

# Representation of the Molecular Mixing Process in a Two-Phase Flow Turbulent Mixing Model

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## 1 Introduction

A turbulence model based on the equations of two-phase flow with diffusion terms added has been used to model the mixing of miscible fluids by Rayleigh-Taylor (RT) instability in 1D and 2D [1, 3]. One important aspect of the mixing process was not represented: the dissipation of concentration fluctuations: the mixing of the two fluids at a molecular level. Mixing at a molecular level inhibits de-mixing and affects many other processes such as chemical reaction and heat flow. The molecular mixing process is represented by mass exchange between the phases. This paper shows results for simple 1D incompressible cases. The next steps will be to include the model in 1D and 2D multifluid compressible turbulent mixing calculations. The Rayleigh-Taylor experiments of Dalziel and Linden (this workshop) show a  $k^{-5/3}$  spectrum for concentration fluctuations. Hence the dissipation of concentration fluctuations should be similar to the behaviour of a passive tracer in high Reynolds number homogeneous turbulence:

$$\frac{d}{dt}(\sigma^2) = -\text{constant} \times \sigma^2 \times \frac{k^{1/2}}{\ell_t} \quad (1)$$

where  $\sigma$  is the s.d. of concentration fluctuations,  $k$  is the turbulence kinetic energy, and  $\ell_t$  is the turbulence length scale.

## 2 The Mass Exchange Term

The aim is to incorporate Equation (1) into the two-fluid turbulence model of [1, 3]. This is achieved by adding terms for mass exchange between the fluids. Such terms have previously been used in two-phase flow models for liquid/vapor mixtures. It is supposed that there are two phases with volume fractions  $f_1$  and  $f_2$  and densities  $\rho_1$  and  $\rho_2$ . Initially **phase 1** consists of pure **fluid 1** with density  $\rho_1^0$ , and **phase 2** consists

of pure **fluid 2** with density  $\rho_2^0$ . When mixing occurs there is a mass exchange between the two phases. **Phase 1** is then rich in **fluid 1** and **phase 2** is rich in **fluid 2**. New variables are needed to define the mixture:  $\alpha_{rs}$  is the fraction by volume of **fluid s** in **phase r**. The density of phase  $r$  is then  $\rho_r = \alpha_{r1}\rho_1^0 + \alpha_{r2}\rho_2^0$ , and the mean volume fraction of **fluid r** for the mixture is  $\hat{f} = f_1\alpha_{1r} + f_2\alpha_{2r}$ .

Youngs [3] gives probability density functions for the dense fluid volume fraction at various plane layers, derived from 3D numerical simulations of RT mixing. The results show that:

- (a) There is a high degree of molecular mixing;
- (b) On the heavy fluid side of the mixing zone, there are highly mixed bubbles of light fluid surrounded by pure heavy fluid;
- (c) On the light fluid side of the mixing zone, there are highly mixed spikes of heavy fluid surrounded by pure light fluid;
- (d) In the middle of the mixing zone, there is little pure light fluid or pure heavy fluid;

The results suggest the following entrainment model. The entrainment rate per unit volume is  $\dot{V} = c_3 f_1 f_2 k^{1/2} / \ell_t$ , where  $c_3$  is a model coefficient. In time  $\Delta t$ , for unit volume,  $\dot{V}\Delta t$  of phase 1 mixes uniformly with  $\dot{V}\Delta t$  of phase 2. A proportion  $p_1$  of the mixture is re-assigned to phase 1, and a proportion  $p_2$  is re-assigned to phase 2. Then, if the advection and diffusion terms are omitted:

$$\begin{aligned} \frac{\partial f_1}{\partial t} &= (p_1 - p_2)\dot{V} \\ \frac{\partial}{\partial t}(f_1\alpha_{11}) &= (p_1\alpha_{21} - p_2\alpha_{11})\dot{V}, \quad \text{etc.} \end{aligned}$$

The choice used here for  $p_1$  and  $p_2$  is  $p_1 = f_2$  and  $p_2 = f_1$ . On the heavy fluid side the bubbles entrain heavy fluid. On the light fluid side spikes entrain light fluid. Then, in accordance with Equation (1), the rate of change of the concentration fluctuation,  $\sigma$ , is given by

$$\frac{d}{dt}\sigma^2 = \frac{d}{dt}f_1f_2(\alpha_{11} - \alpha_{21})^2 = -(\alpha_{11} - \alpha_{21})^2\dot{V} = -c_3\sigma^2\frac{k^{1/2}}{\ell_t}$$

### 3 Modifications to the Two-Phase Flow Equations

A number of additions are required to the two-phase flow model with turbulent diffusions added, as described in [1, 3]. The main changes are summarized below.

