Recent Developments in the Theory and Simulation of Turbulent Mixing

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Outline

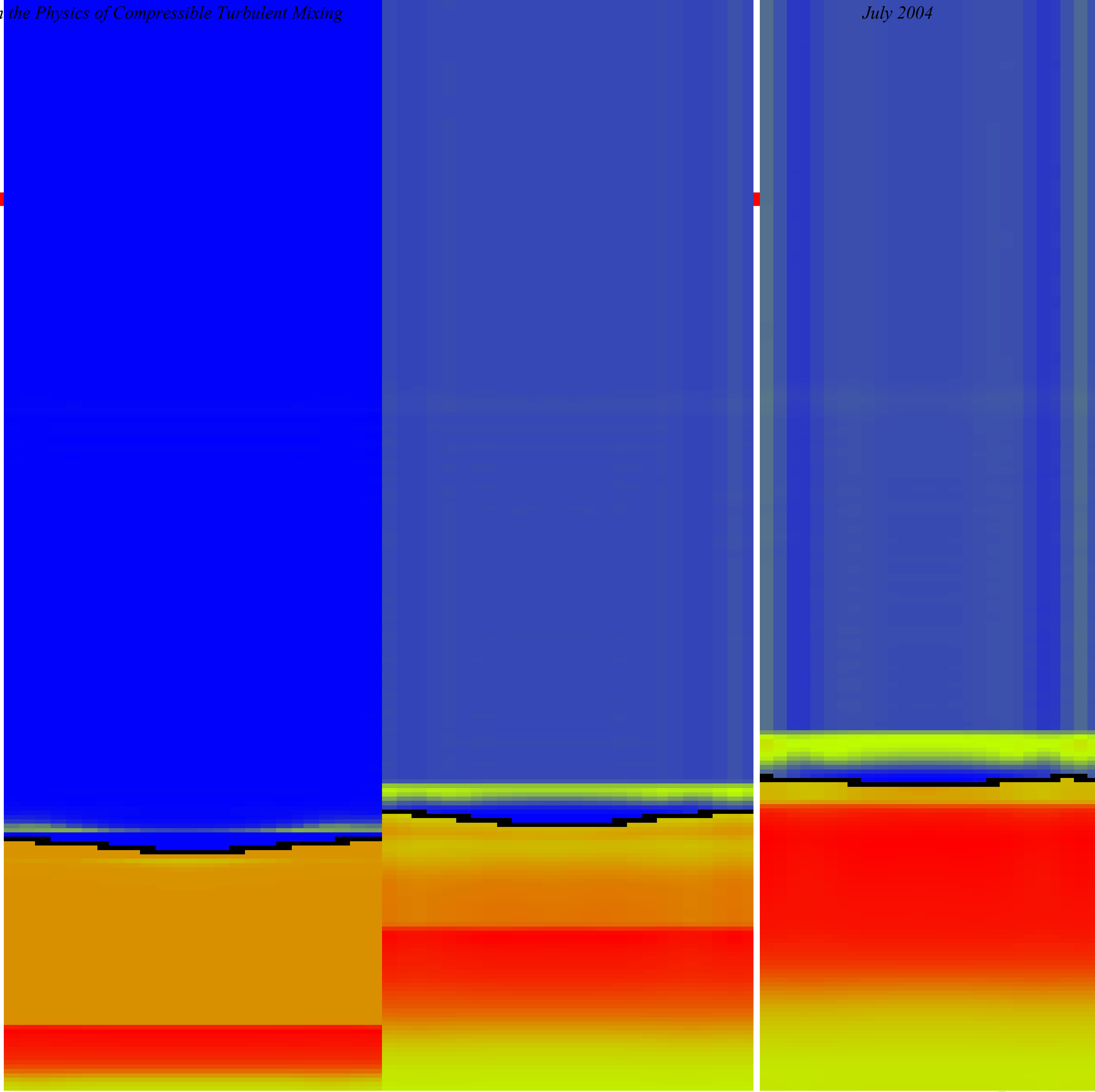
- Turbulent Mixing
  - Comparison to Laser Experiments
  - Numerical Mass Diffusion
  - Compressible Effects
  - Averaged Equations
    - An entropy inequality
    - N > 2 fluids
- Front Tracking
  - Locally Grid Based
  - Conservative

