

Turbulent Mixing and Beyond, The Abdus Salam International Centre for Theoretical Physics , Trieste, Italy, 27 July-07 August, 2009.

THE DENSITY RATIO DEPENDENCE OF SELF-SIMILAR RAYLEIGH-TAYLOR MIXING

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OUTLINE OF TALK

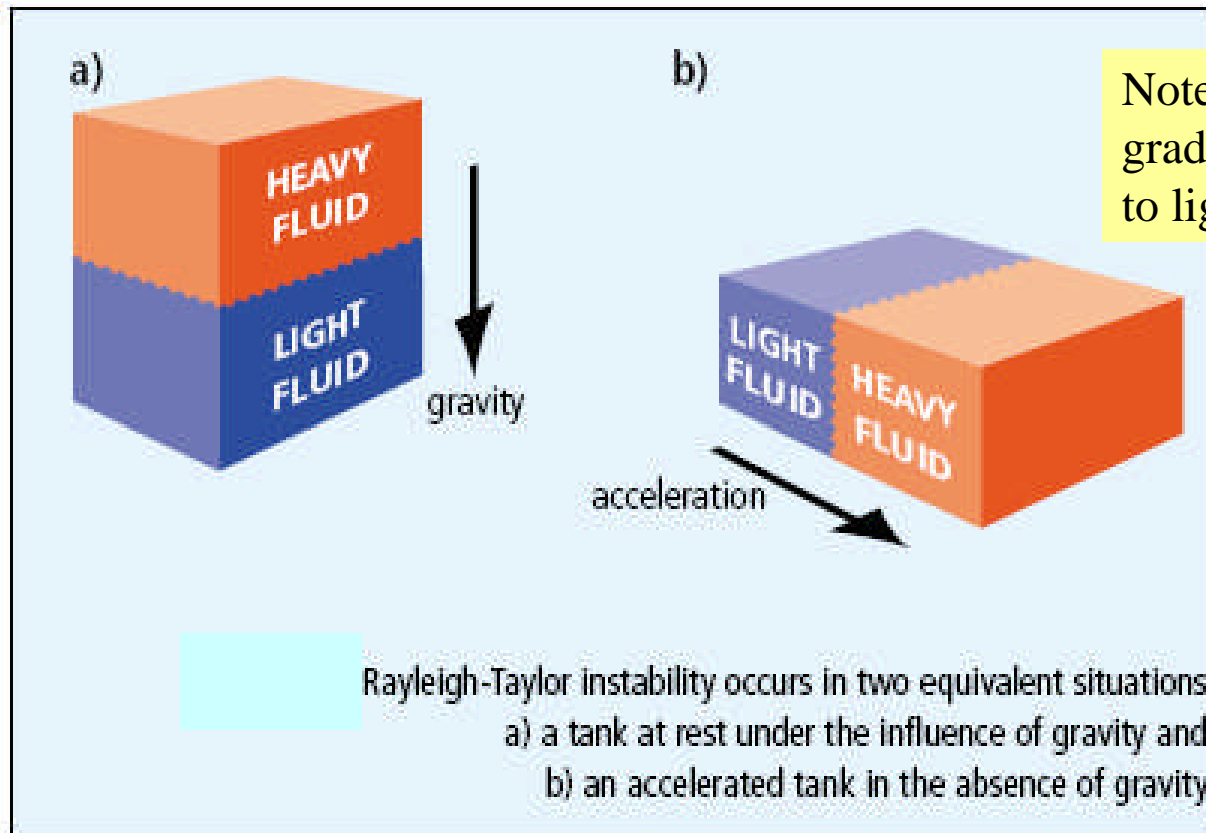
- What is Rayleigh-Taylor instability and where does it occur?
- Self-similar turbulent mixing with constant acceleration

Some historical background, previous simulations, importance for engineering modelling.

The current (ongoing) series of high-resolution simulations – effect of mesh size, influence of density ratio and initial conditions on growth rate and internal structure.

- Application to a simple spherical implosion
- Concluding remarks
- References

What is Rayleigh-Taylor (RT) instability?



