Theoretical Methods for the Determination of Mix

Baolian Cheng, James Glimm and David Sharp

Los Alamos National Laboratory
Los Alamos, NM
Department of Applied Mathematics & Statistics
State University of New York
Stony Brook, NY 11794-3600
Center for Data Intensive Computing
Brookhaven National Laboratory
Upton, NY 11973-5000

- in collaboration with -

Hyeonseong Jin
Main Results

1. Buoyancy drag mixing edge motion equations —
   Agree with bubble merger model, experiments, FT simulation and $A = 1$ theory
   Spike -- bubble coupling (Center of Mass)
   All drag coefficients determined
   Lower than leading order asymptotics

2. Improved two phase mix model equations --
   mathematically stable and thermodynamically determinate
   Closure specified from asymptotic analysis

3. Turbulent diffusivity derived from mix model
Comparison of Bubble Merger Model with Experiments, Simulation

\[ Z_b(t) = \text{penetration distance of light fluid into heavy} \]

\[ = \alpha_b Agt^2 \]

\[ \alpha_b = 0.05 - 0.06 \quad \text{(Theory)} \]

\[ 0.05 - 0.077 \quad \text{(Experiment)} \]

\[ 0.07 \quad \text{(Simulation - tracked)} \]

Bubble height / bubble width = 3.3 (experiment)

\[ = 2.3 \quad \text{(theory)} \]
A Bubble Merger Model

Statistical Models of Interacting Bubbles

Bubble Merger Models

Bubble velocity = single mode velocity + envelope velocity
Bubble Merger Criterion

Envelope velocity > 0  advanced bubble

Envelope velocity < 0  retarded bubble

Remove bubble from ensemble where velocity = 0:

\[ \text{single mode velocity} = \left| \text{envelope velocity} \right| \]

\[ \alpha_b \approx 0.5 - 0.6 \]
Scaled Variables

\[ r = \text{mean bubble radius} \]

\[ t_m = \text{time to bubble merger} \]

\[ t'_m = \text{scaled time to merger} \]

\[ dt' = \left( \frac{Ag}{r} \right)^{1/2} dt \]

\[ \langle \rangle^* = \text{fixed point expectation} \]
Renormalization group (RNG) fixed point equation for bubble radius

\[
\frac{dr}{dt} = \Delta r \times \text{merger rate} = kr \times \text{merger rate}
\]

\[
= kr \left\langle \frac{1}{t_m} \right\rangle = k \sqrt{Ag} \left\langle \frac{1}{t_m'} \right\rangle r^{1/2}
\]

\(k\) = fractional increase in radius due to one merger event; \(t_m\) = time to merger

\[
r = \frac{k^2}{4} \left\langle \frac{1}{t_m'} \right\rangle Ag t^2 ; \quad \alpha_r = \frac{k^2}{4} \left\langle \frac{1}{t_m'} \right\rangle *
\]
Derive rate equation for $h$ in RNG scaling
RNG Bubble Height Equation

\[ \alpha_b = \frac{1}{2} C_b \alpha_r^{1/2} + \left[ \frac{1}{2k} + \frac{1}{2} \right] \alpha_{hm} \]

\( C_b \) = terminal velocity coefficient for single (periodic) bubble

Average of three Smeeton and Youngs experiments:

LHS = 0.067; RHS = 0.0695;
Fixed Point Calculation = 0.056
Center of Mass (COM) Hypothesis

\[ Z_{\text{COM}} = \alpha_{\text{COM}} Ag t^2 \]

\[ \alpha_{\text{COM}} = \frac{7}{60} \alpha_s A^\gamma; \quad \gamma = 3 - 17 \]

\[ \approx 0 \text{ unless } A \approx 1 \]

fits data and theory \((A = 1)\). \(\alpha_s / \alpha_b = \text{solution of quadratic equation} \)

\[ \alpha_s = \alpha_s (\alpha_b) \]
Free Fall

- LEM Data (Dimonte & Schneider[8])
- $\gamma = 3$
- $\gamma = 10$
- $\gamma = 17$

$\alpha_s/\alpha_b$

$A$

Brookhaven Science Associates
U.S. Department of Energy
Mixing Zone Edge Models

\[ Z_{b,s}(t) = h_{b,s} = a_{bs} \ A g t^2 \text{ in RT case} \]