Validation from OMEGA, NIF mix experiments

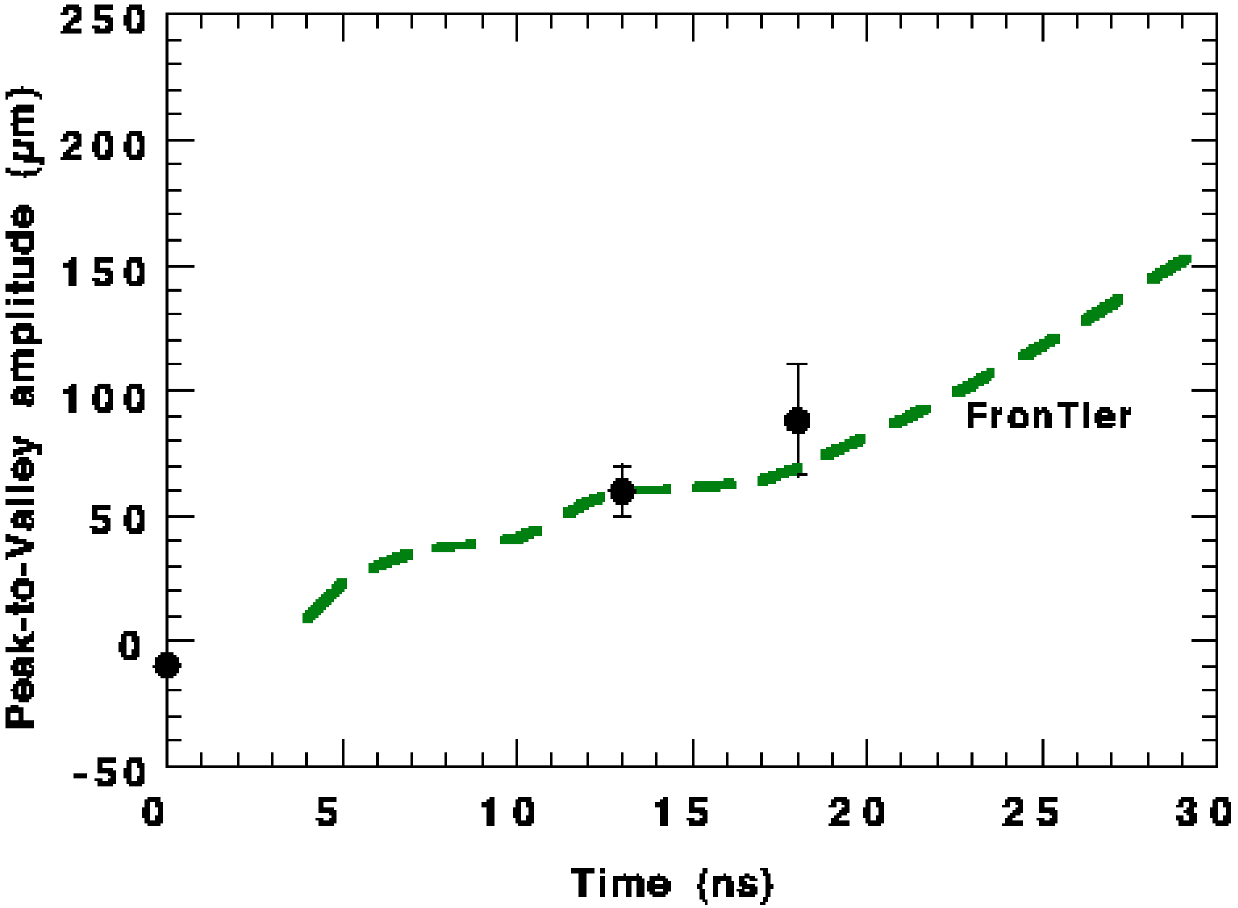
- Experiments by P. Drake (U. MIch.), B. Remington (LLNL) to test single mode Rayleigh-Taylor mixing and transition to mode breakup, chaos, and turbulent mixing
  - Radiation preheat modifies initial data
  - 1D Rad hydro data from HYADES code
- Preshot Frontier predictions
  - Use 1D data in slices to get rad hydro heating
  - Use FronTier to get accurate interface motion
  - Predict pre-hydro initial conditions due to preheat and influence on hydro instabilities
- Post shot comparison to experimental data: excellent

Preshot:

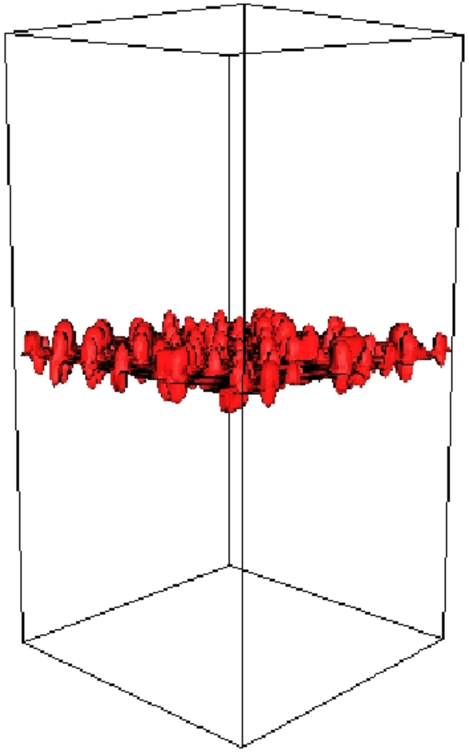
- Data after preheat motion (far right). Perturbation is compressed 2X, compared to the as machined sine wave (left). Shape change modifies hydro instability development.



