

# **BHR Development: Initial Conditions and Molecular Mix Measurements for Rayleigh-Taylor Turbulence**

**Malcolm J. Andrews<sup>1</sup>, Robert Gore<sup>1</sup>, Bertrand Rollin<sup>1</sup>,  
Yuval Doron<sup>2</sup>, Andrew Duggleby<sup>2</sup>,**

**<sup>1</sup>Los Alamos National Laboratory, NM.**

**<sup>2</sup>Department of Mechanical Engineering, Texas A&M University,  
College Station, TX.**

**LA-UR 09-04608**

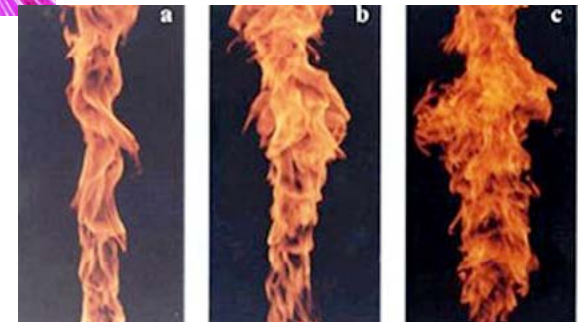
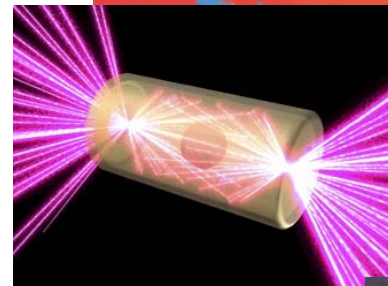
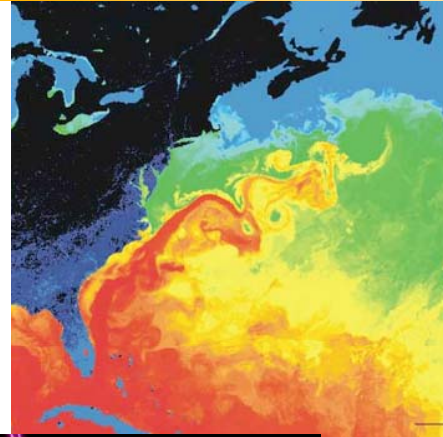
# Outline

---

- Introduction to the BHR turbulence model
- Current research related to BHR
- Molecular mixing measurements at high Schmidt number
- Incorporating Initial Conditions into BHR

# Goal: accurate and cost/time effective calculations of variable density turbulent mixing

- **Broad spectrum of flow conditions**
  - Rayleigh - Taylor
  - Richtmyer - Meshkov
  - Kelvin - Helmholtz with different fluids
- **Broad spectrum of physical regimes**
  - $Sc$  from  $10^{-4}$  to  $10^4$
  - $Re$  to  $10^8$
  - $A$  from  $10^{-4}$  to near 1
  - Large range of space & time scales
- **Questions to be answered**
  - How much mass is mixed
  - How much of that mass is molecularly mixed
  - We look to experiments to define where our models work and where they don't work & why



# Three main avenues of modeling variable density turbulent mixing; all start in the same place

$$\mathbf{F} = m\mathbf{a}$$

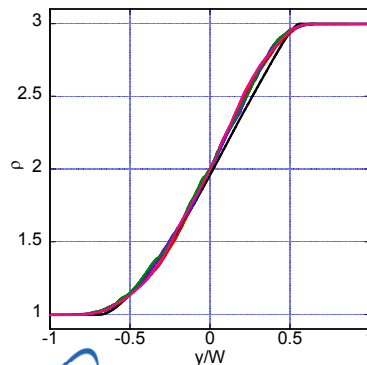
$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i$$

