Theoretical Methods for the Determination of Mix

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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

$Z_b(t) =$ penetration distance of light fluid into heavy

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

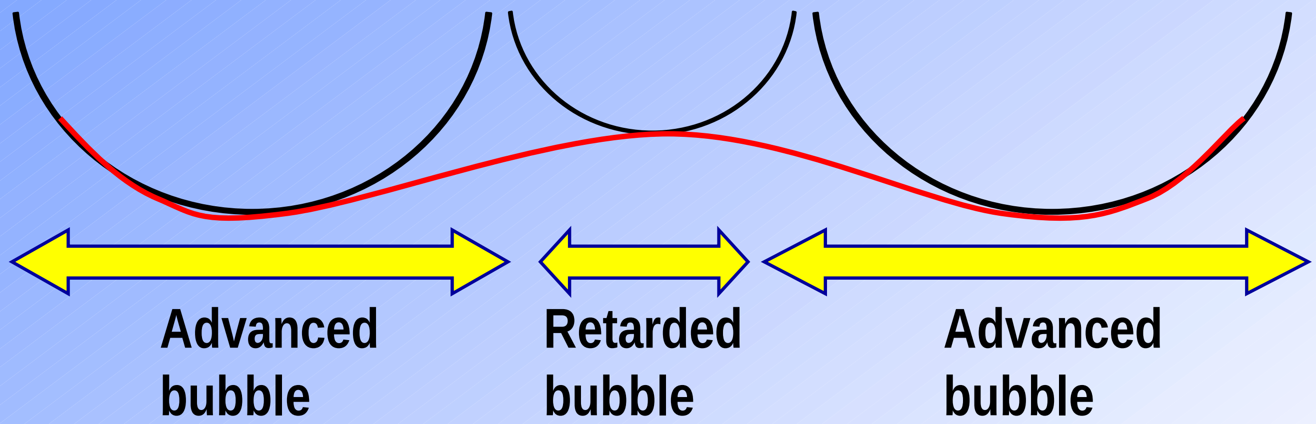
$\alpha_b =$ 0.05 -- 0.077 (Experiment)
0.05 -- 0.06 (Theory)
0.07 (Simulation - tracked)

Bubble height / bubble width = 3.3 (experiment)
= 2.3 (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:

| single mode velocity | = | envelope velocity |

$$\alpha_b \approx 0.5 \text{ -- } 0.6$$

Scaled Variables

$$r = \text{mean bubble radius}$$

$$t_m = \text{time to bubble merger}$$

$$t_m' = \text{scaled time to merger}$$

$$dt' = (Ag/r)^{1/2}\, dt$$

$$\langle \ \rangle_* = \text{fixed point expectation}$$

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

$$r = \frac{k^2}{4} \left\langle \frac{1}{t_m{}'} \right\rangle_* Agt^2; \quad \alpha_r = \frac{k^2}{4} \left\langle \frac{1}{t_m{}'} \right\rangle_*$$

Bubble height variables

$$k = \text{geometric factor}, \approx .43$$

$$\bar{h} = \text{mean bubble height}$$

$$h_m = \text{bubble height separation for merger}$$

$$h = \bar{h} + h_m / 2$$

Derive rate equation for h in RNG scaling

RNG Bubble Height Equation

$$\alpha_b = \frac{1}{2} c_b \alpha_r^{1/2} + \left[\frac{1}{2k} + \frac{1}{2} \right] \alpha_{h_m}$$

