p}_2 - \overline{p}_1)}{\alpha_S + \alpha_B} + 2(\alpha_S\rho_2 - \alpha_B\rho_1) + \frac{\rho_1 + \rho_2}{A_t}. \tag{16}$$

These equations can be integrated in closed form, introducing two new integration constants, C_1 and C_2, into the solution.

In the absence of information about the pressures at the mixing zone boundaries, we can make an approximation that the fluid outside the mixing zone, which is stagnant at $t = 0$, remains stagnant for all t. In other words, the pressure in a pure phase region is governed by a hydrostatic, time independent equation, and is therefore determined by the initial data. This modeling assumption provides two boundary pressures, $\overline{p}_1(\alpha_S) = \rho_1\alpha_S/A$ and $\overline{p}_2(-\alpha_B) = -\rho_2\alpha_B/A$, which one would expect to determine the integration constants C_1 and C_2. Actually these two boundary conditions determine a linear system

for C_1 and C_2 which is degenerate. Solvability is then a constraint on the right hand side of this system, *i.e.*, the terms independent of C_1 and C_2 which, after some algebra, can be written in the form

$$(1 + A_t)\alpha_B x^2 + (2A_t\alpha_B - 1)x + 1 - (1 - A_t)\alpha_B = 0, \tag{17}$$

where $x = \alpha_S/\alpha_B$. This quadratic equation has two real roots over the interval $0 \leq A_t \leq 1$, for $\alpha_B \leq 0.085$. The lower root appears to be the physically meaningful one. This root satisfies $x = 1$ ($\alpha_S = \alpha_B$) for $A_t = 0$, as should be the case. If $0 < A_t$, the roots depend on α_B. Substituting $\alpha_B = 0.06$, we obtain the value $x = 1.07$ for $A_t = 0.23$, $x = 1.16$ for $A_t = 0.5$, and $x = 1.3$ for $A_t = 0.8$ for the lower root, which can be compared to the experimental values $x = 1$, $x = 1.3$, and $x \approx 1.5$–1.8 respectively, for the same A_t values, given by Read [13] and Youngs [15].

The agreement with experiment is promising but not perfect. The discrepancy can be attributed to the approximation of stagnant conditions outside the mixing region. Equation (13) contains a non-zero term, $\beta_k v_k$, which is not present in the $t = 0$, hydrostatic equation for the (unscaled) pressure. Since $v_1 = \alpha_S - \alpha_B$ and $v_2 = \alpha_S - \alpha_B$ in the light and heavy fluid regions, respectively, the error in the approximation is $O(\alpha_S - \alpha_B)$ for small A; thus it is zero at $A = 0$ and it increases with increasing A. This trend is consistent with the comparison reported above. Again, we emphasize that this approximation is made in the absence of accurate drag information and is not an intrinsic aspect of our model.

5 Conclusion

We have proposed a new two-phase closure for chaotic fluid mixing by Rayleigh-Taylor instability. This model has been validated by comparison with two-phase turbulent mixing data obtained from numerical solution of the two-fluid Euler equations, which itself is in agreement with experiment. The one-dimensional two-phase flow equations derived from our model have a RNG fixed-point solution in the incompressible limit. Our model is closed in the interior of the mixing zone, but not at the edges. A physical law for the boundaries, involving form drag and buoyancy, would supply the missing data associated with the incoming sound wave of the phase of vanishing volume fraction.

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