▪ Full averaging

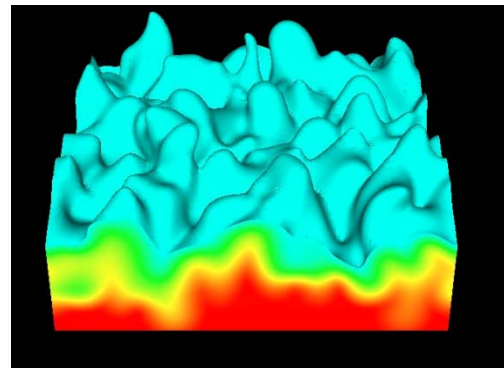
▪ Partial averaging

▪ No averaging

URANS



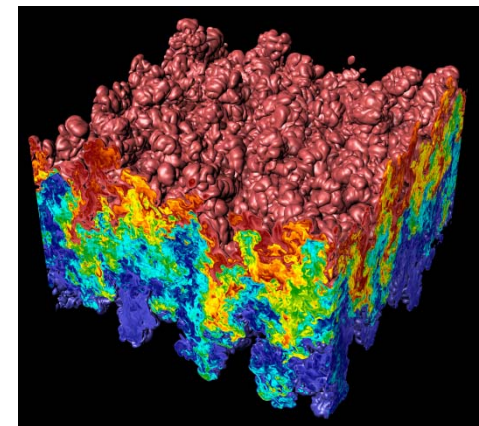
LES



Plus description of small scales

UNCLASSIFIED

DNS



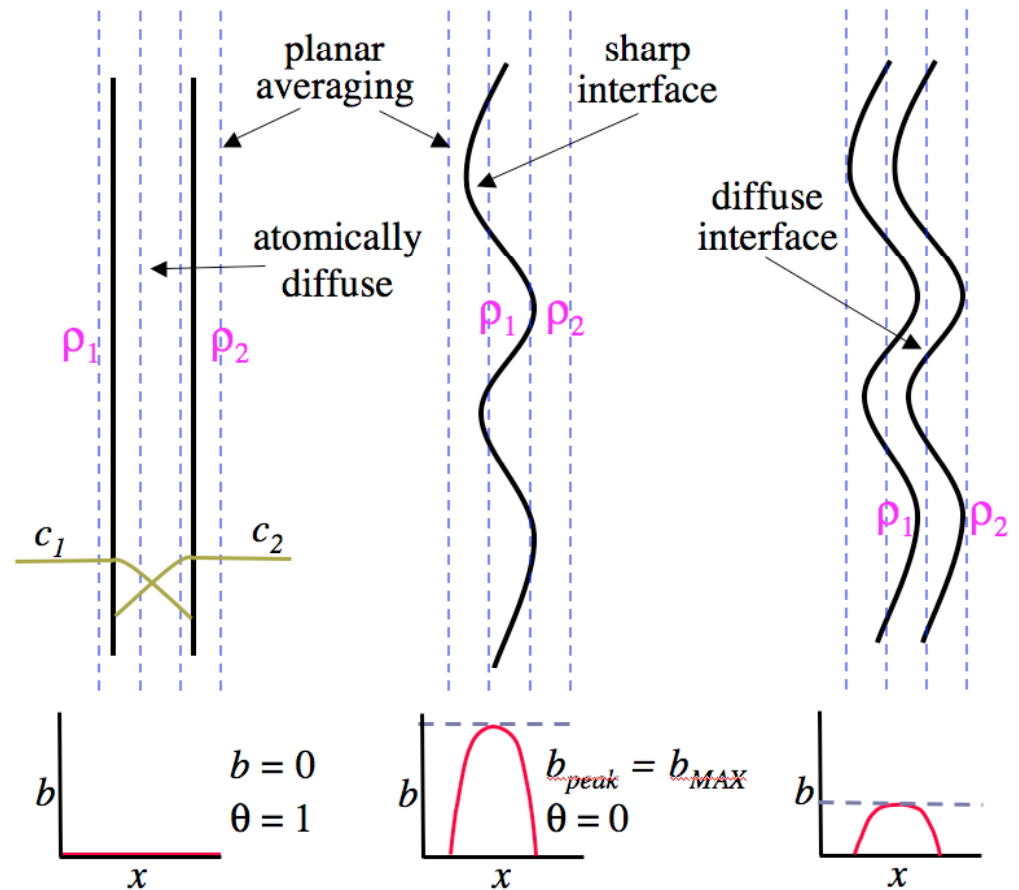
Turbulent Mixing & Beyond, 2009

# Definitions of the important quantities of interest for modeling variable density flows (averages of fluctuating quantities)-BHR

- $R_{ij}$ , Reynolds Stress
- $K$ , Turbulent Kinetic energy
- $a$ , Turbulent mass flux
- $b$ , Density fluctuation

$$R_{ij} = \overline{\rho u_i' u_j'} \quad K = R_{nn} / 2\bar{\rho}$$

$$a_i = \overline{\rho' u_i'} / \bar{\rho} \quad b = -\rho' \left( \frac{1}{\rho} \right)'$$



## From averaging Navier-Stokes we get the fundamental equations for variable density flows

---

$$\frac{D\bar{\rho}K}{Dt} = a_n \frac{\partial \mathcal{P}}{\partial x_n} - R_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} + \text{DIFFUSION} - \text{DISSIPATION}$$

$$\frac{D\bar{\rho}a_i}{Dt} = b \frac{\partial \mathcal{P}}{\partial x_i} - R_{ij} \frac{\partial \rho}{\partial x_j} + \text{DIFFUSION} - \text{DISSIPATION}$$

$$\frac{D\bar{\rho}b}{Dt} = 2\bar{\rho}a_n \frac{\partial b}{\partial x_n} - 2(b+1)a_n \frac{\partial \rho}{\partial x_n} + \text{DIFFUSION} - \text{DISSIPATION}$$

$$\frac{D\bar{\rho}c^k}{Dt} = \frac{\partial}{\partial x_n} \left( \frac{\rho \nu_T}{\sigma_c} \frac{\partial c^k}{\partial x_n} \right)$$

## Diffusion and dissipation are modeled in a simple fashion

---

$$DIFFUSION \Rightarrow \frac{\partial}{\partial x_n} \left( \frac{\bar{\rho} \nu_T}{\sigma_X} \frac{\partial X}{\partial x_n} \right) \quad X \Rightarrow K, a, b, S$$

$$DISSIPATION \Rightarrow \frac{C_X \bar{\rho} X}{S / \sqrt{K}}$$

- For example, the dissipation of turbulent kinetic energy

$$D_K = \mu \overline{\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i}}$$

