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This article was submitted to 2000 Nuclear Explosives Code
Development Conference, Oakland, CA, October 23 – 27, 2000

U.S. Department of Energy

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October 1, 2000

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Implementation of a Simple Model for Linear and Nonlinear Mixing at Unstable Fluid Interfaces in Hydrodynamics Codes ¹ (U)

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A simple model was recently described for predicting the time evolution of the width of the mixing layer at an unstable fluid interface [J. D. Ramshaw, Phys. Rev. E 58, 5834 (1998); ibid. 61, 5339 (2000)]. The ordinary differential equations of this model have been heuristically generalized into partial differential equations suitable for implementation in multicomponent hydrodynamics codes. The central ingredient in this generalization is a non-diffusional expression for the species mass fluxes. These fluxes describe the relative motion of the species, and thereby determine the local mixing rate and spatial distribution of mixed fluid as a function of time. The generalized model has been implemented in a two-dimensional hydrodynamics code. The model equations and implementation procedure are summarized, and comparisons with experimental mixing data are presented.

Keywords: mixing, instability, Rayleigh-Taylor, Richtmyer-Meshkov, Kelvin-Helmholtz

Introduction

There is considerable current interest in material interpenetration and mixing at unstable fluid interfaces, particularly those driven by the normal acceleration of adjacent fluid layers with different densities. Such processes occur, for example, in the implosion of inertial confinement fusion capsules and in certain astrophysical problems. These processes can in principle be computed in detail by direct numerical simulations with multidimensional hydrodynamics codes, and recent advances in computer technology and numerical methodology now make this feasible in some problems. In most practical applications, however, computer time and/or storage limitations still preclude a complete simulation of the very wide range of length and time scales involved in such instabilities. In particular, the development of the instabilities, at least at early times, is sensitive to the amplitude and length scales of the initial perturbations, which are frequently too small to resolve in a practical computing mesh.

In order to simulate the effects of interfacial instabilities and material mixing with reasonable accuracy on present-day computers, it is therefore necessary to develop submodels which capture the essential physics of these effects in a form and framework suitable for implementation into hydrodynamics codes. Conventional turbulence models are not well suited for this purpose, as they are usually developed and calibrated for single homogeneous materials rather than a mixture of different materials with significantly different densities. Multiphase turbulence models allow for the different materials but tend to be much more complicated, which makes them difficult to validate and implement. Ease of implementation is a major consideration, since modern hydrodynamics codes are becoming ever more

¹This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

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sophisticated and difficult to modify. Thus there is a particular need for mixing models which are simple enough to be installed into existing hydrodynamics codes on a relatively short time scale. Such models should clearly be as simple and easy to retrofit as possible, but not of course so simple that they fail to capture the essential physics. Models of this type will necessarily be phenomenological, but they should be as fundamentally based as their simplicity allows. They should attempt to maximize the physics while minimizing the empiricism and the number of free parameters.

These requirements imply that the model must allow for an arbitrary time-dependent acceleration history $a(t)$, and it must reproduce the known linear and nonlinear growth behavior of the incompressible Rayleigh-Taylor (RT) and Richtmyer-Meshkov (RM) instabilities as special cases. Other desirable features include the ability to represent compression effects, shock waves, and Kelvin-Helmholtz (KH) instabilities resulting from tangential velocity discontinuities. A simple model with these features has recently been constructed based on the general concepts of energy conservation and scale invariance (Ramshaw 1998, 2000). This model takes the form of a second-order ordinary differential equation (ODE) (or two coupled first-order ODEs) for the time evolution of the penetration depth h of the light fluid into the heavier one (see Fig. 1). The model correctly reproduces the known linear and nonlinear growth behavior of the RT, RM, and KH instabilities, and gives results in good agreement with the experimental data of Dimonte and Schneider (1996) for four different time-dependent acceleration histories. It therefore seems a promising candidate to represent the effects of interfacial instabilities and mixing in hydrodynamics codes.

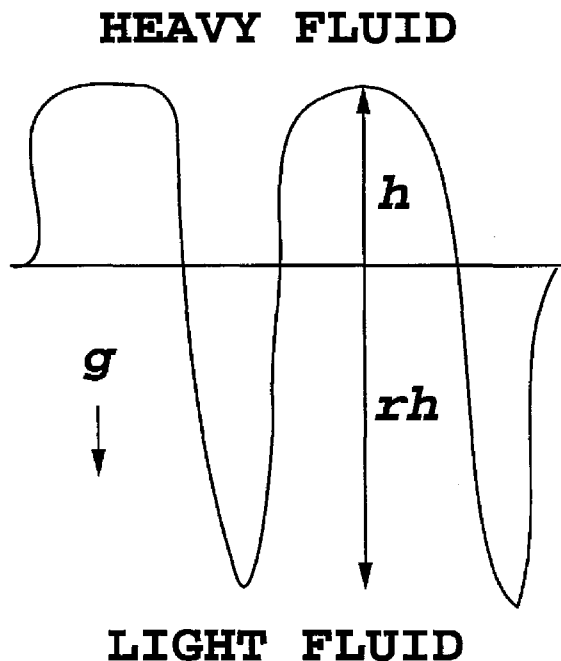


Figure 1: Schematic of mixing layer.

However, it is by no means obvious how best to incorporate ODE models of this general type into the partial differential equations (PDEs) of hydrodynamics. The central problem is that ODE models and the variables therein (like h) are global in nature, whereas the

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PDEs of hydrodynamics are local. In particular, the description of mixing in hydrodynamics requires expressions for the local mass fluxes of the different materials relative to the mean fluid velocity. The mixing model must supply these expressions, and this requires the introduction of additional ingredients and assumptions. A variety of new issues arise and must be addressed, and there is considerable ambiguity (or freedom!) about how to resolve them and proceed. Here we propose and describe a particular procedure for extending the ODE model into a local model for predicting local material mass fluxes in a hydrodynamics code. We do not claim that the present procedure is unique or even optimal, but it is straightforward, easy to implement, and works well in the test problems performed to date. This procedure has been used to incorporate the model in a relatively simple multicomponent hydrodynamics code (Cloutman 1990) for testing purposes. The resulting code has been used to simulate a set of incompressible linear electric motor experiments (Dimonte and Schneider 1996), as well as a shock tube experiment performed by Zaytsev *et al.* (Mügler and Gauthier 1998). In both cases the agreement with experiment is quite satisfactory. Further development and testing of this model and implementation procedure in other hydrodynamics codes therefore seems worthwhile.