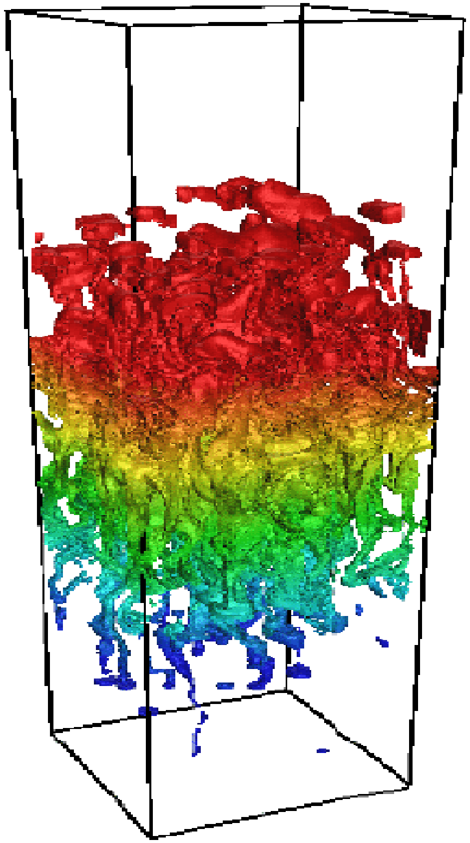
Postshot Comparison of *FronTier* Simulations with Remington et al Experiment



The FronTier Fluid Mixing Simulation



Early time FronTier simulation of 3D RT mixing layer.



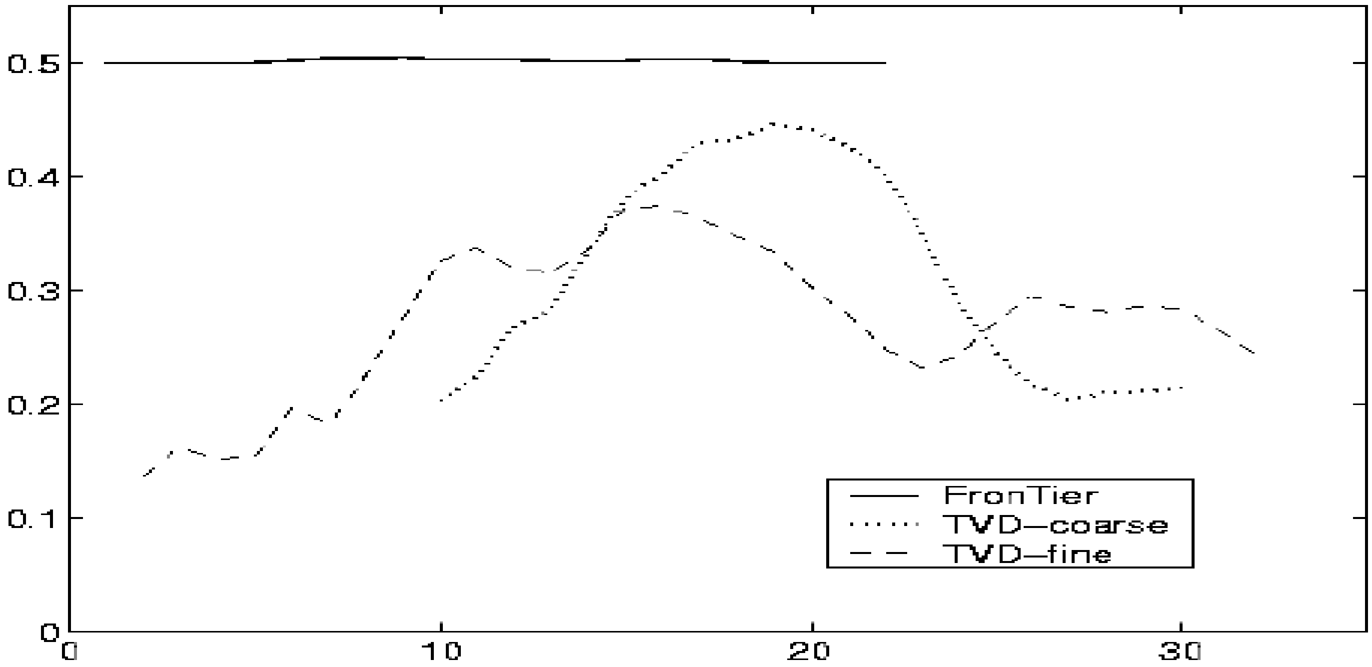
Late time FronTier simulation of a 3D RT mixing layer.

Time Dependent Atwood Number

- For each z
  - Compute the maximum and minimum density
  - Form a space and time dependent A(z,t) from min/max
- Average A(z,t) over bubble region to get A(t)
- Untracked A(t) is about ½ nominal value due to mass diffusion; tracked A(t) is virtually constant
- If A(t) is used in definition of alpha, all simulations agree (with each other, with experiment, with theory)