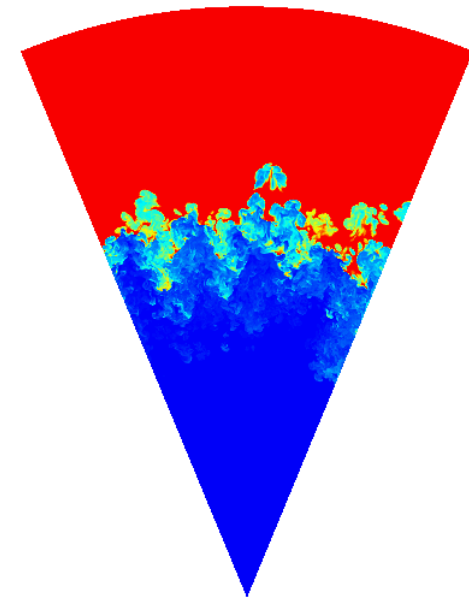
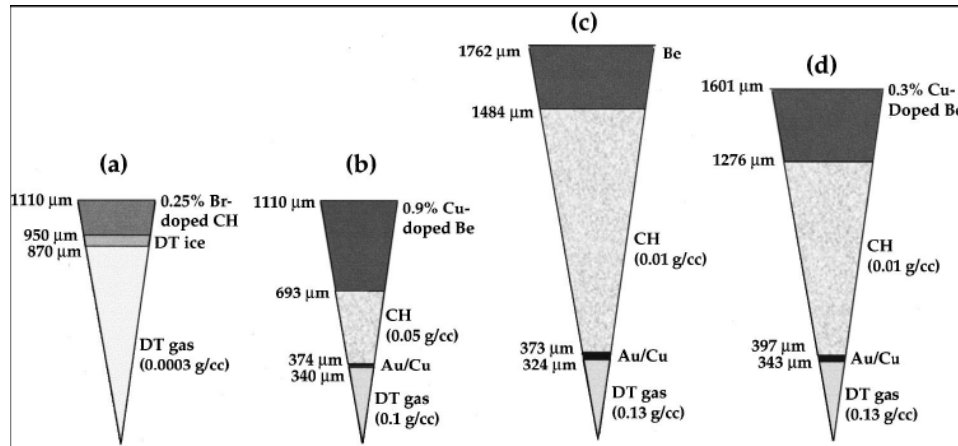
- Astrophysics
- Ocean/Atmosphere
- Geological flows
- Combustion
- ICF

First publication, Rayleigh (1883)

Became an important research topic after the paper of G.I. Talyor (1950)

(related process – Richtmyer-Meshkov instability occurs when shock waves pass through perturbed interfaces)

Inertial Confinement Fusion (ICF) – nanosecond time-scale

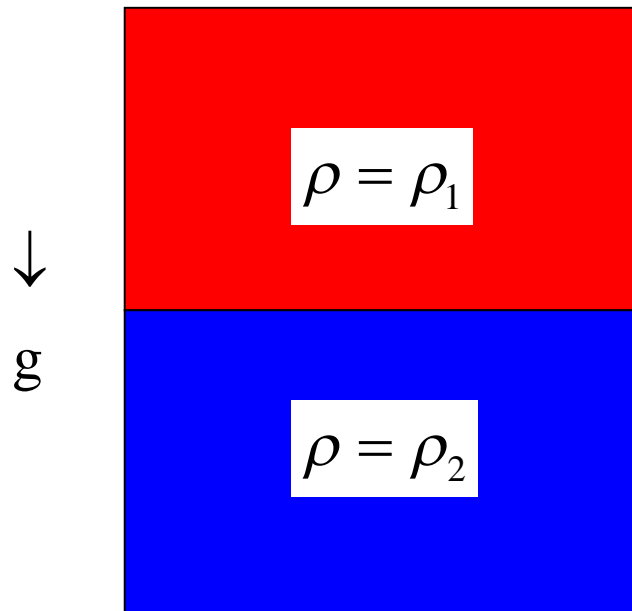


Amendt et al. Physics of Plasmas (2002) –
degradation of capsule performance.

Focus of the present talk will be high-Reynolds no. mixing at initially sharp interfaces.

Flows may be compressible, but turbulence Mach no. (u'/c) is low \Rightarrow most key aspects of the RT process can be understood via incompressible experiments and simulations.