Summary of the ODE Mix Model

The ODE mix model used in this work is based on the general concepts of energy conservation and scale invariance. The model was constructed by a heuristic procedure consisting of three main steps: (1) The first step is to derive a time evolution equation for the kinetic energy of an inhomogeneous fluid subjected to a slow uniform but anisotropic compression or expansion. (2) The various terms in this equation are then evaluated using the linear potential flow solution for two fluids separated by a sinusoidally perturbed interface with amplitude h and wavelength λ . This ensures that we properly capture the correct linear stability behavior for small perturbations. (3) Finally, the formulation is extrapolated into the nonlinear regime by means of a wavelength renormalization hypothesis (WRH), according to which the effective value of λ becomes proportional to $|h|$ at late times. The WRH embodies the scale invariance that mixing layers are expected to exhibit in the nonlinear regime. The reader is referred to the literature for the derivation and further discussion. Here we shall simply summarize the model and a few post-publication improvements, so that we can concentrate on the implementation issues in subsequent sections. It should be noted that the general model (Ramshaw 2000) includes the effects of KH instability resulting from transverse shear, but these effects are neglected here for simplicity.

The model may be expressed in the form of the following two coupled ODEs:

$$\dot{h} = D_n h + v \quad (1)$$

$$\sqrt{\lambda} \frac{d}{dt} (\sqrt{\lambda} v) = 2\pi[a(t)Ah - c|v|v] - \frac{1}{4}D_t \lambda v \quad (2)$$

where $a(t)$ is the acceleration normal to the interface, A is the Atwood number, D_n and D_t are the normal and transverse expansion rates, λ is a function of $b|h|$ (defined below), and

$$b = \frac{\pi\theta}{\alpha(2-\theta)} \quad (3)$$

$$c = \frac{2-3\theta}{4\alpha(2-\theta)} \quad (4)$$

where α and θ are parameters in the nonlinear RT and RM growth laws $h_{RT} = \alpha A g t^2$ and $h_{RM} \sim t^\theta$. The term involving $a(t)$ represents the growth of the instability due to buoyancy forces, while the term involving c represents the viscous dissipation of mixing energy to thermal energy.

In this model, the effective perturbation wavelength λ undergoes a transition from its initial value λ_0 for $|h| \ll \lambda_0$ to the WRH value $b|h|$ when $|h| \gg \lambda_0$. This transition was originally effected suddenly at the point $|h| = m\lambda_0$, where $m \sim 1/2$ is set at the user's discretion. This is clearly unrealistic, as there is a weakly nonlinear transitional regime during which the instability has become nonlinear but λ_0 remains the dominant length scale. We therefore now allow for a smooth transition between linear and fully nonlinear behavior over the range $m_1\lambda_0 < |h| < m_2\lambda_0$. This can be done by replacing c by fc and letting

$$\lambda = (1 - f)\lambda_0 + fb|h| \quad (5)$$

where $f = 3x^2 - 2x^3$ and $x = (|h|/\lambda_0 - m_1)/(m_2 - m_1)$, subject to the constraint $0 \leq x \leq 1$. However, one intuitively suspects that the damping coefficient c should come into play before λ changes much, and this can be accomplished by raising f to different powers in the two quantities; i.e., replacing c by $f^y c$ and letting

$$\lambda = (1 - f^z)\lambda_0 + f^z b|h| \quad (6)$$

Test calculations to date have been performed with $m_1 = 0.1$, $m_2 = 1$, $y = 0.1$, and $z = 2$, but more detailed comparisons with weakly nonlinear $h(t)$ data are needed to determine the values of m_1 and m_2 and/or the form of f .

The Treatment of Shock Waves

This model presents two known problems when shock waves are present. The first is that hydrodynamics codes typically treat shock waves by shock smearing or capturing techniques, which artificially thicken the shock by means of a shock viscosity. This in turn artificially prolongs the duration of the shock, which may then become gradual rather than impulsive compared to the natural time scale for h to change in the mixing model. This would allow a significant but unphysical change in the value of h during the shock, and the shock would not then deposit the correct energy in the mixing layer. Fortunately, this problem can easily be avoided by monitoring the shock viscosity within the mixing layer to detect the presence of a shock, and replacing v by zero in Eq. (1) while the shock is present. This has the physically appropriate effect of freezing h (except for compression effects) at its value when the shock arrives until the shock has passed by.

The second problem is more insidious: if a perturbed interface is subjected to a slowly varying $a(t) < 0$, $h(t)$ will undergo stable oscillations about $h = 0$. If a shock wave then strikes the mixing layer, its effect will be highly sensitive to its arrival time relative to the phase of the oscillations (see Fig. 2). In particular, if the shock arrives at a time when $|h|$ is very small or zero, it will have little or no effect. This behavior is actually physical for a single-mode perturbation in the linear regime, but will rarely occur in practical problems due to the inevitable presence of other modes and the fact that it is highly unlikely that all the associated mode amplitudes would be very small at the same time.