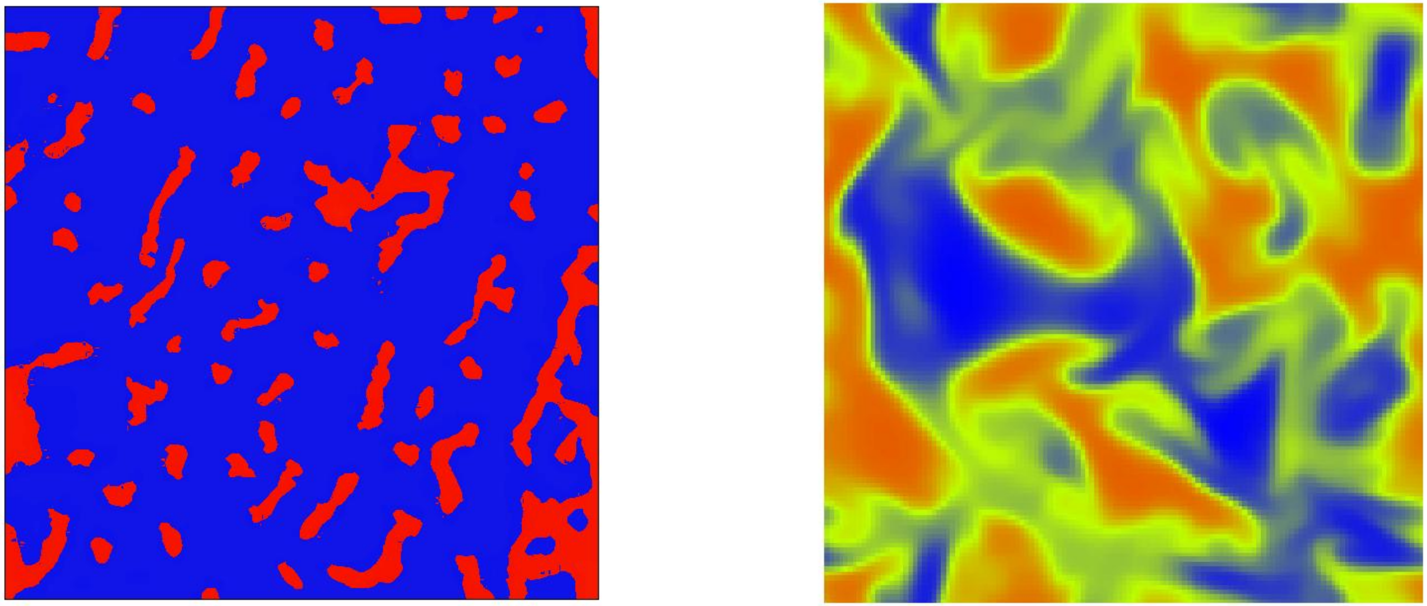
Time Dependent Atwood Numbers
Comparison of tracked and untracked simulations

A(t)



Time

Density at Z = const. Cross section. Comparison of FronTier (left) and TVD (right)