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

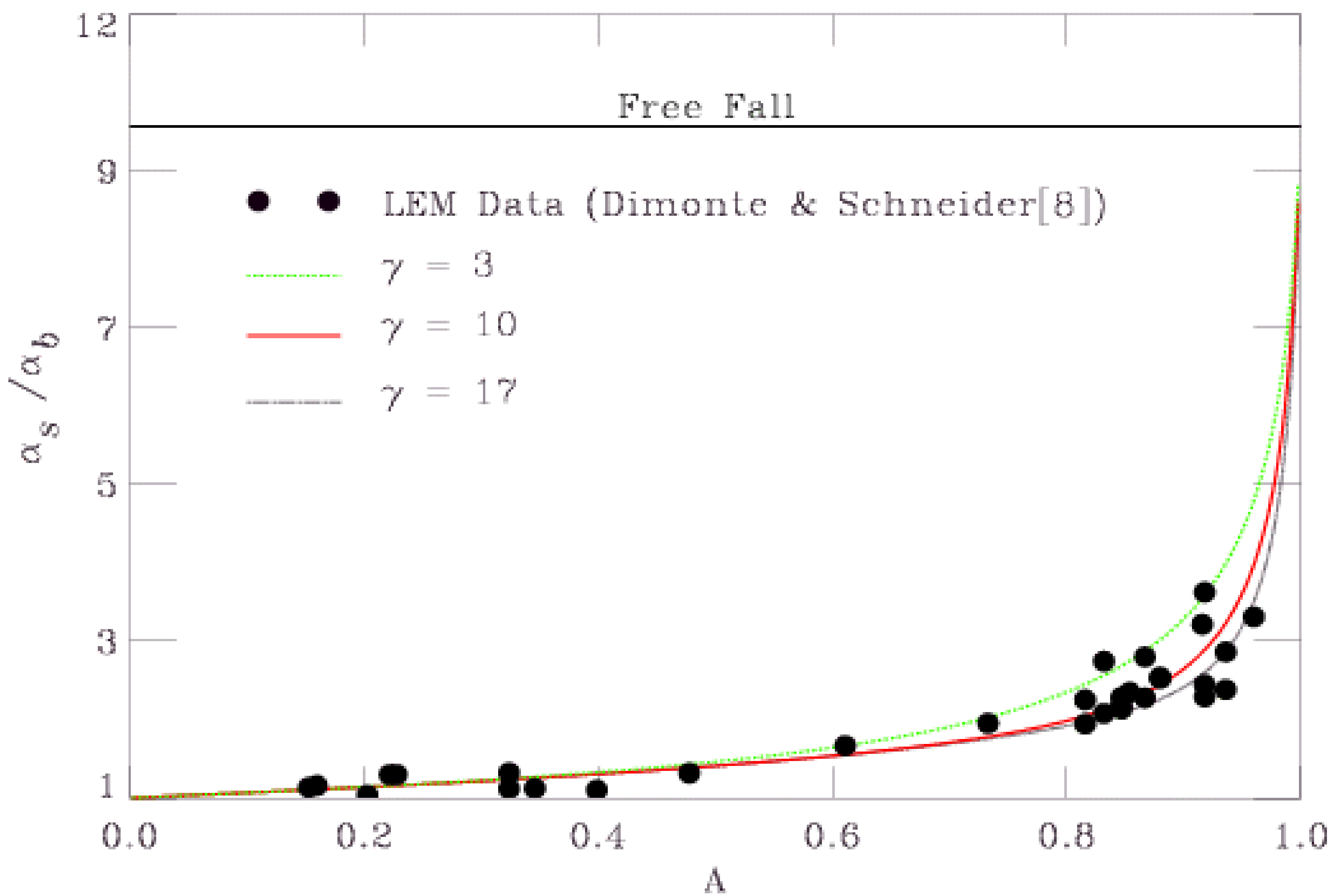
$$Z_{\mathrm{COM}} = \alpha_{\mathrm{COM}} A g t^2$$

$$\alpha_{\mathrm{COM}} = \frac{7}{60} \alpha_s A^{\gamma}; \quad \gamma = 3 - 17$$

$$\approx 0 \text{ unless } A \approx 1$$

fits data and theory (A = 1). α_s / α_b **= solution of quadratic equation**

$$\alpha_s = \alpha_s(\alpha_b)$$


Free Fall
LEM Data (Dimonte & Schneider[8])
γ = 3
γ = 10
γ = 17
α_s /α_b
A
12
9
7
5
3
1
0.0
0.2
0.4
0.6
0.8
1.0