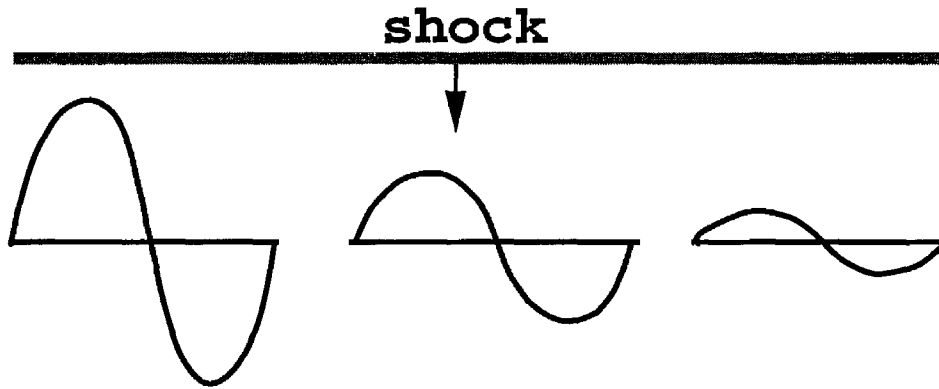


Figure 2: Sensitivity to shock arrival time during stable oscillations.

Unfortunately, there is no obvious way to cure this problem properly without generalizing the model to include a true multimode capability, which would entail a great deal of additional complexity. However, the problem can be ameliorated or prevented from occurring by means of various simple *ad hoc* fixes such as the following:

- (a) Set $v = 0$ whenever $hv < 0$. This completely prohibits demixing.
- (b) Replace $a(t)A$ by $\max(a(t)A, 0)$ when shocks are absent. This ignores accelerations in the stable direction except when shocks are present, when they cannot be ignored without losing the RM instability.
- (c) Greatly increase the dissipation coefficient c when $hv < 0$ to retard the rate of demixing.
- (d) Reverse the sign of h whenever $hv < 0$. This completely prohibits demixing but preserves the sign information contained in v and \dot{v} , which seems important in problems with multiple or reflected shocks.

We emphasize, however, that none of these fixes is fully satisfactory, and all of them produce other unphysical behavior in some situations. They should therefore be used with care and caution to ensure that the cure does not produce worse symptoms than the disease. At present we are leaning toward (d) above, which seems to do the minimum violence to the remaining physics, but further investigation is needed.

Implementing ODE Mix Models in Hydrodynamics Codes

A number of new issues must be addressed in order to implement ODE mix models of the present type in hydrodynamics codes. The situation is complicated by the fact that the variables in ODE mix models (such as h and v) are inherently global in nature, while the PDEs of hydrodynamics are inherently local. It is by no means obvious (at least to the present author) how best to convert between these two very different types of description. It is evidently necessary to compute and store h and v as local variables in every cell of the computing mesh (or at least every cell containing mixed materials) while maintaining their interpretation as semi-global quantities associated with a larger region containing the cell in question. Since h and v are not local densities of conserved quantities, they need not

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be transported conservatively (or even differentially!), but their values must nevertheless be transported or propagated between cells in some sensible way consistent with their semi-global nature. The computation of h and v also requires the quantities $a(t)$, A , D_n , and D_t , so it is necessary to specify the manner in which these quantities are to be evaluated in terms of the hydrodynamic variables.

Even if we have sensible local or semi-local values for h and v , these variables are not themselves directly useful in hydrodynamics. The basic quantities required in a hydrodynamic description are the local material or species mass fluxes, which are required to describe the local transport of materials and predict local species concentration profiles and distributions. The mix model must supply these mass fluxes, and this requires further modeling assumptions. These fluxes can be expressed in terms of the relative velocities between species, which are evidently closely related to v . However, v is a scalar while the mass fluxes are vectors, so it is necessary to define the direction they point in as well as their precise dependence on v and other variables. It is natural to identify this direction with the local normal to the mixing layer, which is also needed for other purposes. This normal direction must be defined in terms of the hydrodynamic variables and their gradients. Moreover, the mix model contains only two materials, light and heavy, whereas realistic problems of interest often involve multiple species. It is therefore necessary to construct logic for grouping multiple species together into light and heavy materials, and conversely for separating the light and heavy mass fluxes into mass fluxes for each individual species.

The primary effect of the mix model on the hydrodynamic equations occurs through the species mass fluxes, which appear in the species continuity equations. This effect is straightforward and is the essence of mixing. However, it is also necessary to determine the form of any required modifications to the other hydrodynamic equations. In particular, the species mass fluxes imply a corresponding additional enthalpy flux which must be accounted for. In addition, the relative motion of materials implies the presence of non-thermal kinetic energy which is not contained in the mean flow. This energy must be included in the overall energy balance, and its dissipation produces thermal energy which also must be accounted for.

Finally, incorporation of the model in a hydrodynamics code requires consideration of numerical issues, including the placement of variables and the numerical scheme used to advance them in time. The numerical treatment is constrained by the requirement of compatibility with the mesh and numerical scheme used for the hydrodynamics, and hence will be somewhat code-specific. Fortunately, these numerical issues present no particular difficulties and are relatively straightforward compared to the more subtle conceptual issues discussed above.

The above are the main issues that needed to be addressed in order to extend the original ODE model into a form suitable for implementation in hydrodynamics codes. The manner in which these issues were treated and resolved will be described in subsequent sections. It should be noted, however, that most of these issues do not admit of a unique resolution. We are constructing a model rather than a theory, and by its very nature a model represents a collection of uncontrolled approximations. These approximations present a variety of different choices, and their validity can only be assessed *a posteriori*. Thus we cannot, and do not, claim that the choices made here are unique or optimal, but it is encouraging that the resulting solutions agree well with experimental data in the test problems performed to

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date. However, more extensive test calculations and implementations in other hydrodynamic codes will be required before a final assessment can be made.