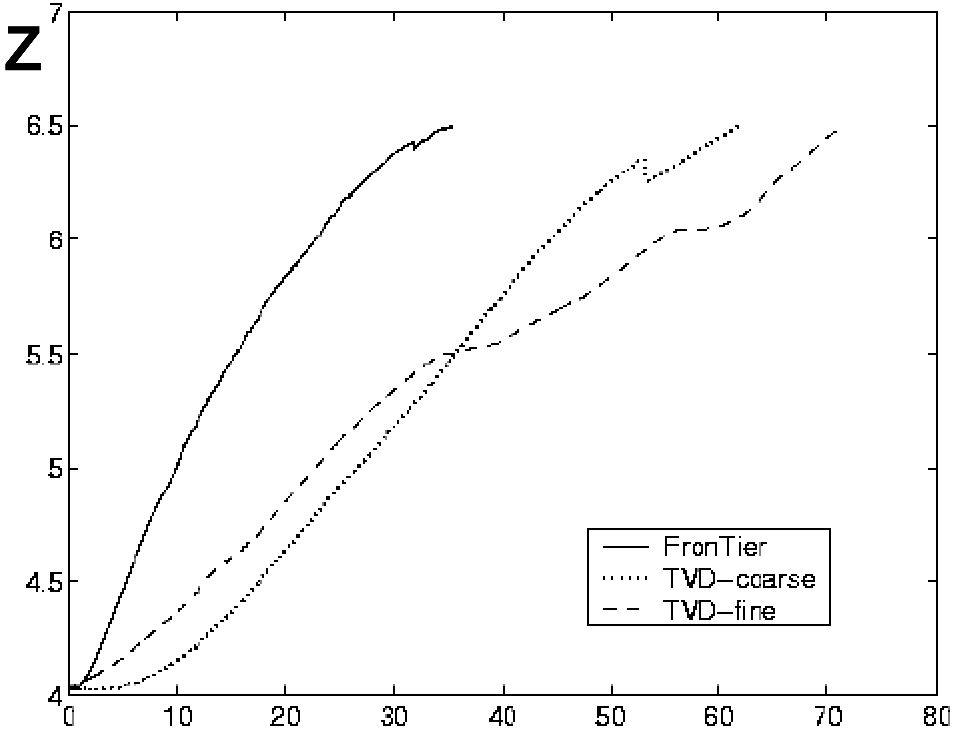


50% reduction of density contrast in untracked simulation

FronTier and TVD Simulations

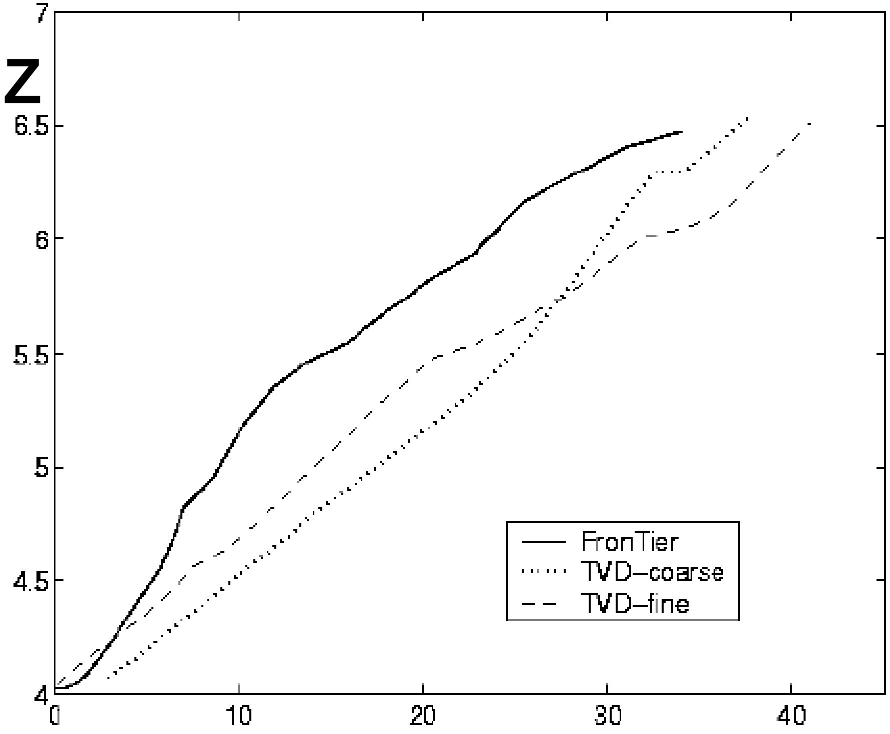
without / with diffusion renormalization of time scales

Alphas from theory, experiment, some simulations agree; most simulations disagree



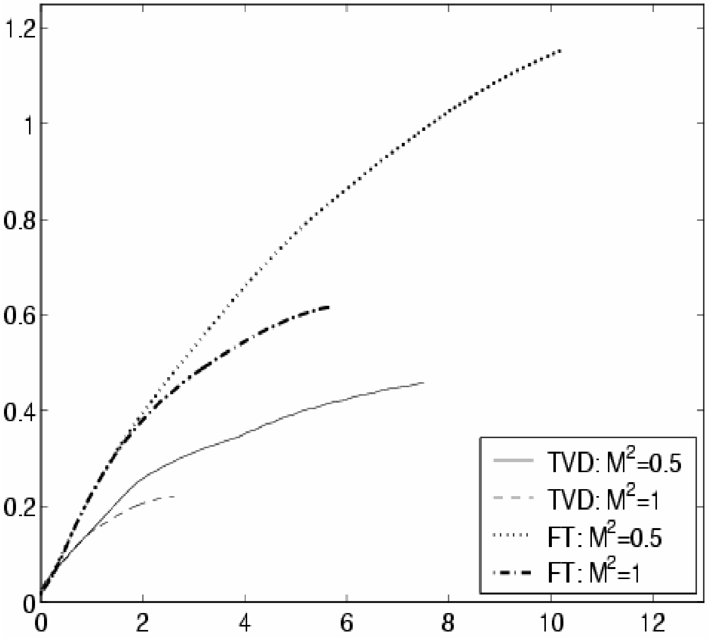
$$Agt^2$$

All alphas agree: theory, experiment, all simulations

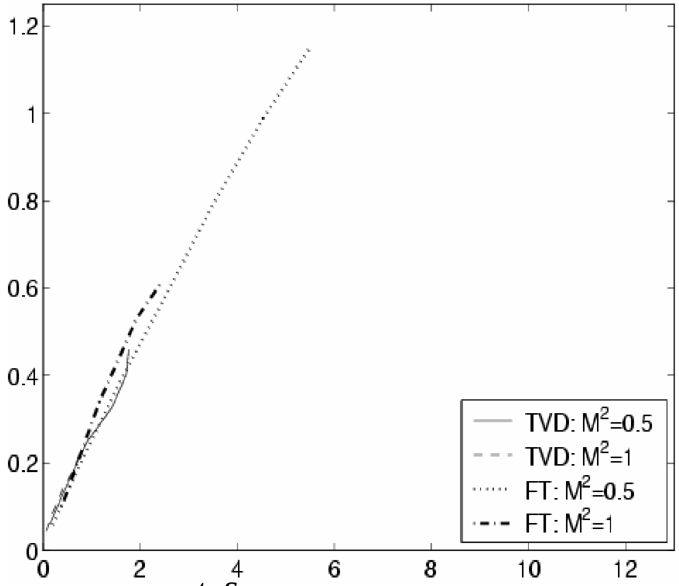


$$2\iint gA(s)dsdt$$

Self Similar Highly Compressible Mixing



$$Agt^2$$



$$2\int_0^t\int_0^{s_1} A(s)\,g\,ds\,ds_1$$

Systematic theoretical and simulation of effects of compressibility on mixing rates: A well defined mixing rate alpha (right frame) is 2X larger than the incompressible value.