Mixing Zone Edge Models

$Z_{b,s}$ (t) = $h_{b,s}$ = α_{bs} Agt^2 in RT case

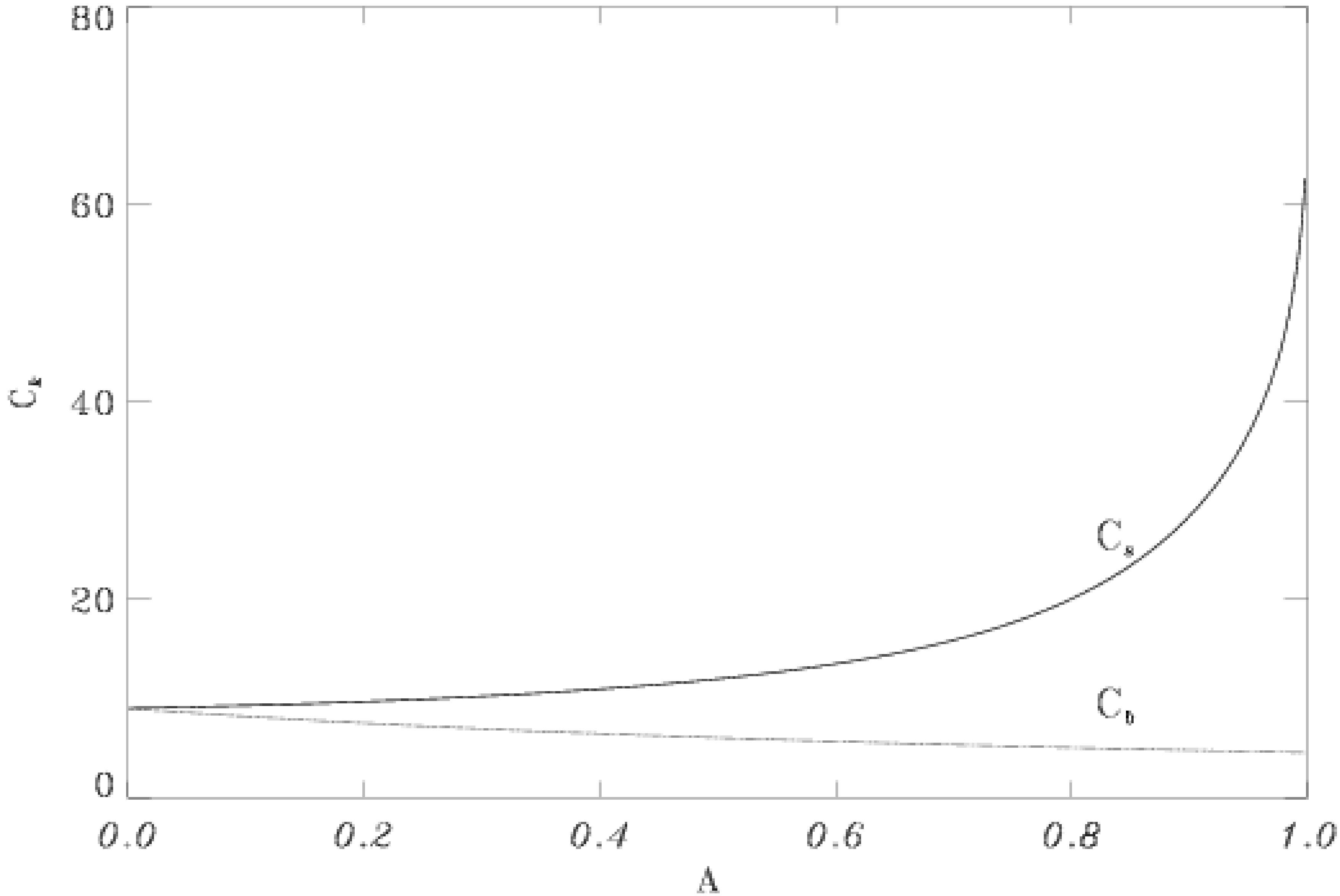
Buoyancy Drag equation for $Z_{b,s}$ (t):

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

Determine $C_{b,s}$ from RT edge motion theory.