Two Materials vs. Multiple Species

A general multicomponent hydrodynamics formulation must allow for an arbitrary number of species or materials, whereas the mix model has only two materials, light and heavy. In order to employ it in more general situations, it is evidently necessary to divide the species into a light subset A and a heavy subset B . This may be done either globally or locally. Once each species has been labeled as being light or heavy, the local partial densities of the light and heavy materials are given by

$$\rho_A = \sum_{i \in A} \rho_i, \quad \rho_B = \sum_{i \in B} \rho_i \quad (7)$$

where ρ_i is the local partial density of species i (i.e., mass of species i per unit total volume). The local volume fraction of species i is $\alpha_i = \rho_i / \rho_i^0$, where ρ_i^0 is the mass density of pure material i (i.e., mass of species i per unit volume of species i). The local volume fractions of the light and heavy materials are then given by

$$\alpha_A = \sum_{i \in A} \alpha_i, \quad \alpha_B = \sum_{i \in B} \alpha_i \quad (8)$$

The local densities of "pure" light and heavy materials may then be defined by

$$\rho_A^0 = \rho_A / \alpha_A, \quad \rho_B^0 = \rho_B / \alpha_B \quad (9)$$

and the local Atwood number is then given by

$$A = \frac{\rho_B^0 - \rho_A^0}{\rho_B^0 + \rho_A^0} \quad (10)$$

Equation (9) breaks down in cells containing pure or nearly pure A or B , so we temporarily insert small virtual quantities of A or B into such cells in order to ensure that ρ_A^0 and ρ_B^0 have reasonable values everywhere.

Normal Vector and Acceleration

The local unit vector normal to the mixing layer (region) is defined by

$$\mathbf{n} = -\nabla \alpha_A / |\nabla \alpha_A| \quad (11)$$

which by construction points from the light material into the heavy material. The local acceleration in the normal direction is then given by

$$a(t) = -(1/\rho) \mathbf{n} \cdot \nabla p \quad (12)$$

where ρ and p are the local mass density and pressure of the fluid.

Mass-Weighted, Volume-Weighted, and Relative Velocities

The local mass weighted fluid velocity \mathbf{u} is determined by the hydrodynamic momentum equation. It is related to the velocities of materials A and B by

$$\rho \mathbf{u} = \rho_A \mathbf{u}_A + \rho_B \mathbf{u}_B \quad (13)$$

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Similarly, the local volume weighted fluid velocity is given by

$$\mathbf{u}_v = \alpha_A \mathbf{u}_A + \alpha_B \mathbf{u}_B \quad (14)$$

and it is easy to show that

$$\rho(\mathbf{u}_v - \mathbf{u}) = (\alpha_A \rho_B - \alpha_B \rho_A)(\mathbf{u}_A - \mathbf{u}_B) = \alpha_A \alpha_B (\rho_B^0 - \rho_A^0)(\mathbf{u}_A - \mathbf{u}_B) \quad (15)$$

Since it is \mathbf{u}_v rather than \mathbf{u} which determines volume changes, the local expansion rates D_n and D_t should evidently be evaluated from \mathbf{u}_v rather than \mathbf{u} . We therefore set

$$D_n = \mathbf{n} \cdot \nabla \mathbf{u}_v \cdot \mathbf{n} \quad (16)$$

$$D_t = \nabla \cdot \mathbf{u}_v - D_n \quad (17)$$

Inspection of Fig. 1 suggests that the relative velocity should be of the form

$$\mathbf{u}_A - \mathbf{u}_B = \mu(1 + r)v \operatorname{sign}(h)\mathbf{n} \quad (18)$$

where μ is an as yet undetermined coefficient of order unity. However, this expression requires *local* values of v and h , which have not yet been defined. The manner in which h and v are determined locally will be discussed below. The spike/bubble height ratio r is given by (Dimonte and Schneider 2000)

$$r = \min[(\rho_B^0/\rho_A^0)^{1/3}, (2\alpha)^{-1}] \quad (19)$$

where we have imposed a constraint to prevent the spike velocity from exceeding the free-fall velocity in a constant gravitational field for large density ratios.

Mass Fluxes and Species Transport

Species transport and mixing in multicomponent hydrodynamics is governed by the individual species continuity equations, which take the form

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}) = - \nabla \cdot \mathbf{J}_i \quad (20)$$

where \mathbf{J}_i is mass flux of species i relative to \mathbf{u} . It is the task of the mix model to supply these fluxes. This will be done by expressing \mathbf{J}_i in terms of the light and heavy material mass fluxes $\mathbf{J}_A = \rho_A(\mathbf{u}_A - \mathbf{u})$ and $\mathbf{J}_B = \rho_B(\mathbf{u}_B - \mathbf{u}) = -\mathbf{J}_A$. Using Eq. (13), we readily obtain

$$\mathbf{J}_A = -\mathbf{J}_B = \left(\frac{\rho_A \rho_B}{\rho} \right) (\mathbf{u}_A - \mathbf{u}_B) \quad (21)$$

To relate \mathbf{J}_i to $\mathbf{J}_{A,B}$, we simply regard materials A and B as mixtures which carry their constituent species along with them, so that

$$\mathbf{J}_i = y_i^A \mathbf{J}_A + y_i^B \mathbf{J}_B = (y_i^A - y_i^B) \mathbf{J}_A \quad (22)$$

where y_i^A and y_i^B are the mass fractions of species i in materials A and B . Ordinarily a given species is considered either light or heavy, so that only one of y_i^A and y_i^B is nonzero for each i . Equations (21) and (22) determine the species mass fluxes in terms of the relative velocity given by Eq. (18).

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The different species have different thermal energies, so a corresponding term $\sum_i h_i \mathbf{J}_i$ must also be added to the heat flux in the energy equation, where h_i is the partial specific enthalpy of species i . This term is often referred to as the “enthalpy diffusion” term when the mass fluxes \mathbf{J}_i are diffusional in nature. Most turbulent mixing models indeed employ diffusional expressions for \mathbf{J}_i , but in the present context this seems inconsistent with the inertial nature of the mixing process. In contrast, the mass fluxes in the present treatment are inertial and reversible, which permits the description of demixing in stable accelerations.