Theoretical Model for Compressible Mixing

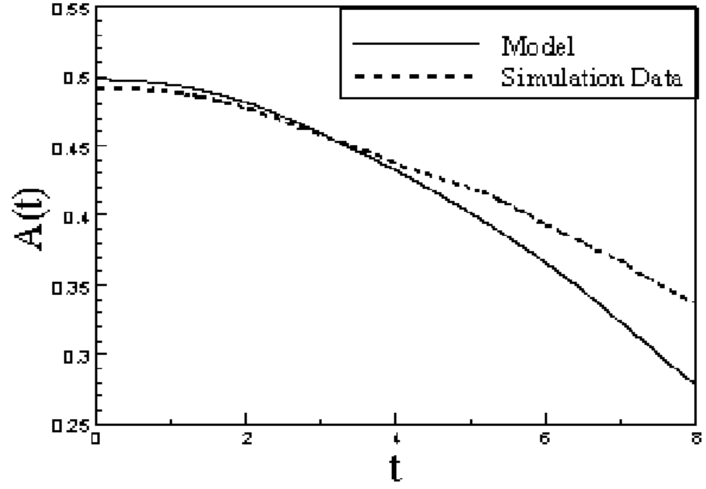
$$(-1)^i Z_i'' = Ag - (-1)^i \frac{\rho_{i'}}{\rho_1 + \rho_2} \frac{CV_i^2}{Z_i}$$

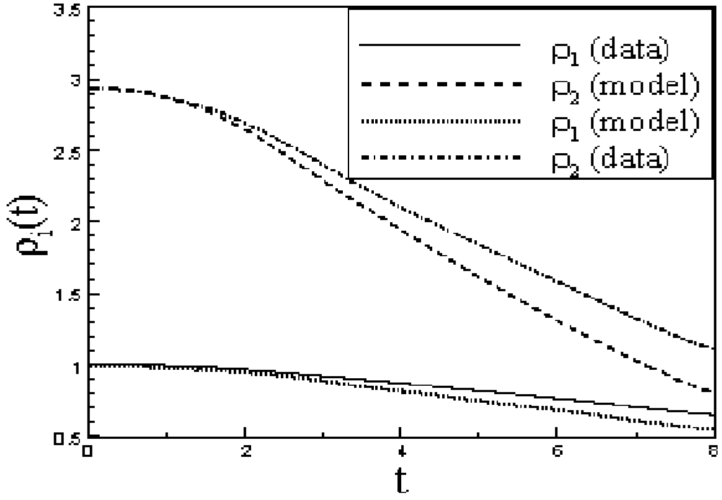
Buoyancy Drag Eq.

$$A = A(Z_i(t))$$

Time Dependent Atwood defined at bubble tip

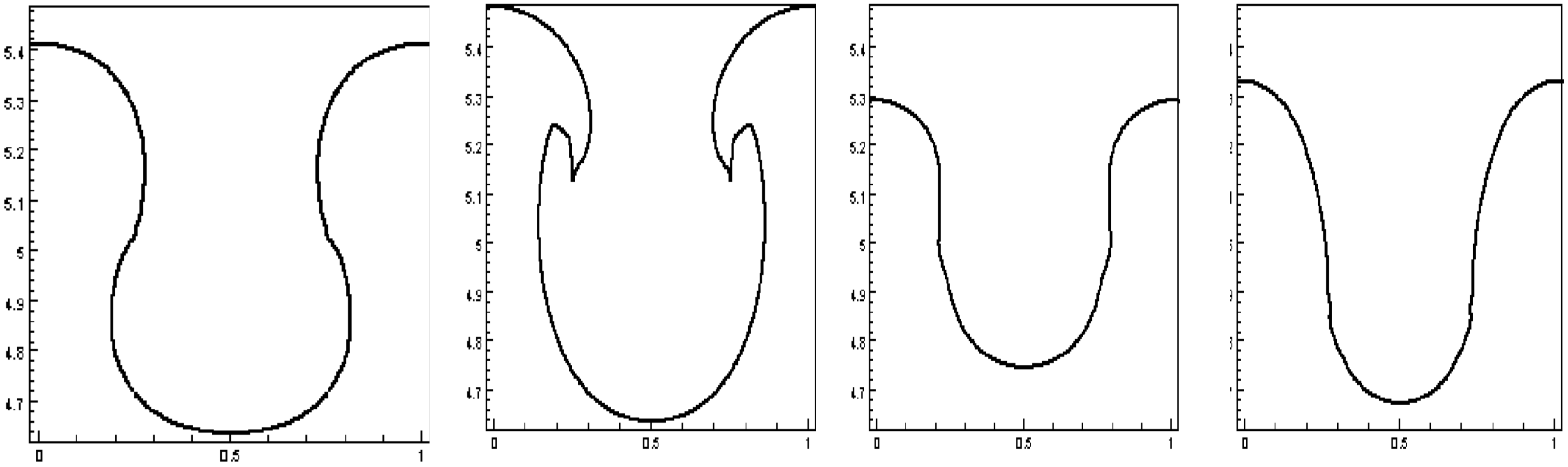
Physics model: Heavy fluid is isothermal at bubble tip from initial conditions; Light fluid is isentropic in its change from original z = 0 value