ODE valid for arbitrary acceleration

k = 1 from standard fluid dynamics and from bubble geometry



80
60
40
20
0
0.0
0.2
0.4
0.6
0.8
1.0
A
C_s
C_b

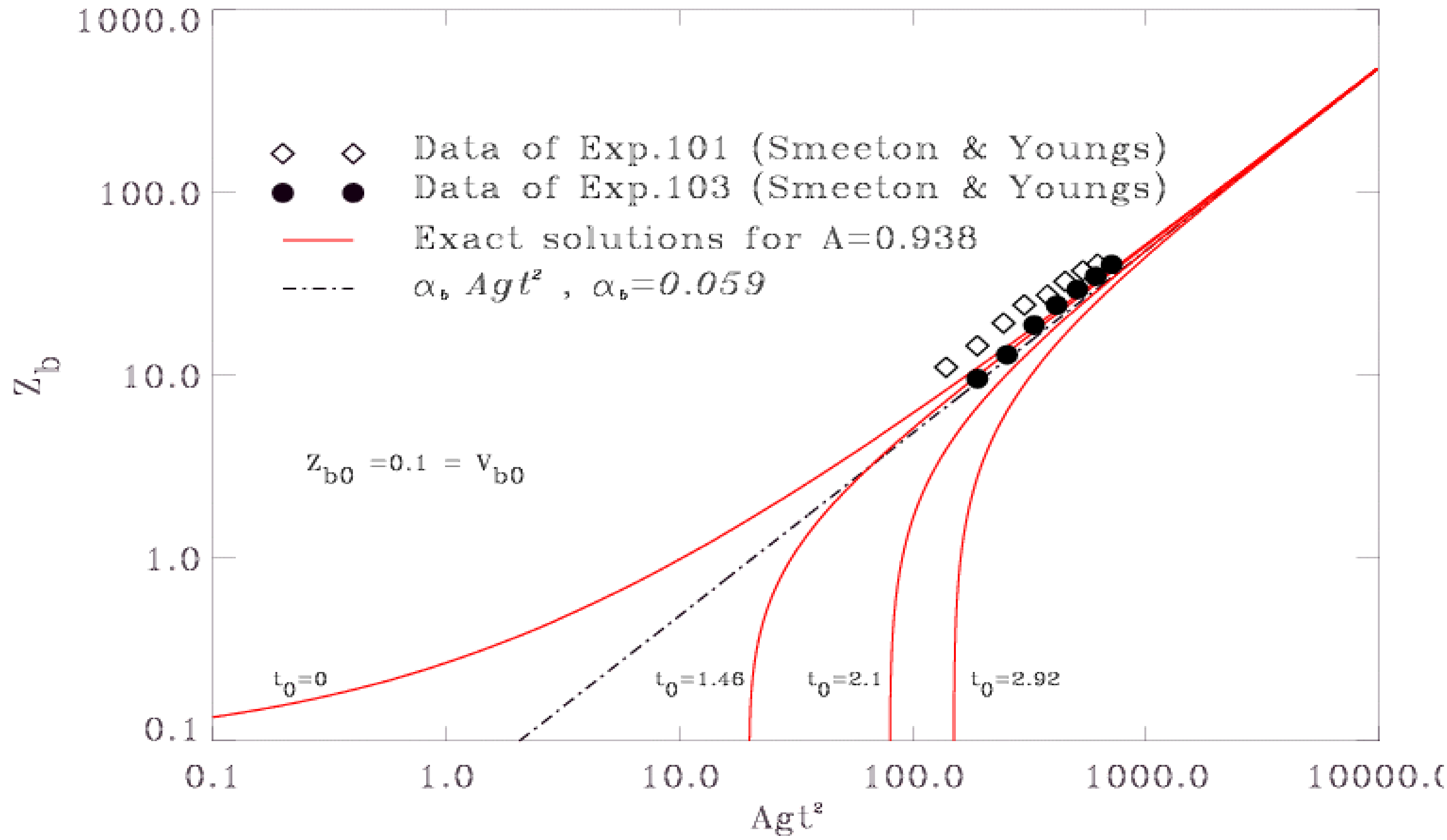
Non-leading Order Terms in RT Asymptotics