Transport equations are needed for the new variables  $\alpha_{rs}$ . These need to include terms for advection, diffusion and mass exchange. The equation for  $\alpha_{11}$  is

$$\frac{\partial}{\partial t}(f_1\alpha_{11}) + \frac{\partial}{\partial x}\{f_1\alpha_{11}(u_1 - w_1)\} = \frac{\partial}{\partial x}\left\{D\frac{\partial}{\partial x}(f_1\alpha_{11})\right\} + (p_1\alpha_{21} - p_2\alpha_{11})\dot{V}$$

$u_r$  is the mass weighted mean velocity of phase  $r$  and  $w_r = -\frac{D}{\rho_r f_r}\frac{\partial}{\partial x}(\rho_r f_r)$  is the value of  $u_r - \bar{u}$  for purely diffusive mixing.

The rates of transfer of mass, per unit volume, from phase 1 to phase 2 and from phase 2 to phase 1 are  $\Delta M_{12} = \rho_1 p_2 \dot{V}$  and  $\Delta M_{21} = \rho_2 p_1 \dot{V}$ , respectively. Extra terms are required in the momentum equation for each phase. The net transfer of momentum from phase 1 to phase 2, in the absence of turbulent diffusion terms, is given by

$$\begin{aligned}\Delta U_{12} &= u_1 \Delta M_{12} - u_2 \Delta M_{21} \\ &= \Delta M(u_1 - u_2) + (m_1 u_2 + m_2 u_1)(\Delta M_{12} - \Delta M_{21})\end{aligned}$$

where  $\Delta M = m_1 \Delta M_{12} + m_2 \Delta M_{21}$  and  $m_r$  is the mass fraction of phase  $r$ .

When turbulent diffusion terms are present, the term involving  $\Delta M$  is replaced by  $\Delta M(u_1 - u_2 - w_1 + w_2)$ . This ensures that high mass exchange  $\Delta M \rightarrow \infty$  gives the required diffusive limit  $u_1 - u_2 = w_1 - w_2$ .

The source term in the length scale equation used in [1, 3] was proportional to the velocity difference  $u_1 - u_2$ . This gave, length scale  $L \sim$  mixing zone width. When the mass exchange terms are included, mixing is partly due to turbulent diffusion within each phase and the velocity difference,  $u_1 - u_2$ , does not fully characterize the mixing rate. Instead it has proved necessary to use the **fluid** velocity difference  $\hat{u}_1 - \hat{u}_2$  in the length scale source term. The fluid velocity,  $\hat{u}_s$ , is defined by

$$\frac{\partial}{\partial t}\hat{f}_s + \frac{\partial}{\partial x}(\hat{f}_s \hat{u}_s) = 0,$$

and is calculated from

$$\hat{f}_s \hat{u}_s = f_1 \alpha_{1s}(u_1 - w_1) + f_2 \alpha_{2s}(u_2 - w_2) - D \frac{\partial \hat{f}_s}{\partial x}.$$

#### 4 Application to RT Mixing at a Range of Density Ratios

The model with mass exchange terms included has been applied to RT mixing of incompressible fluids at a plane boundary with constant gravity  $g$ . The initial density is  $\rho = \rho_1^0$  for  $x < 0$ ,  $\rho = \rho_2^0$  for  $x > 0$ . Two density ratios  $\rho_1^0/\rho_2^0 = 1.01$  and 20 are considered. Model coefficients are chosen to give (a) growth rate  $h_1^{0.95} = 0.05 A g t^2$  where  $A$  is the Atwood number, (b) molecular mixing fraction  $\Theta \sim 0.84$ , and (c) turbulence

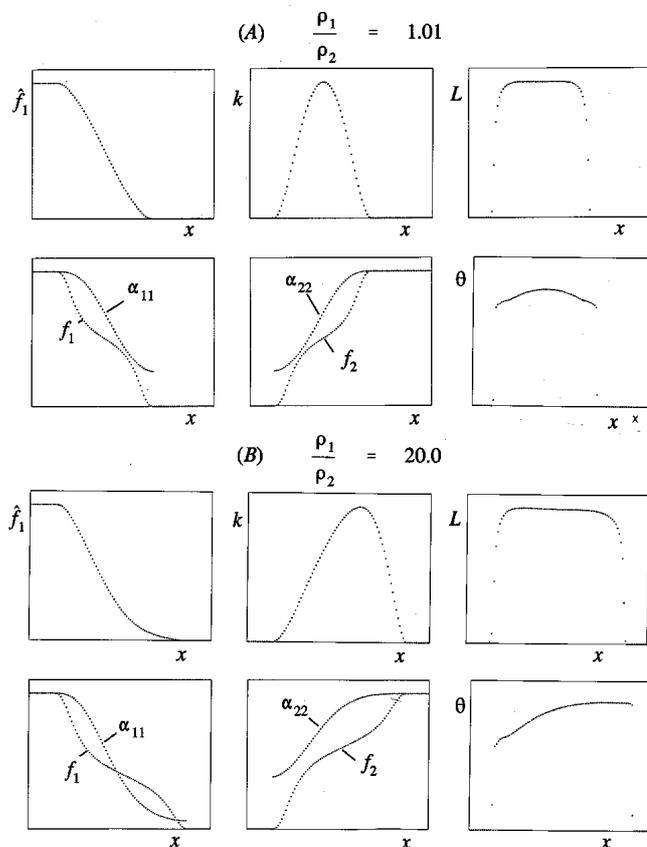


Figure 1: Application to Rayleigh-Taylor mixing.