- For these modeled terms we are always looking for shortcomings of our approach and ways to improve

# Validation and model development requires information from a lot of sources; none are perfect, all are needed

Relevance

- **First and foremost is always the application of interest**
  - No universal turbulence model; most applicable experiment usually most lacking in detailed data for model validation
- **Partially integrated (HEDP e.g., CyIMix, Ignition applications)**
  - Give some detailed information but is complicated by the integration and lack of complete data
    - data - width's but not K; complication could be EoS
- **Small scale experiments**
  - Scaling an issue; data acquisition is easier but still incomplete
    - TAMU & LANL-P23 shock tube we can get K,a,b but not all the individual modeled terms
    - Aren't always universal
- **DNS**
  - Some regimes/IC are easier, others harder
  - "data" is complete
  - "data" isn't data

Information



# We use a large data suite to validate our turbulence models

## ■ DNS

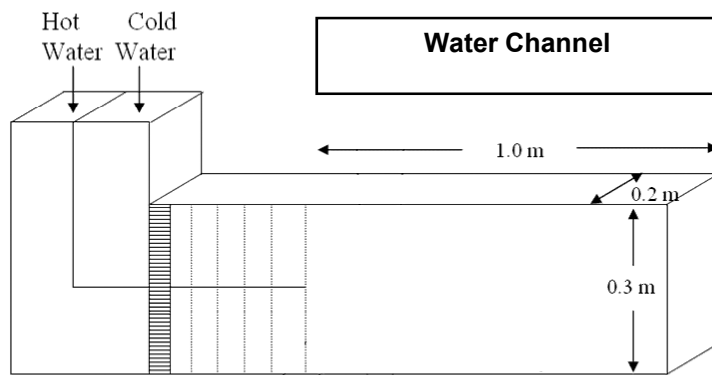
- Cabot & Cook (LLNL)
- Livescu (LANL)
- CalTech LES / D. Pullin

## ■ Small scale

- TAMU gas & water RT channel
- P23 shock tube (LANL)
- PRad (LANL)
- University of Wisconsin/ R.Bonnazza
- Arizona/ J. Jacobs
- Open literature
  - CEA/French
  - VINEEF/Russian
  - AWE/British
  - Others

coefficient	RT-DNS	RT-TAMU	RM-all	origin
C1	1.44	1.44	1.44	Free shear
C2	1.92	1.92	1.92	Iso-decay
C4	1.05	.75	0.75	RT growth
$\sigma_b$	3.0	3.0	3.0	RT/TAMU
$\sigma_c$	0.6	0.6	0.6	global
$\sigma_s$	0.1	0.1	0.1	Top hat
$C_\mu$	0.28	0.28	0.28	RT/TAMU
Cb2	2.5	2.5	0.25	RT/RM
Ca1	6.0	6.0	6.0	RT/TAMU
bij_n	0	0	0	stability

# Large Schmidt Number, Liquid-Phase Molecular Mix Measurements



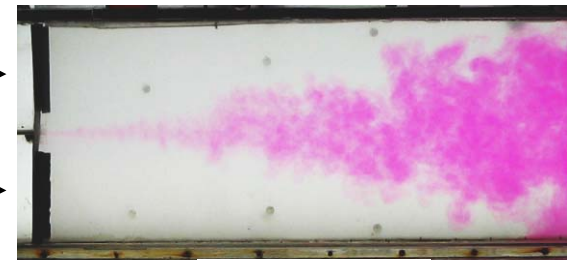
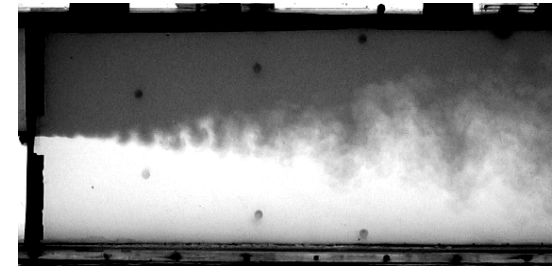
Camera:  
1600H × 1200V  
Pixels  
3 Channel CCD

Salt water (fluid 1) + Nigrosine dye

Fresh water (fluid 2)

Salt water + NaOH;  
 $\text{pH}_1 = 11.5$

Fresh water + HCL;  
 $\text{pH}_2 \leq 7$ ;  
 $[\text{In}]_2 = 6 \times 10^{-6}$