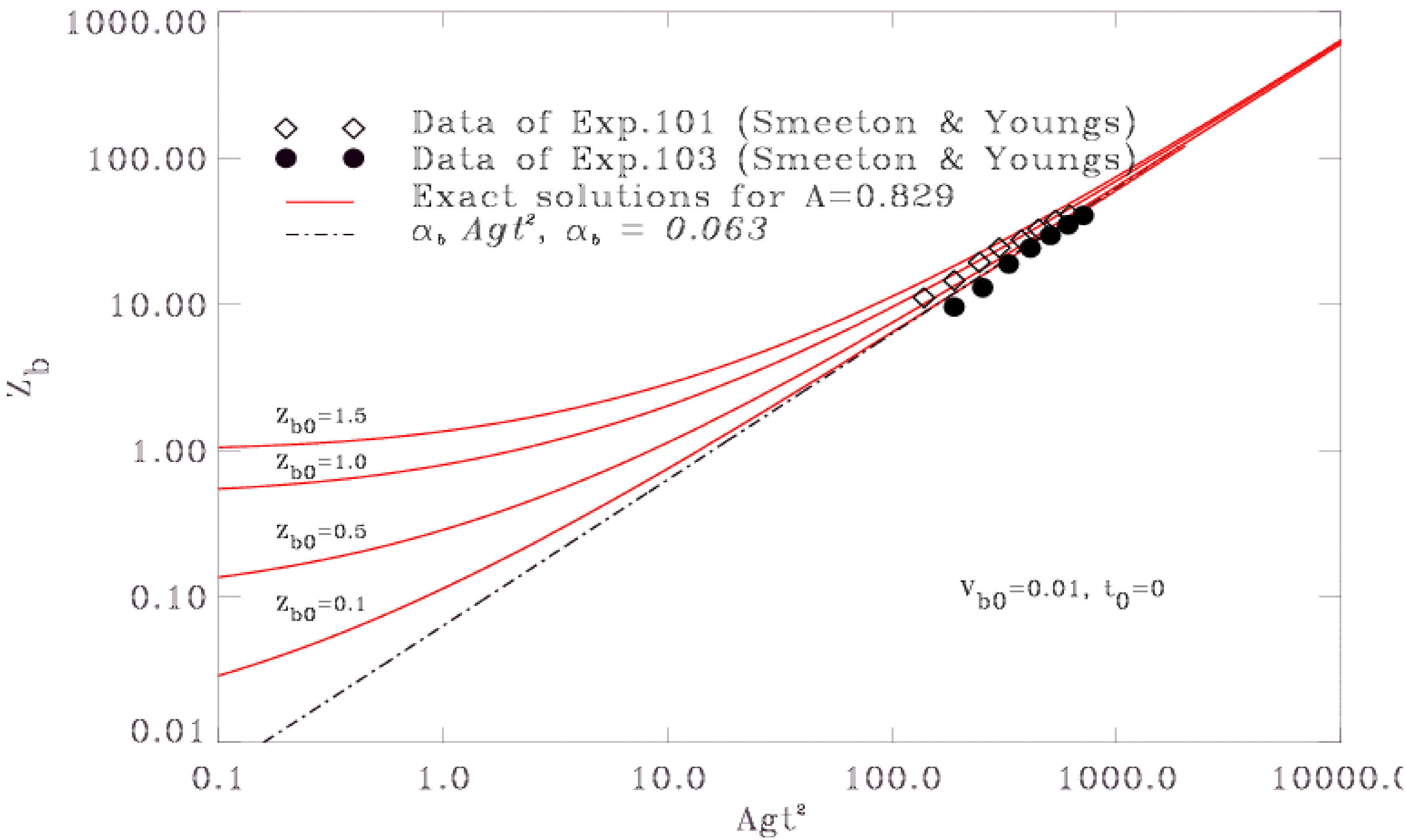
$$Z(\mathrm{t}) = \alpha \; Agt^{2} + \beta t + \gamma$$

β, γ depend on initial data :

$$t_{0}, Z_{0}, \; V_{0}$$

α does not depend on initial data


1000.0
100.0
10.0
1.0
0.1
Z_b
Data of Exp.101 (Smeeton & Youngs)
Data of Exp.103 (Smeeton & Youngs)
Exact solutions for A=0.938
$\alpha_b\ Agt^2$, α_b=0.059
Z_{b0} =0.1 = V_{b0}
t_0=0
t_0=1.46
t_0=2.1
t_0=2.92
0.1
1.0
10.0
100.0
1000.0
Agt^2