Compressible EOS Effects on Mix: Single Mode RT in 2D

- Strongly compressible: EOS effects are not important
- Weakly compressible
  - Form drag and terminal velocities: insensitive
  - Pressure drag: highly sensitive
  - Shape highly: sensitive



$$\gamma_1 = 2.0 \quad \gamma_2 = 1.1 \quad P_{1\infty}/P_0 = 0 \quad P_{1\infty}/P_0 = 0$$

$$\gamma_1 = 1.1 \quad \gamma_2 = 2.0 \quad P_{1\infty}/P_0 = 10 \quad P_{1\infty}/P_0 = 10$$

$$\gamma_1 = 4.0 \quad \gamma_2 = 1.1 \quad P_{1\infty}/P_0 = 0 \quad P_{1\infty}/P_0 = 10$$

$$\gamma_1 = 1.1 \quad \gamma_2 = 4.0 \quad P_{1\infty}/P_0 = 10 \quad P_{1\infty}/P_0 = 0$$

Low compressible flow at time of terminal velocity

Mixing Rate Summary
Time Dependent Density Contrast

- All incompressible mixing rates are equal after allowing for effects of numerical mass diffusion
  - Experimental, theoretical, numerical
- Highly compressible mixing is self similar after allowing for effects of stratification
- Mixing rate thus defined has a strong dependence on compressibility
- Weakly compressible
  - Strong EOS effects for some variables, not for others

Theoretical Prediction of Mixing Rate

- Bubble merger (small bubbles removed, large ones grow to fill space)
- Merger leads to fewer but larger bubbles
- Variation in bubble height adds to velocity of bubbles
- New equation derived to relate:
  - Mixing rate
  - Fluctuations in bubble height
  - Mean bubble diameter

Bubble Merger Model

$\alpha_b =$ Growth rate constant for mixing zone

$\alpha_r =$ Growth rate constant for bubble radius

$\alpha_{h'} =$ Growth rate constant for height fluctuations

(*) $\alpha_b = a\alpha_r^{1/2} + b\alpha_{h'}$

$a, b =$ Computable quantities

Eq. (*) validated by direct comparison to experimental data

$\alpha_r, \alpha_{h'}$ determined by renormalization group fixed point analysis

$\alpha_b = 0.06$

Two-Pressure Two-Phase Flow Model

- The averaged equations

$$\frac{\partial \beta_k}{\partial t} + v^* \frac{\partial \beta_k}{\partial z} = 0, \qquad \beta_1 + \beta_2 = 1$$

$$\frac{\partial(\beta_k \rho_k)}{\partial t} + \frac{\partial(\beta_k \rho_k v_k)}{\partial z} = 0$$

$$\frac{\partial(\beta_k \rho_k v_k)}{\partial t} + \frac{\partial(\beta_k \rho_k v_k v_k)}{\partial z} = -\frac{\partial(\beta_k p_k)}{\partial z} + p^* \frac{\partial \beta_k}{\partial z} + \beta_k \rho_k g$$

$$\frac{\partial(\beta_k \rho_k E_k)}{\partial t} + \frac{\partial(\beta_k \rho_k v_k E_k)}{\partial z} = -\frac{\partial(\beta_k p_k v_k)}{\partial z} + (pv)^* \frac{\partial \beta_k}{\partial z} + \beta_k \rho_k v_k g \qquad \text{(Total energy closure)}$$

- $k = 1, 2$: the light and heavy fluid
- $g = g(t) > 0$: acceleration

β_k, v_k , ρ_k , p_k , S_k , e_k , E_k : the volume fraction, velocity, density, pressure, entropy, internal energy and total energy of fluid k

Energy averaged equations

- Entropy is a nonlinear function of other variables (density, internal energy)
- The entropy of the averages (of these other variables) is not equal to the average of the (microphysical) entropy
- Difference, the entropy of averaging, has a definite sign (positive).

New closure for *(pv)**

- Positivity of entropy
  - Assume an entropy of averaging, must be positive
  - New constraint introduces coupling between two edges of mixing zone
  - Analytic basis for previous edge coupling conclusions based on center of mass assumptions
- New closure satisfies all conservation and boundary constraints
- Improved physical and mathematical basis

New N > 2 Materials Closure

$$\frac{\partial \beta_k}{\partial t} + v_k^* \frac{\partial \beta_k}{\partial t} = 0;$$

$$v_k^* = \text{ average intfc velocity}$$

$$v_k^* = \sum \Psi_{jk} v_{kj}$$

$$v_{kj} = \mu_{kj}^v v_k + \mu_{jk}^v v_j$$

$$\mu_{kj}^v = \frac{\beta_j}{\beta_j + \sigma_{kj}^v \beta_k}$$

Front Tracking: Grid free vs. Grid based

- **Grid free**: interface and interior (volume) grid are unrelated
- **Grid based**: the interface is directly tied to the volume grid.
  - The interface is defined by its intersections with the grid cell edges.
  - In the interior of the cell, the interface is reconstructed from its cell edge crossings.