For the case of one-dimensional mixing of two incompressible materials with a uniform value of $v(t)$, an analytical similarity solution can be derived for the volume fraction profile. The result is

$$\alpha_A = \frac{1}{2} \left[1 - \frac{1}{\mu(1+r)} \left(\frac{x}{h} \right) \right] \quad (23)$$

The total width of the mixing layer from $\alpha_A = 0$ to $\alpha_A = 1$ is seen to be $2\mu(1+r)h$. Equating this width to $(1+r)h$ (see Fig. 1) then gives $\mu = 1/2$, thereby roughly determining the value of μ .

The use of a constant value of μ in Eq. (18) therefore results in a linear volume fraction profile in this situation, which is the simplest qualitatively reasonable possibility. However, this profile becomes more and more unrealistic as the Atwood number increases, as it does not properly reflect the asymmetry between spike and bubble penetration. Fortunately, a generalized similarity solution shows that other profiles can be accommodated by introducing an appropriate volume fraction dependence into $\mathbf{u}_A - \mathbf{u}_B$. This provides a mechanism whereby experimentally determined volume fraction profiles can be incorporated into the model if desired.

Computing “Local” Values of h and v

Having defined local values for the quantities $a(t)$, A , D_n , and D_t , we are now in a position to advance h and v in time by means of Eqs. (1) and (2). However, this requires us to confront our central dilemma: by their very nature h and v are not local variables, and yet they must be computed locally in a hydrodynamics code. We shall attempt to evade this dilemma by the simple expedient of defining and computing local values of h and v within each cell of the computing mesh, but interpreting these values as semi-global (or semi-local) parameters which pertain to the part of the mixing layer in the neighborhood or vicinity of that cell. However, it is not sensible to compute h and v in unmixed cells containing pure or nearly pure A or B , so we set $h = v = 0$ in such cells. We consider a cell unmixed if its value of α_A is less than 0.01 or greater than 0.99.

The interpretation of h and v as semi-global quantities implies that their gradients *within* the mixing layer should remain small. To ensure this, we smooth the h and v fields by an artificial diffusional process which tends to equalize nonzero values of h and v in neighboring cells. However, this process is not allowed to produce nonzero values of h or v in unmixed cells where $h = v = 0$, so it does not tend to spread out the mixing region. The expansion of the mixing region occurs entirely through the action of the mass fluxes, which are nondiffusional in character as discussed above. The smoothing of h and v therefore does not diffuse species or materials.

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As the mixing layer grows, or as it moves through the mesh due to mesh motion and/or convection of the fluid as a whole, it is necessary to transport or propagate h and v between cells accordingly. Since h and v are not densities of conserved quantities, there is no need or incentive to transport them conservatively. Indeed, since h and v are not really local variables, it is even dubious to transport them in the usual local manner involving convective derivatives. If this were done, h and v would tend to be smeared out by numerical diffusion, which would reduce their amplitudes and introduce undesirable gradients in their values within the mixing region. We therefore use an entirely different approach based on the idea that h and v are inherently attached to, and hence transported along with, the mixed material which they produce. This idea can be implemented simply by switching on h and v when the mass fluxing causes a previously unmixed cell to acquire a significant amount of the other material. When an unmixed cell with $h = v = 0$ acquires a value $0.01 < \alpha_A < 0.99$, we therefore set h and v in that cell equal to an average of the nonzero values in neighboring cells.

Energy Conservation

The relative motion of materials implies the presence of additional kinetic energy which is not contained in the kinetic energy of the mean flow. This kinetic energy of mixing is closely analogous to the turbulent kinetic energy appearing in turbulence models. The total energy of the flow is of course still conserved, but now includes mixing energy as well as thermal and mean flow kinetic energy. A transport equation for the mean flow kinetic energy density $\frac{1}{2}\rho|\mathbf{u}|^2$ can readily be derived from the momentum equation in the usual way. When this is subtracted from the total energy equation, one obtains an internal energy equation which looks formally the same as the usual one. This is deceptive, however, because the resulting "internal" energy is no longer purely thermal, but now includes the kinetic energy of mixing as well.

The present model therefore requires two modifications to the energy equation: (a) inclusion of the additional term $\sum_i h_i \mathbf{J}_i$ in the heat flux as previously noted, and (b) reinterpretation of the internal energy as the sum of mixing and thermal energies as described above. Once (a) has been implemented, the "internal" energy may be computed in the usual way. However, (b) implies that it is then necessary to subtract out the local mixing energy in order to obtain the local thermal energy for use in the thermodynamic state relations. Unfortunately, the local mixing energy density cannot be directly evaluated in the present model, since h and v are not local variables. This problem is not peculiar to the present model, but occurs in any model in which the kinetic energy of turbulence or mixing is not computed and stored locally. In particular, the same situation occurs (but has rarely been discussed) in the original Smagorinsky/Deardorff subgrid-scale turbulence models, which do not compute the turbulent kinetic energy either. These models simply presume that the internal energy is purely thermal, and hence they implicitly assume that turbulent energy is negligible compared to thermal energy. This is always the case at low Mach number, but cannot safely be assumed at higher Mach numbers.

Even though the local kinetic energy of mixing cannot be directly evaluated in the present model, it can nevertheless be approximated in the following manner. The approximation is based on the fact that in contrast to h and v , the material velocities \mathbf{u}_A and \mathbf{u}_B really are local variables, so the material kinetic energy densities $Q_A = \frac{1}{2}\rho_A|\mathbf{u}_A|^2$ and $Q_B = \frac{1}{2}\rho_B|\mathbf{u}_B|^2$

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can be evaluated locally. One might at first think that the mixing energy density is simply $Q_A + Q_B - \frac{1}{2}\rho|\mathbf{u}|^2$, but this would be wrong because it neglects the contributions of the small-scale secondary flows which contribute to the mixing energy but not to \mathbf{u}_A and \mathbf{u}_B . These contributions cannot be evaluated exactly, but their effect may be approximated by inserting a correction factor based on the relative magnitudes of the normal and transverse contributions to the kinetic energy tensor in the linearized potential flow solution (Ramshaw 2000). However, this solution was obtained in a frame moving with \mathbf{u}_v rather than \mathbf{u} , so this difference must also be accounted for. The net result is the following approximate expression for the local mixing energy per unit volume Q ,

$$Q = \frac{\mu^2(1+r)^2v^2}{2\rho} [(\alpha_A\rho_B - \alpha_B\rho_A)^2 + 2\rho_A\rho_B] \quad (24)$$

The local thermal energy density can then be approximately evaluated simply by subtracting Q from the local internal energy density computed from the energy equation.