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_{b0}=1.5
Z_{b0}=1.0
Z_{b0}=0.5
Z_{b0}=0.1
V_{b0}=0.01, t_0=0
Z_b
Agt^2
1000.00
100.00
10.00
1.00
0.10
0.01
0.1
1.0
10.0
100.0
1000.0

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: $\overline{U}_t + \nabla \overline{F(U)} = 0$

$$\overline{F(U)} \neq F(\overline{U})$$

$$F_{ren}(\overline{U}) \approx \overline{F(U)}$$

$$\overline{U}_t + \nabla F_{ren}(\overline{U}) = 0$$

Closure Problem: Determine F_{ren}

Ensemble Averages

Assume two fluids, labeled k=1 (light) and k=2 (heavy). Define

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

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

Microphysics

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

Macrophysics

$$\boldsymbol{\beta}_\mathbf{k} = \langle \mathbf{X_k} \rangle$$

$$\frac{\partial \boldsymbol{\beta}_\mathbf{k}}{\partial \mathbf{t}} + \langle \upsilon \cdot \nabla \mathbf{X_k} \rangle = \mathbf{0}$$

Define υ^*:

$$\langle \upsilon \cdot \nabla \mathbf{X_k} \rangle \equiv \upsilon^* \nabla \boldsymbol{\beta}_\mathbf{k}$$

Thus

$$\frac{\partial \boldsymbol{\beta}_\mathbf{k}}{\partial \mathbf{t}} + \upsilon^* \cdot \nabla \boldsymbol{\beta}_\mathbf{k} = \mathbf{0}$$

Closure

Assume: v* depends on v_1 and v_2 and spatially dimensionless quantities only.

Assume: regularity of v*.

Theorem: $$\upsilon^* = \mu_2^{\upsilon}\upsilon_1 + \mu_1^{\upsilon}\upsilon_2$$

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

Assume: all μ's depend on β_k and t only.

Explicit Model: Zero Parameters

Exact calculation: μ_k^{υ} is fractional linear. Assume same for μ_k^{p}.
Assume dependence on β_k alone. Then

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

with k' denoting the other fluid index and $c_1^q c_2^q = 1 \qquad q = \upsilon \quad \text{or} \quad q = \text{p}.$

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

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

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

$$\ddot{Z}_k(t) = \text{Drag + buoyancy}$$

Analytic Solution: Incompressible Case

$$\upsilon_k(\beta_k, t) = V_k \mu_{k'}^{\upsilon}$$

$$\upsilon^*(\beta_k, t) = \frac{V_k V_{k'}(V_k \beta_k^2 + V_{k'} \beta_{k'}^2)}{(|V_k|\beta_k + |V_{k'}|\beta_{k'})^2}$$

$$z(\beta_k, t) = z_0(\beta_k) + \int_0^t \upsilon^*(\beta_k, s)ds$$

Let

$$\overline{p} = \beta_1 p_1 + \beta_2 p_2, \qquad p_{diff} = \frac{p_2}{\rho_2} - \frac{p_1}{\rho_1},$$

$$\frac{D_k}{D_t} = \frac{\partial}{\partial t} + \upsilon_k \frac{\partial}{\partial_z} \quad .$$

Then

$$\overline{p}(z, t) = p_2(Z_1) + \int_{Z_1}^{z} \sum_{k=1}^{2} \beta_k \rho_k \left(g - \frac{D_k \upsilon_k}{Dt}\right)dz$$

$$p_{diff} = p_{diff}(Z_1) - \int_{Z_1}^{z} \left(\frac{D_2 \upsilon_2}{Dt} - \frac{D_1 \upsilon_1}{Dt}\right)dz$$