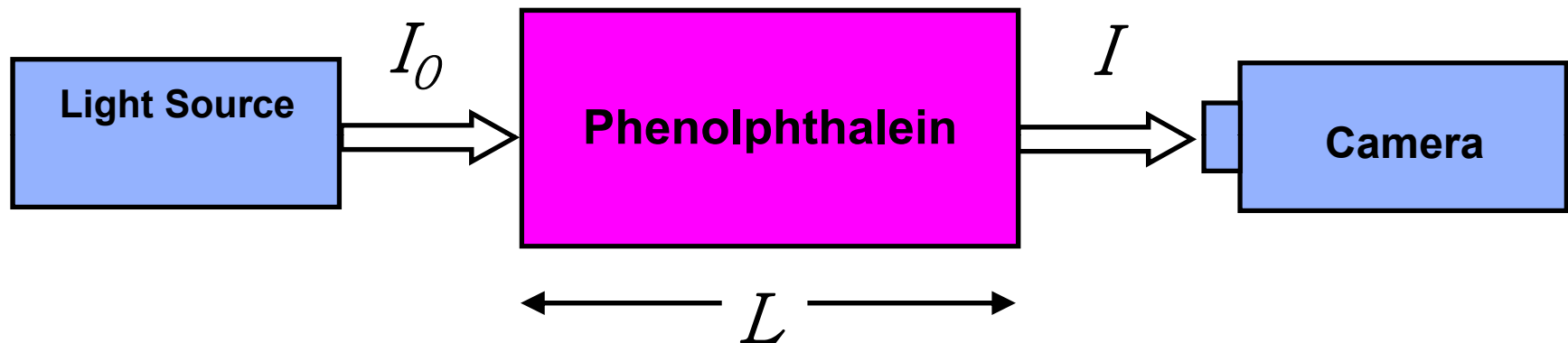


$$\tau = \frac{x}{U_m} \sqrt{\frac{Ag}{H}}$$

- Current research examines the degree of molecular mixing in a high Schmidt number ( $Sc \sim 10^3$ ) Rayleigh–Taylor mixing layer using chemical indicators (color change at  $\text{pH}=9.53$ )
- Light absorption techniques used to measure mean concentration of passive scalar (Nigrosine dye) and reacting scalar (phenolphthalein)
- Measurement techniques free of probe-resolution requirements

## Product Formation Measurements

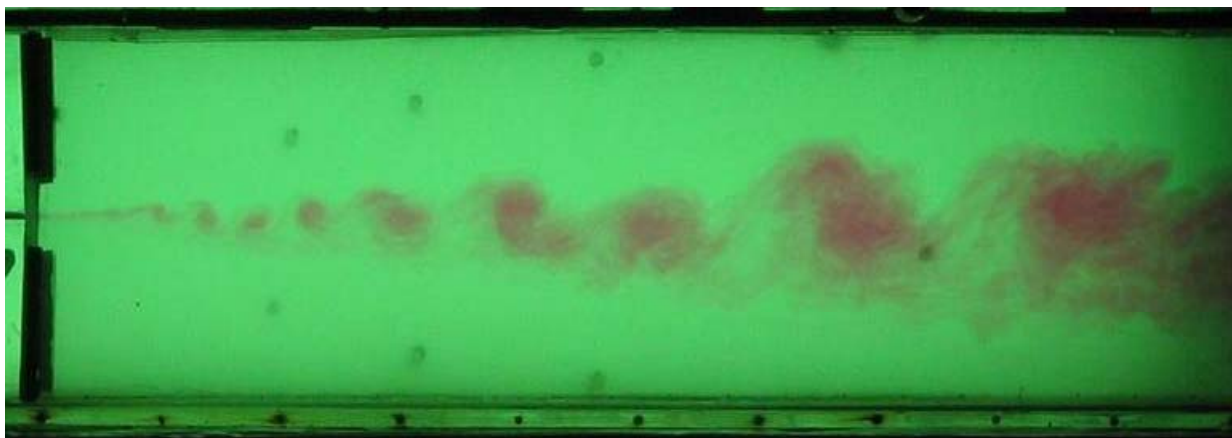
- Measure formation of  $\text{In}_{IV}$  using backlit imaging techniques



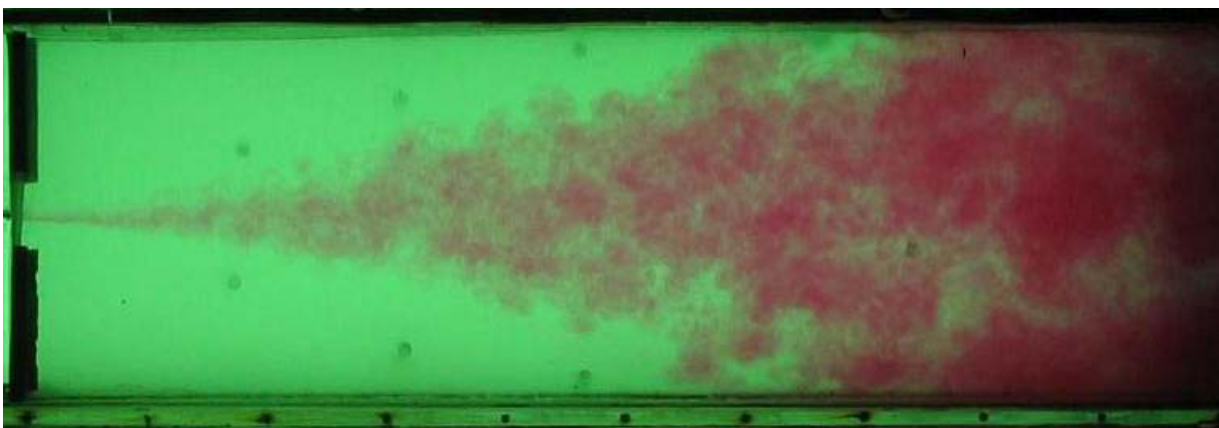
- Light absorption related to average concentration of indicator by Beer's Law

$$\sigma = -\ln \left( \frac{I}{I_0} \right) = \epsilon L \overline{[\text{In}_{IV}]}$$