Numerical Scheme

The time advancement of h and v requires an approximate solution of Eqs. (1) and (2) in each mixed cell. This is done by means of the same scheme originally used for the previous incompressible model (Ramshaw 1998), augmented by a suitable treatment of the compression terms. We evaluate h in the compression term in Eq. (1) as either h^n or h^{n+1} according as $D_n > 0$ or $D_n < 0$, respectively. Similarly, we evaluate v in the compression term in Eq. (2) as either v^{n+1} or v^n according as $D_t > 0$ or $D_t < 0$, respectively. This treatment preserves the essential physical property that these terms cannot change the sign of h or v , no matter how large the time step becomes.

It is also necessary to specify the placement of the variables in the computing mesh so that the spatial differencing may be defined. This will of course depend on the type of mesh and the placement of the hydrodynamic variables therein, so no general procedure can be given. In most hydrodynamics codes, thermodynamic variables such as pressure and densities are located at cell centers, and a spatial difference approximation to Eq. (20) is obtained by integrating over the volume of a typical cell and using the divergence theorem to convert volume integrals to surface integrals. When this is the case, the mass fluxes \mathbf{J}_A and \mathbf{J}_i are required on cell faces. Regardless of where h and v are located, some averaging or interpolation is required to obtain them and/or the other quantities at places where they are not fundamentally defined. At present we simply locate h and v at cell centers. Quantities required to compute cell face values of \mathbf{J}_A and \mathbf{J}_i from Eqs. (18), (21) and (22) are obtained by averaging or interpolation from the adjacent cell centered quantities, except that we use whichever of the two adjacent values of v is larger in magnitude in Eq. (18). This is done to ensure that the relative velocity has its full value even on faces where one of the adjacent cells is unmixed and consequently has $v = 0$.

Pilot Implementation and Test Calculations

The present model has been implemented in the COYOTE code (Cloutman 1990) for testing purposes. COYOTE is a rectangular-mesh Eulerian code for computing multicomponent hydrodynamics problems in two space dimensions. Test calculations have been performed corresponding to the experimental data of Dimonte and Schneider (1996) on the growth

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of a mixing layer between two incompressible fluids subjected to four different acceleration histories. All calculations were performed with the fixed parameter values $\alpha = 0.06$, $\theta = 0.3$, and $\mu = 0.5$. The bubble penetration depth h was defined as the distance from the original unperturbed interface to the point where $\alpha_A = 0.07$. It is convenient to plot h vs. the interface displacement z defined by $d^2z/dt^2 = a(t)$. Comparisons between the computed and measured values of $h(z)$ are shown in Fig. 3. The agreement is seen to be quite satisfactory.