Asymptotic Expansion in Powers of M = Mach Number

0th order = incompressible v, β

1st order = correction v, β

2nd order = incompressible p_1, p_2

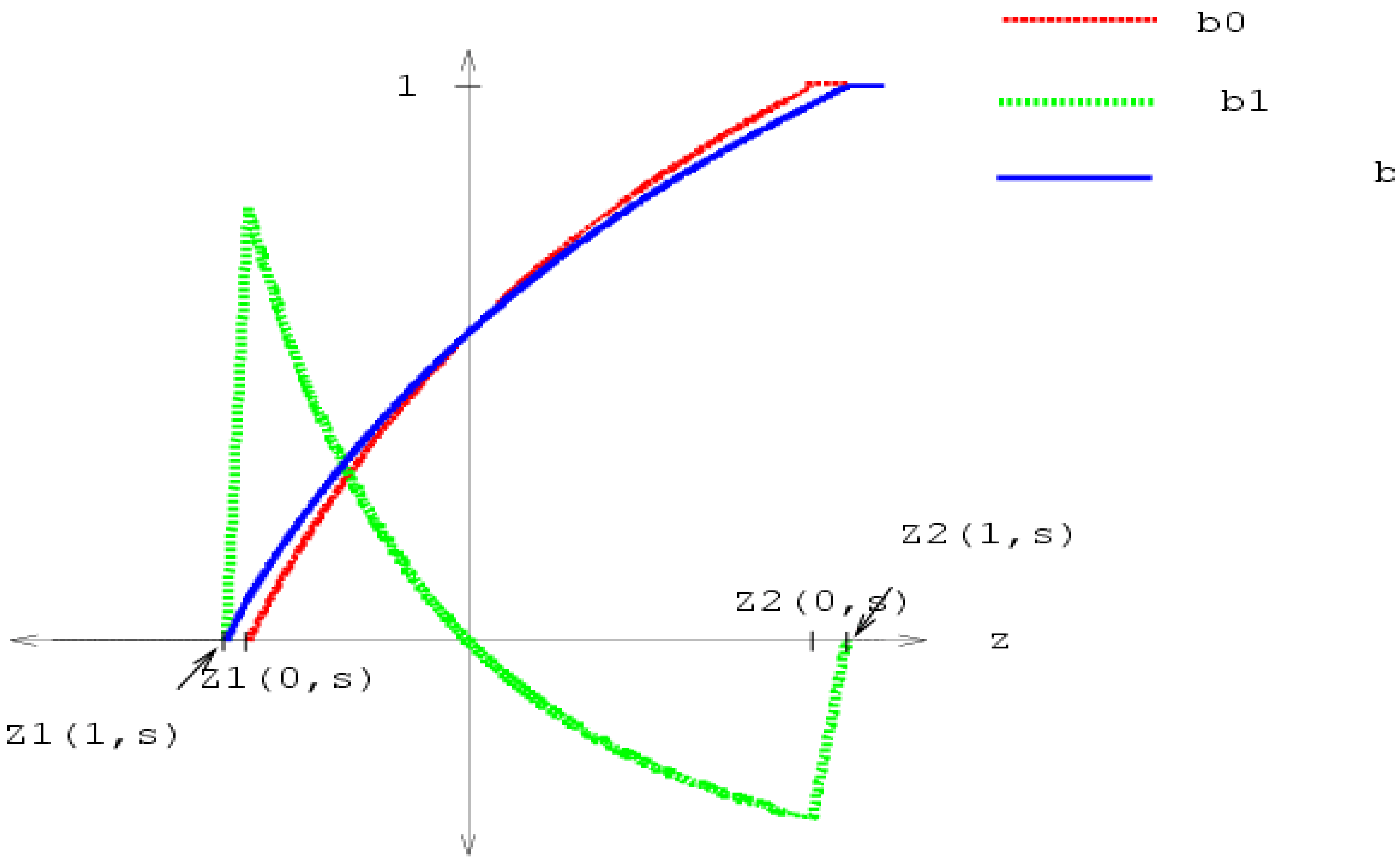
+ v, β correction

2nd order p_1, p_2 = incompressible p_1, p_2

$\Rightarrow$ constraint:

"missing" incompressible pressure equation

Also resolves "missing" compressible closure.


b0
b1
b
1
z
z2(1,s)
z2(0,s)
z1(0,s)
z1(1,s)