Buoyancy Drag equation for \( Z_{b,s}(t) \):

\[
\left( \rho_{b,s} + k \rho_{s,b} \right) \ddot{Z}_{b,s}(t) = \left( \rho_b - \rho_s \right) g - \rho_{s,b} C_{b,s} \dot{Z}_{b,s}^2 / Z_{b,s}
\]

Determine \( C_{b,s} \) from RT edge motion theory.
ODE valid for arbitrary acceleration

\( k = 1 \) from standard fluid dynamics and from bubble geometry
The graph shows two curves labeled $C_\alpha$ and $C_b$. The curve $C_\alpha$ starts at a lower value and increases rapidly as $A$ increases, approaching infinity as $A$ approaches 1. The curve $C_b$ starts higher and decreases gradually as $A$ increases.
Non-leading Order Terms in RT Asymptotics

\[ Z(t) = \alpha \ Agt^2 + \beta t + \gamma \]
\[ \beta, \gamma \] depend on initial data:
\[ t_0, Z_0, V_0 \]
\[ \alpha \] does not depend on initial data
Data of Exp.101 (Smeeton & Youngs)
Data of Exp.103 (Smeeton & Youngs)

Exact solutions for $A=0.938$

$\alpha_b A g t^2$, $\alpha_b=0.059$

$z_{b0} = 0.1 = v_{b0}$

$t_0=0$  $t_0=1.46$  $t_0=2.1$  $t_0=2.92$
Data of Exp.101 (Smeeton & Youngs)
Data of Exp.103 (Smeeton & Youngs)
Exact solutions for $A=0.829$

$\alpha_b \, Agt^2$, $\alpha_b = 0.063$

$Z_b$

$Z_{b0}=1.5$
$Z_{b0}=1.0$
$Z_{b0}=0.5$
$Z_{b0}=0.1$

$v_{b0}=0.01$, $t_0=0$
Chunk Mix Model

- Complete fluid variables for each fluid
  - Mathematically stable equations

- Improved physics model for mix
  - Pressure difference forces ~ drag

- Thermodynamics is process independent

- New closure proposed and tested
  - Zero parameters (incompressible flow)

- Analytic solution for incompressible case
Multiphase Averaged Equations

**Microphysics:** \[ U_t + \nabla F(U) = 0 \]

**Macrophysics:** \[ \bar{U}_t + \nabla \bar{F}(U) = 0 \]

\[ \bar{F}(U) \neq F(\bar{U}) \]

\[ F_{\text{ren}}(\bar{U}) \approx \bar{F}(U) \]

\[ \bar{U}_t + \nabla F_{\text{ren}}(\bar{U}) = 0 \]

**Closure Problem:** Determine \( F_{\text{ren}} \)
Assume two fluids, labeled $k=1$ (light) and $k=2$ (heavy). Define

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

Let $\langle \cdot \rangle$ denote (ensemble) average.

**Microphysics**

$$\frac{\partial X_k}{\partial t} + \nu \cdot \nabla X_k = 0$$

Define $\nu^*$:

$$\langle \nu \cdot \nabla X_k \rangle \equiv \nu^* \nabla \beta_k$$

**Macrophysics**

$$\frac{\partial \beta_k}{\partial t} + \langle \nu \cdot \nabla X_k \rangle = 0$$

Thus

$$\frac{\partial \beta_k}{\partial t} + \nu^* \cdot \nabla \beta_k = 0$$
Closure

Assume: $v^*$ depends on $v_1$ and $v_2$ and spatially dimensionless quantities only.
Assume: regularity of $v^*$.

Theorem: $v^* = \mu_2 v_1 + \mu_1 v_2$

(convex combination) and related expressions for $p^*$ and $(pv)^*$

Assume: all $\mu$'s depend on $\beta_k$ and $t$ only.
Explicit Model: Zero Parameters

Exact calculation: $\mu_k^\nu$ is fractional linear. Assume same for $\mu_k^p$. Assume dependence on $\beta_k$ alone. Then

$$\mu_k^q = \frac{\beta_k}{\beta_k + c_k^q \beta_{k'}}$$

with $k'$ denoting the other fluid index and $c_1^q c_2^q = 1$ \( q = \nu \) or \( q = p \).