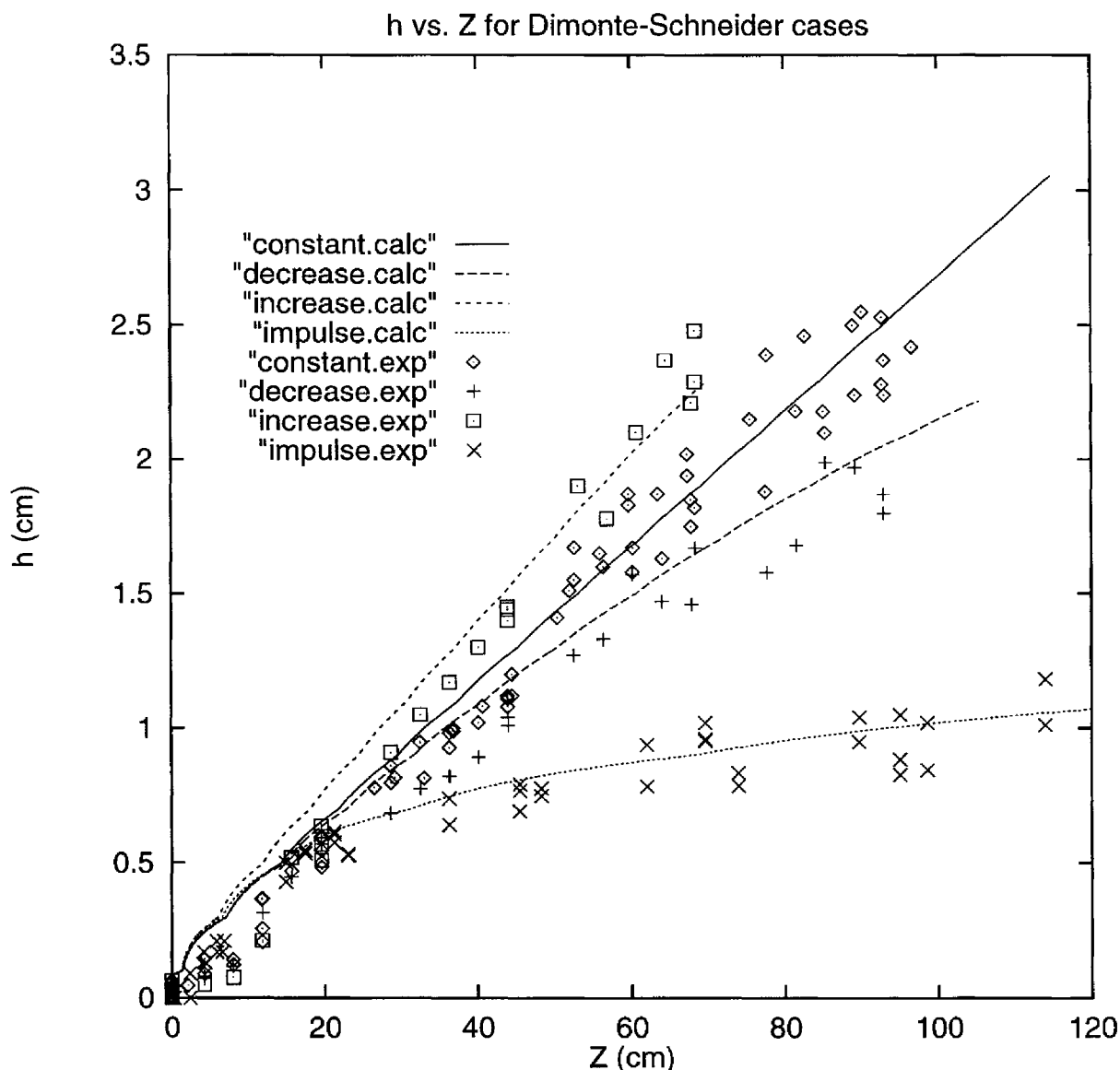


Figure 3: Comparison of computed and measured bubble penetration depths for four different acceleration histories.

The time evolution of the computed volume fraction profiles for the "constant" acceleration case is shown in Fig. 4. As expected from the similarity solution, the profiles are seen to be nearly linear except for the rounding of the corners by the numerics.

We also performed a RM simulation corresponding to a shock tube experiment by Zaytsev (Mügler and Gauthier 1998), in which a Mach 3.5 shock wave impinges on a perturbed

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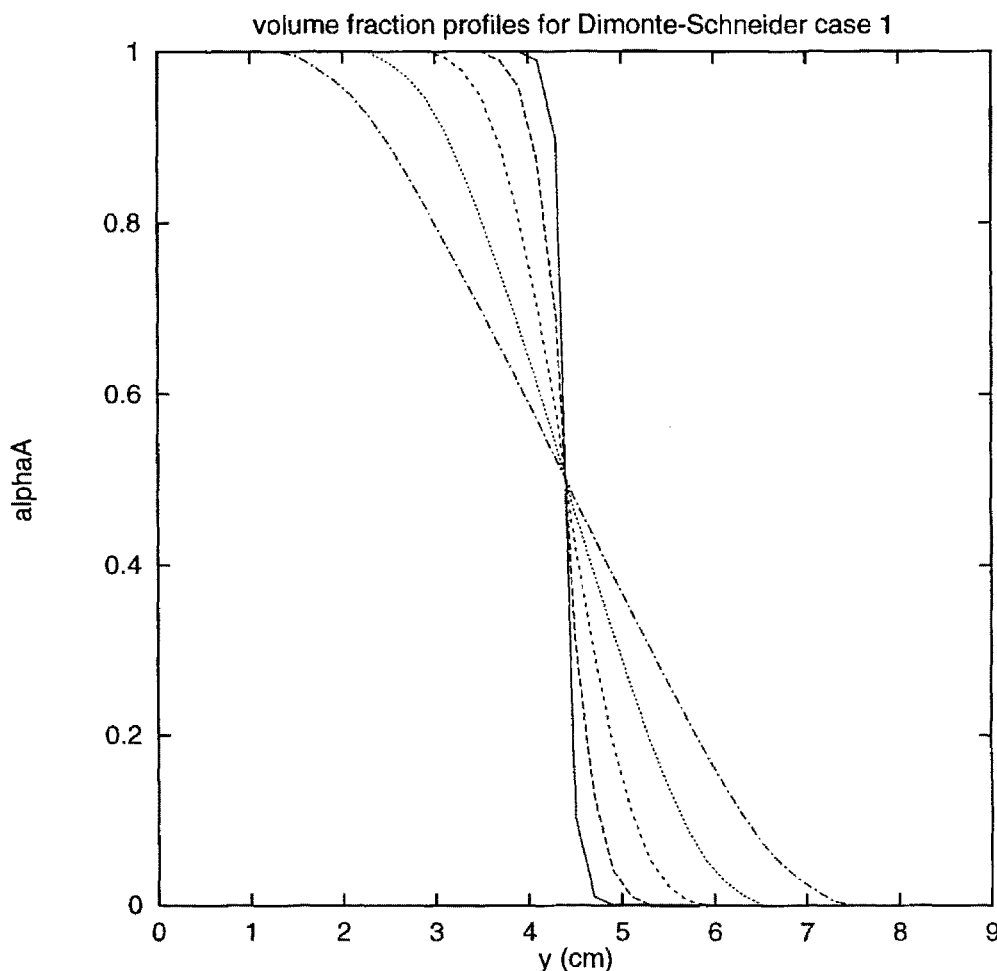


Figure 4: Volume fraction of light material vs. normal distance y at $t = 10, 20, 30, 40$, and 50 ms.

interface between Kr and Xe. The initial perturbation is sinusoidal with amplitude $h_0 = 0.5$ cm and wavelength $\lambda_0 = 3.6$ cm. The mixing layer width is defined, both experimentally and computationally, as the distance between the points at which $\alpha_A = 0.05$ and 0.95 . The calculation was performed using the same values of α , θ , and μ as before, and the parameters defining the weakly nonlinear transitional regime parameters were arbitrarily taken to be $m_1 = 0.1$, $m_2 = 1$, $y = 0.1$, and $z = 2$. Figure 5 compares the computed and measured mixing layer widths, and the agreement is again quite satisfactory.