Reduced Models:
Equilibrated Pressures and Velocities

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

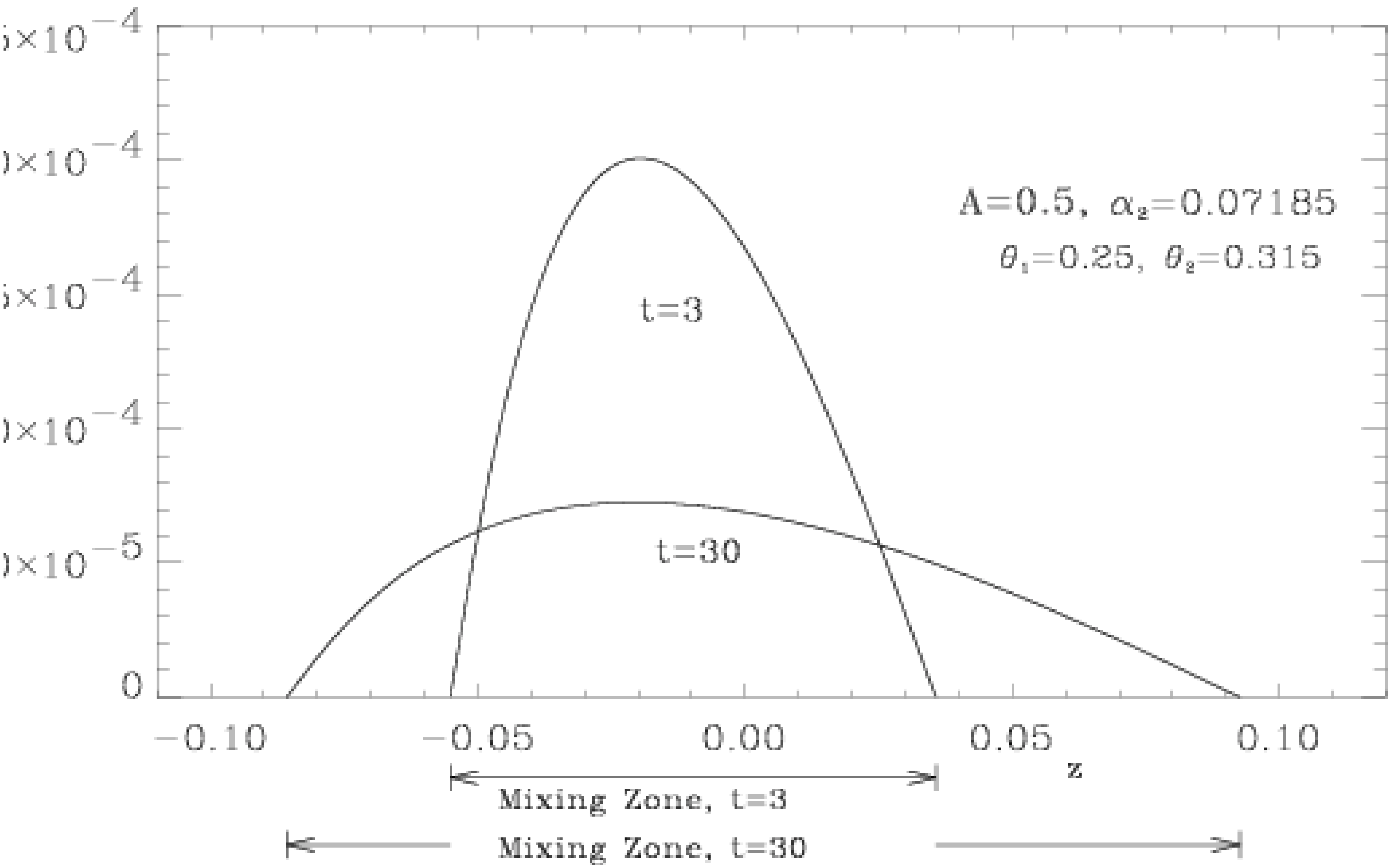
RT diffusion coefficient:

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

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, α_2=0.07185
θ_1=0.25, θ_2=0.315
t=3
t=30
z
−0.10
−0.05
0.00
0.05
0.10
Mixing Zone, t=3
Mixing Zone, t=30

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 intial conditions
- Improved mix model equations: Stable mathematically and thermodynamically determinate
- Asmptotics defined; closure improved