With the mixing zone boundaries $Z_k(t)$, and velocities $V_k(t)$,

$$c_k^n = \frac{|V_{k'}|}{|V_k|}, \quad c_k^p = \frac{\rho_{k'}}{\rho_k}$$

for incompressible flow. Boundary accelerations $\ddot{Z}_k(t)$ must be supplied externally to this model.

$$\ddot{Z}_k(t) = \text{Drag + buoyancy}$$
Analytic Solution: Incompressible Case

\[ \nu_k (\beta_k, t) = V_k \mu_k \nu \]

\[ \nu * (\beta_k, t) = \frac{V_k V_k' (V_k \beta_k^2 + V_k \beta_k^2)}{(|V_k \beta_k| + |V_k' \beta_k'|)^2} \]

\[ z (\beta_k, t) = z_0 (\beta_k) + \int_0^t \nu * (\beta_k, s) ds \]

Let

\[ \overline{p} = \beta_1 p_1 + \beta_2 p_2, \quad p_{\text{diff}} = \frac{p_2}{\rho_2} - \frac{p_1}{\rho_1}, \]

\[ \frac{D_k}{D_t} = \frac{\partial}{\partial t} + \nu_k \frac{\partial}{\partial z}. \]

Then

\[ \overline{p} (z, t) = p_2 (Z_1) + \int_{z_1}^z \sum_{k=1}^2 \beta_k \rho_k (g - \frac{D_k \nu_k}{D_t}) dz \]

\[ p_{\text{diff}} = p_{\text{diff}} (Z_1) - \int_{z_1}^z \left( \frac{D_2 \nu_2}{D_t} - \frac{D_1 \nu_1}{D_t} \right) dz \]
Asymptotic Expansion in Powers of \( M = \text{Mach Number} \)

0\(^{\text{th}}\) order \( = \) incompressible \( v, \beta \)

1\(^{\text{st}}\) order \( = \) correction \( v, \beta \)

2\(^{\text{nd}}\) order \( = \) incompressible \( p_1, p_2 \)

\[ + v, \beta \quad \text{correction} \]

2\(^{\text{nd}}\) order \( p_1, p_2 = \) incompressible \( p_1, p_2 \)

\( \Rightarrow \) constraint:

“missing” incompressible pressure equation

Also resolves “missing” compressible closure.
Equilibrated pressures \((p_1 = p_2)\) requires equilibrated velocities for hyperbolic equations.

Equilibrated velocities requires a diffusion term to move phase particles.

Diffusion can be computed within the Chunk Mix model.
RT and RM Diffusion Coefficients

RT diffusion coefficient:

\[ D = 2A^2 g^2 t^3 \left[ \beta_2 \alpha_2^2 \left( \frac{\alpha_1 \beta_1}{\alpha_1 \beta_1 + \alpha_2 \beta_2} \right)^3 + \beta_1 \alpha_1^2 \left( \frac{\alpha_2 \beta_2}{\alpha_1 \beta_1 + \alpha_2 \beta_2} \right)^3 \right] \]

RM diffusion coefficient (s = entrainment time, obtained from solution of ODE):

\[ D = \frac{\alpha_2^2 \theta_2 \beta_2 s_1^{\theta_2}}{1 + \tau} t^{\theta_2 - 1} + \frac{\alpha_1^2 \theta_1 \beta_1 \tau s_2^{\theta_1}}{1 + \tau} t^{\theta_1 - 1} \]

\[ \tau = \frac{\alpha_2 \beta_2 \theta_2}{\alpha_1 \beta_1 \theta_1} t^{\theta_2 - \theta_1} \]
\( A = 0.5, \alpha_2 = 0.07185 \)
\( \theta_1 = 0.25, \theta_2 = 0.315 \)
Summary: A Predictive Science for Mix

Consistent theory, simulation and experiment for 3D Rayleigh-Taylor fluid mixing

Determine the mixing zone edge motions for general accelerations in agreement with experiment and $A = 1$ theory

Lower than leading order asymptotics with explicit dependence on initial conditions

Improved mix model equations: Stable mathematically and thermodynamically determinate

Asymptotics defined; closure improved