Unresolved Issues and Missing Physics

Although the model now contains many of the ingredients needed to perform nontrivial simulations of practical problems, it still requires further development and improvement in several areas, including the following:

- The present model is limited to single-mode perturbations in the linear regime. The generalization to allow for multimode perturbations and mode coupling would be highly desirable. In particular, this would remove the model's most serious deficiency in deal-

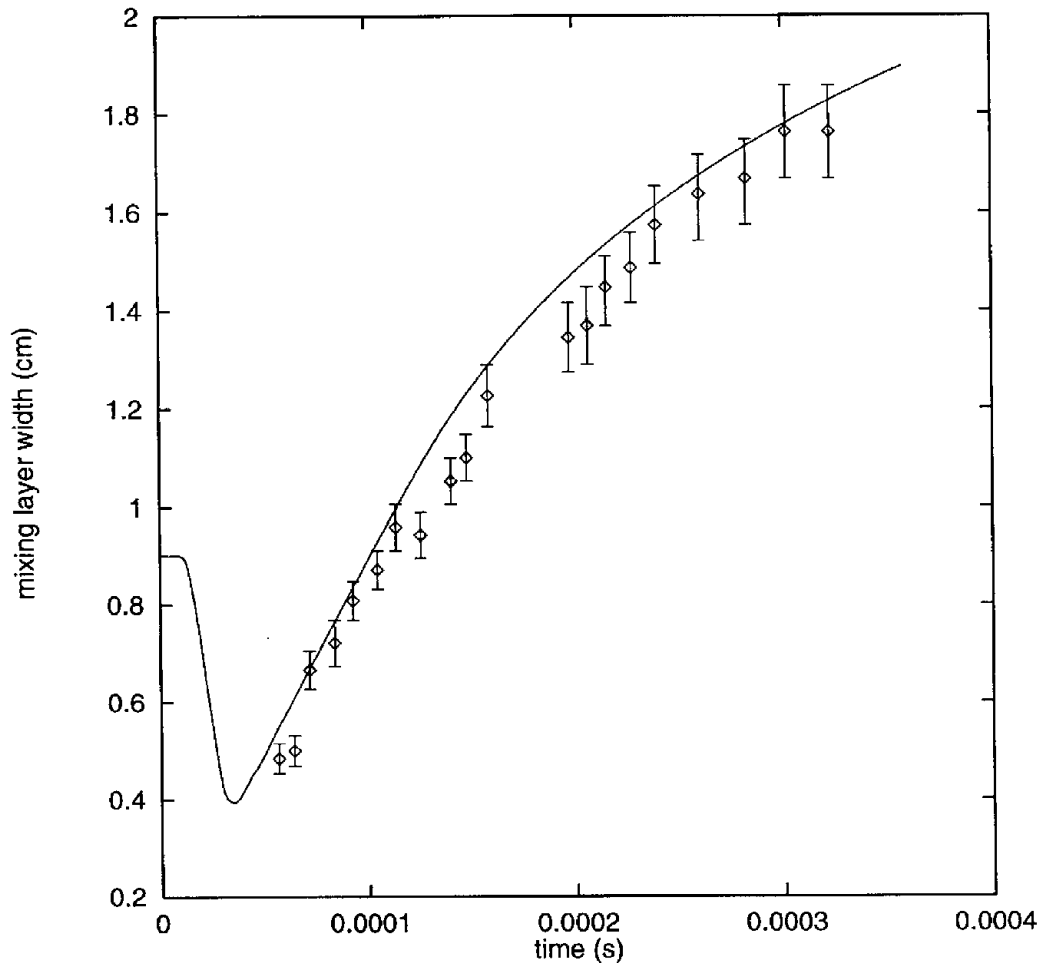


Figure 5: Comparison of computed and measured mixing layer width in Zaytsev shock tube.

ing with shock waves. Unfortunately, it is not clear how to accomplish this generalization without a substantial increase in complexity.

- When $Aa(t) < 0$ the model properly predicts demixing (reseparation) of the two fluids, but at a rate which is expected to be too fast (Ramshaw 1998). Modifications to reduce the rate of demixing should be developed and validated by comparisons with experimental data on demixing rates.
- In its present form, the model neglects surface tension and assumes the two fluids are immiscible. It therefore does not allow for molecular diffusion and does not compute the transition from reversible inertial to irreversible diffusive mixing. Removal of this restriction will probably require the introduction of additional variables to represent information about the spectrum of length scales and the rate at which molecular mixing occurs.
- In some problems the accelerating interface is simultaneously ablating, and this will affect the instability growth in ways that the model cannot currently represent.

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- As discussed above, the model in its present form produces linear or nearly linear volume fraction profiles. Such profiles are not realistic at large Atwood number, where the spike-bubble asymmetry becomes pronounced. The generalization of Eq. (18) to accommodate more general volume fraction profiles therefore requires further consideration.

Concluding Remarks

We have described a heuristic procedure for generalizing a simple ODE mix model into a form suitable for implementation in hydrodynamics codes. This procedure was used to implement the model in the COYOTE code for development and testing purposes. Test calculations and comparisons with experimental data were performed for incompressible linear electric motor experiments and a shock tube experiment, and in all cases good agreement with the data was obtained using a single set of model parameters.

Although implementation details are inevitably code-specific to some degree, the implementation procedure that we have described is sufficiently general that it should be equally applicable to a variety of other hydrodynamics codes and numerical schemes. In particular, the basic procedure is equally applicable in Lagrangian, Eulerian, or ALE codes in one, two, or three space dimensions. It would be relatively straightforward to implement this model in other hydrodynamics codes by essentially the same procedure, and this will indeed be required to address a wider range of problems and assess the overall utility of the model.

Acknowledgments

I am grateful to Larry Cloutman for the original implementation coding and many helpful discussions, and to Guy Dimonte, Dan Klem, Chuck Leith, Tom McAbee, Karnig Mikaelian, Oleg Schilling, Pete Stry, Bob Tipton, and George Zimmerman for various types of assistance and many helpful discussions during the course of this work.

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