K.E. dissipation/loss of potential energy  $\sim 0.55$ . The molecular mixing fraction for the mixing zone as a whole is defined by

$$\Theta = \int (f_1 \alpha_{11} \alpha_{12} + f_2 \alpha_{21} \alpha_{22}) dx / \int \hat{f}_1 \hat{f}_2 dx.$$

The values used for  $\Theta$  and for turbulence dissipation are those indicated by direct 3D numerical simulation [2, 3]. The bubble penetration,  $h_1^{0.95}$ , is measured to the point where  $\hat{f}_1 = 0.95$ . The growth rate used here corresponds to the lower limit of the observed values. Figures 1(a), (b) show plots of  $\hat{f}_1$ ,  $k$ ,  $L$ ,  $f_1$ ,  $\alpha_{11}$ ,  $f_2$ ,  $\alpha_{22}$  and the molecular mixing fraction  $\Theta = (f_1 \alpha_{11} \alpha_{12} + f_2 \alpha_{21} \alpha_{22}) / (\hat{f}_1 \hat{f}_2)$  at the end of each calculation. The profile of  $\Theta$  is symmetrical at  $\rho_1^0 / \rho_2^0 = 1.01$ , but at  $\rho_1^0 / \rho_2^0 = 20$ ,  $\Theta$  is significantly higher on the spike side than on the bubble side. This is in accordance

with results of the 3D simulations [2]. The plots of  $\alpha_{11}$  versus  $x$  show that the spikes of dense fluid become more and more mixed as they penetrate the light fluid. This represents, in an approximate manner, the behaviour seen in the 3D simulations.

## 5 Application to the Overturning of Two Layers of Fluid

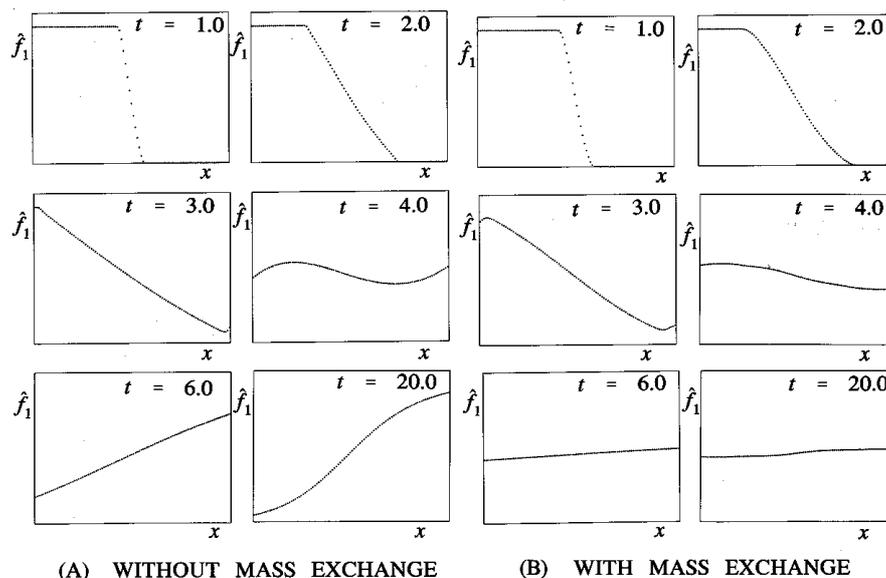


Figure 2: The overturning of two layers of fluid.

This is similar to the previous application. The calculations are continued to a later stage beyond the time when the mixing zone fills the computational region. The initial density is given by  $\rho = \rho_1^0$  for  $-1/2H < x < 0$  and  $\rho = \rho_2^0$  for  $0 < x < 1/2H$ . Rigid walls are present at  $x = \pm 1/2H$ , and gravity is chosen to give  $Ag/H = 1$ . The density ratio is  $\rho_1^0/\rho_2^0 = 1.01$ . The calculations correspond approximately to the experiments of Linden, et al, (these proceedings) - which use brine and water. Two calculations have been performed, with and without mass exchange. In both cases model coefficients were adjusted to give the same growth rate,  $h_1 = 0.05Ag t^2$ . Figures 2(a) and (b) show plots of  $\hat{f}_1$  versus  $x$  at various times. For  $t < 3$ , before the mixing zone fills the computational domain, the calculations with and without mass exchange give similar results. However, at late times,  $t \sim 20$ , there is a marked difference. Without mass exchange there is a high degree of de-mixing. This is not observed in the experiments where de-mixing is inhibited by a high degree of mixing at a molecular level. When

the mass exchange terms are included there is little de-mixing, and this is closer to the experimental behaviour.

### **References**

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- [3] D. L. Youngs, *Laser and Particle Beams*, Vol. 12, p. 725 (1994).