## Shear and RT



$$r=U_2/U_1=0.606$$



$$A_t=7.5 \times 10^{-4}$$

$$\text{pH}_1=11.52, \text{pH}_2=2.44$$

$$f_2^{50\%}=0.471$$

## Molecular Mixing Parameter

- Examining density fluctuations is one means of quantifying molecular mixing

$$\bar{f}_1 = \frac{\bar{\rho} - \rho_2}{\rho_1 + \rho_2} \quad \bar{f}_1 + \bar{f}_2 = 1 \quad \overline{f_1'^2} = \frac{\overline{\rho'^2}}{(\Delta\rho)^2}$$

- Need measurement for density (volume fraction) fluctuations

$$\theta = 1 - \frac{\overline{f_1'^2}}{\bar{f}_1 \bar{f}_2} \quad \theta = \begin{cases} 1 & \text{Molecularly Mixed} \\ 0 & \text{Segregated} \end{cases}$$

Derivation of relationship between  $\overline{[\ln IV]}$  and  $\theta$  is nontrivial

$\overline{[\ln IV]}$

UNCLASSIFIED

Turbulent Mixing & Beyond, 2009

# Product Formation Measurement

- Start with total amount of colored product integral

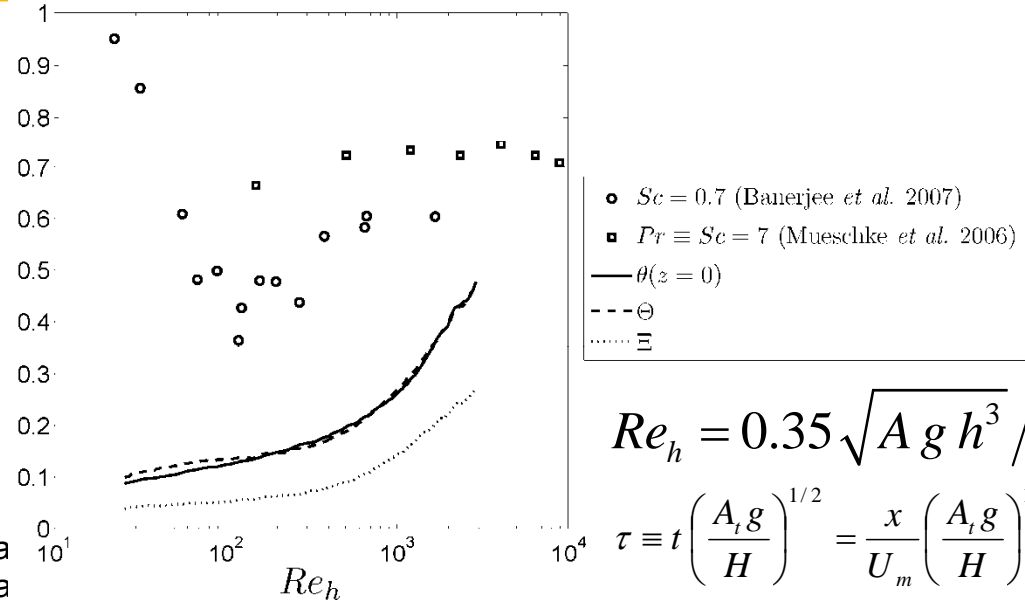
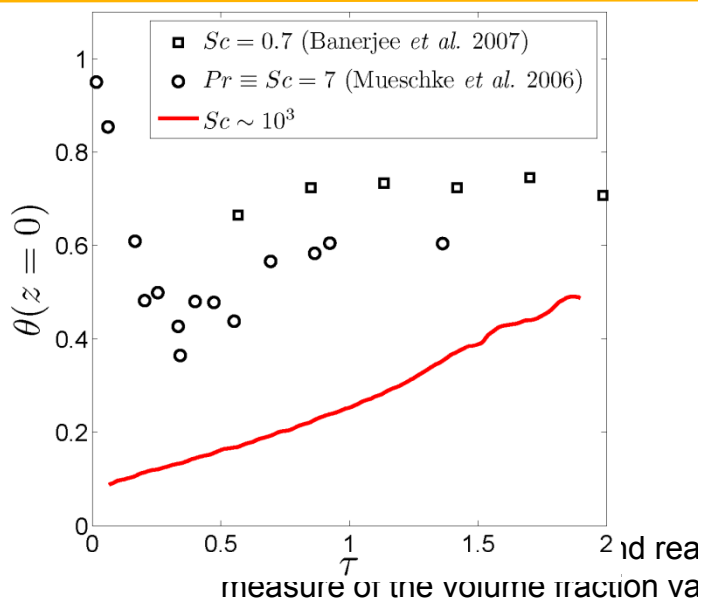
$$C = \frac{[\text{In}_{IV}]}{[\text{In}]_2} = \int_0^1 \alpha_{\text{In}_{IV}}(\text{pH}) f_2 P(f_2) df_2$$