Grid free vs. Grid based

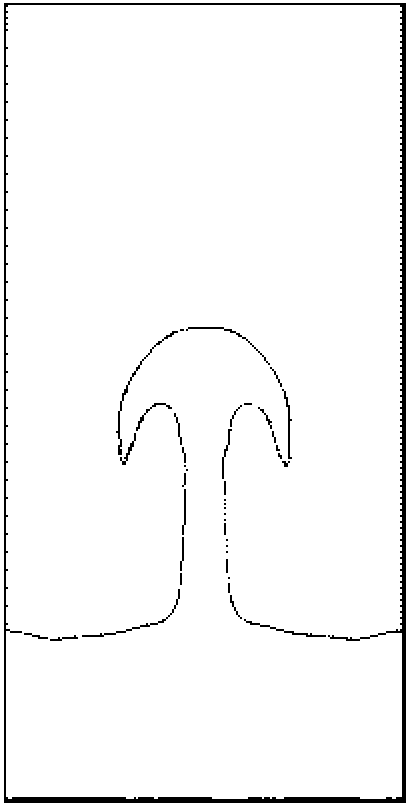
- Grid free
  - more accurate
  - less robust
- Grid based
  - highly robust
  - less accurate
- Locally grid based; Hybrid
  - best of both algorithms

Grid based vs locally grid based

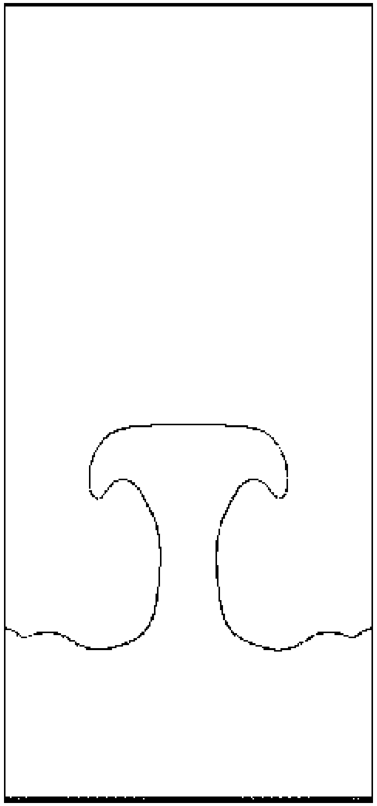
Conservative Tracking

- Track space time interface
- Solution is discontinuous across space time interface but space time flux is continuous
  - This statement is exactly the Rankine-Hugoniot relations for the discontinuity
- Use finite volume differencing in irregular space time volumes
- 1st order accurate at tracked front
- Replaces ghost cell extrapolation
  - Glimm, Marchesin, McBryan, 1980

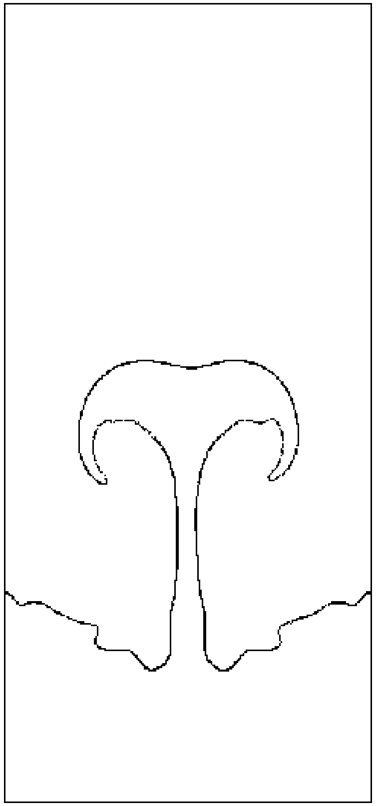
Conservative tracking (40 cells) vs. Nonconservative tracking, 40, 80, 160 cells



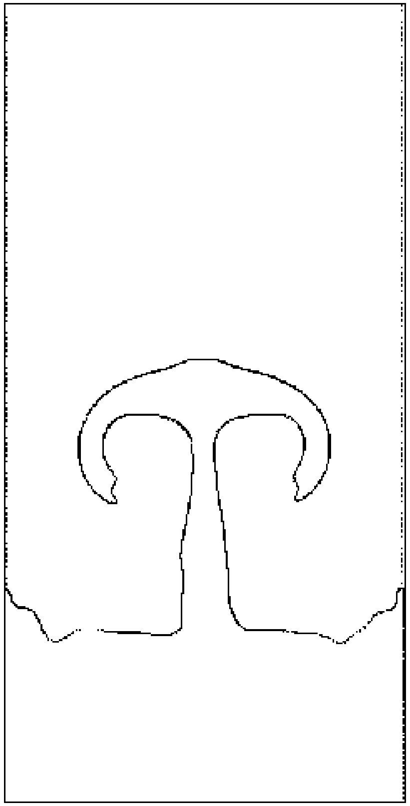
C 40



NC 40



NC 80



NC 160

Comparison of growth rates: 40, 160 cell Cons. Tracked and 160 noncons. Tracked are similar; 40 cell Noncons. Tracked has slower growth