- Replace fraction of dissociation with step function approximation, and integrating over all values of yields

$$\int_0^1 C(f_2^{50\%}) df_2^{50\%} = \alpha_{\text{In}_{IV}}^{max} \bar{f}_1 \bar{f}_2 \theta$$

- First resolution-independent measurement of  $\theta$  for high Schmidt number Rayleigh–Taylor mixing

# Calculation of Molecular Mixing Parameters



$$Re_h = 0.35 \sqrt{A g h^3 / \nu}$$

$$\tau \equiv t \left( \frac{A_t g}{H} \right)^{1/2} = \frac{x}{U_m} \left( \frac{A_t g}{H} \right)^{1/2}$$

- Measurement of various mixing parameters demonstrates large influence of Schmidt number of degree of molecular mixing

$$\theta = 1 - \frac{\overline{f_1'^2}}{\overline{f_1} \overline{f_2}}$$

$$\Theta = 1 - \frac{\int \overline{f_1'^2} dz}{\int \overline{f_1} \overline{f_2} dz}$$

$$\Xi(\varphi_{In}) = \frac{\int [\overline{In_{IV}}] dz}{\int [\overline{In_{IV}}]_{max} dz}$$

## Initial Conditions for RT and RM

---

- Goal is to provide BHR initial conditions that capture initial perturbations
- Linear stability analysis could provide velocities etc. for initial profiles for use in BHR, but linear-to-non-linear can be expected to be better
- Use of Goncharov/Layzer potentials provides a means to obtain velocities, kinetic energy etc. in the early stages of RT/RM development
- Preliminary work is described next to compare a ODE solver with 3-D Miles



## Goncharov's Model

**Velocity potentials near the tip of the bubble:**

$$\phi^h = a(t) J_0(kr) e^{-k(z-\eta_0)}$$

$$\phi^l = b_1(t) J_0(kr) e^{k(z-\eta_0)} + b_2(t) z$$

**Interface amplitude at the tip of the bubble:**

$$\eta = \eta_0(t) + \eta_2(t) r^2$$

$$\ddot{\eta}_0 \frac{k^2 - 4A_T k \eta_2 - 32A_T \eta_2^2}{4(k - 8\eta_2)} + \dot{\eta}_0^2 k^2 \frac{(5A_T - 4)k^2 + 16(2A_T - 3)k\eta_2 + 64A_T \eta_2^2}{8(k - 8\eta_2)^2} + A_T g \eta_2 = 0$$

**k - Bubble height:**  $h_{b,k}(t) = \eta_{0,k}(t) - \eta_{0,k}(0)$

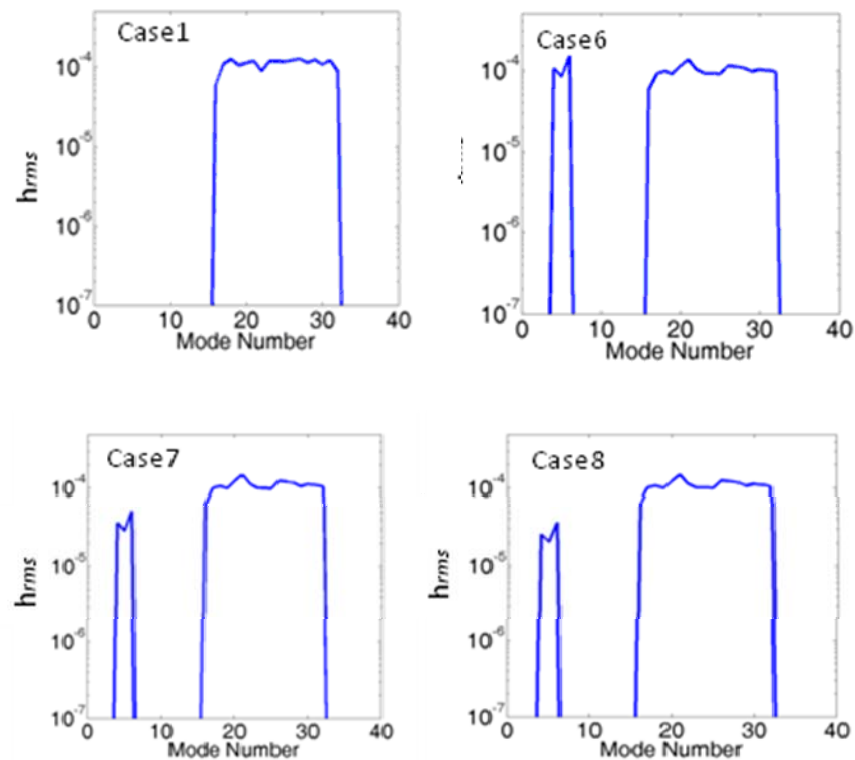
**Multi-mode case:**  $h_b(t) = \max_k (h_{b,k}(t))$

No mode coupling

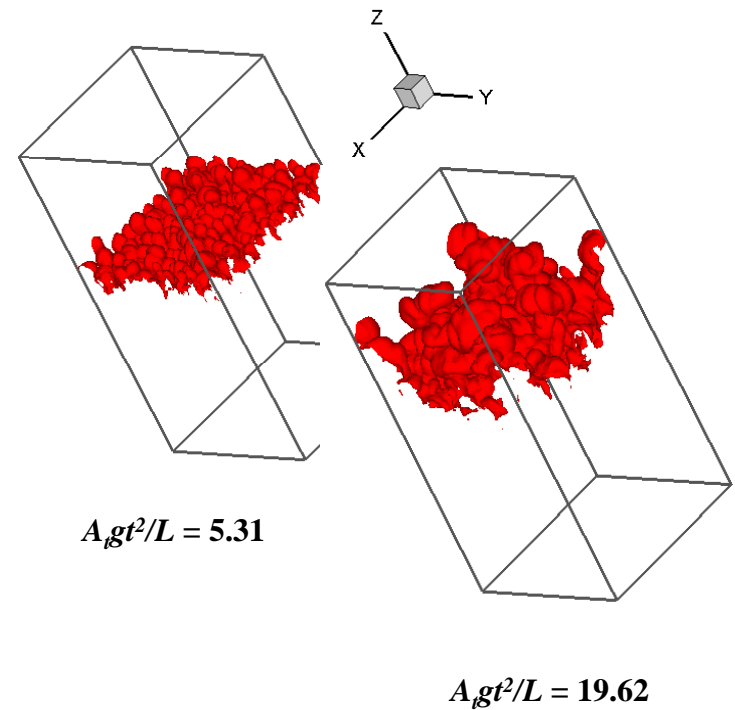
UNCLASSIFIED

# Multi-Mode Study

## Initial Spectrum

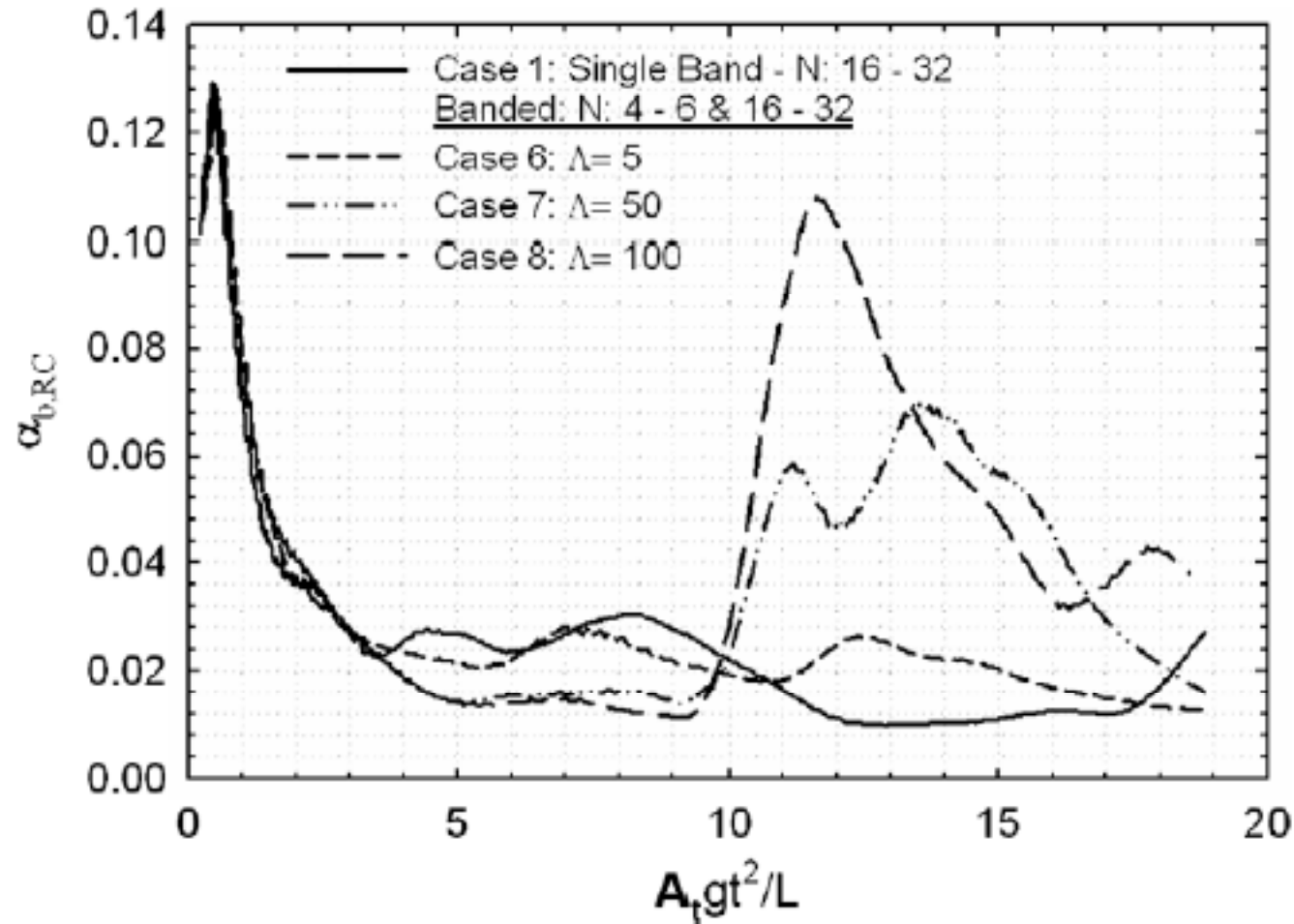


## 3-D MILES Simulations



## Bubble Iso-Surfaces

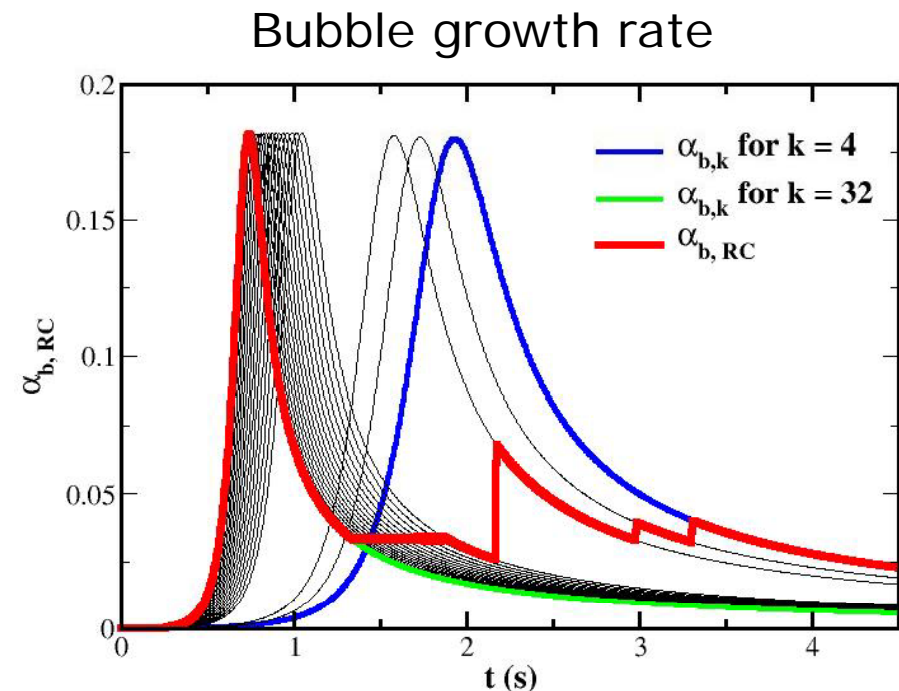
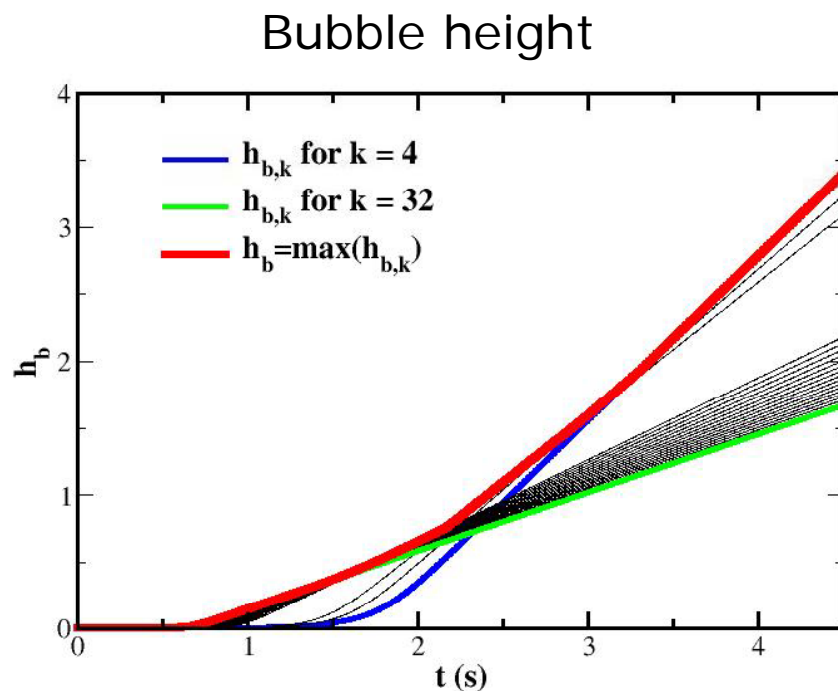
## 3-D MILES from Banerjee & Andrews (2009)



$$h = \alpha A_t g t^2$$

$$\alpha = \frac{\dot{h}^2}{4 A_t g h}$$

## Multi-mode study – ODE's



- At late time,  $h_b$  is governed by the longest wavelength evolution
- Each band of the initial spectrum is 'seen' in the growth rate

# Conclusions

---

- **Our modeling approach relies on fundamental equations for guidance and gives us a strong base for model improvement**
  - The model is not static nor perfect
- **Looking for new/better experimental diagnostics and flow regimes**
- **Molecular Mix Diagnostic**
  - Quantitative diagnostic – molecular resolution
  - $Sc$  significantly affects  $\theta$  at low RT Reynolds numbers, but this dependence is weakened at higher Reynolds numbers
- **Initial conditions and how those are manifested in the model evolution are important**
  - Use of linear-to-non-linear analysis can provide a means to setup initial conditions for BHR