Main focus of the talk



3D incompressible (or near incompressible)

random perturbations

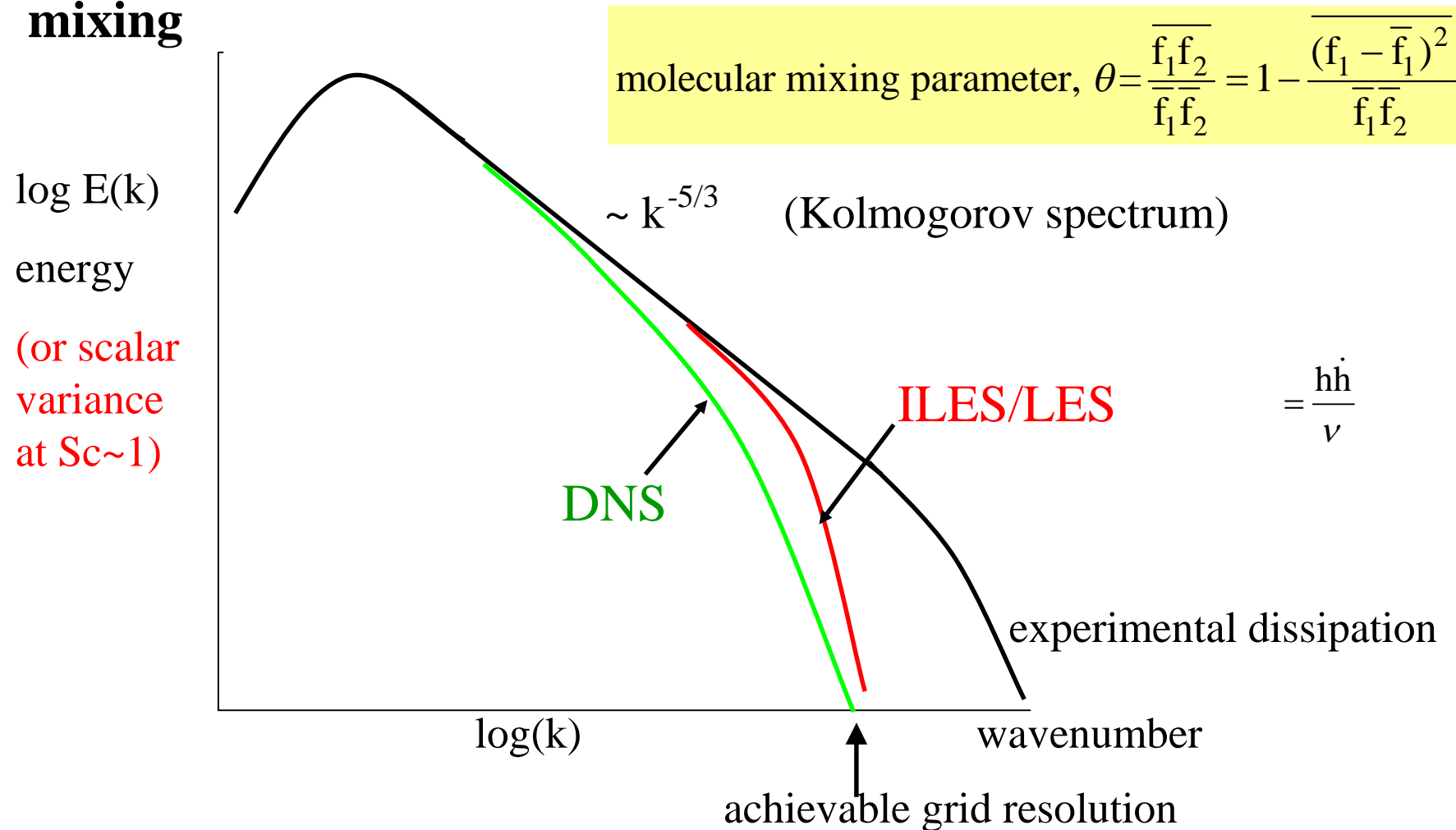
ρ_1 ρ_2 g constant

simulations are for miscible fluids

For self-similar mixing:

$$\text{mixing zone width} = f\left(\frac{\rho_1}{\rho_2}\right)gt^2$$

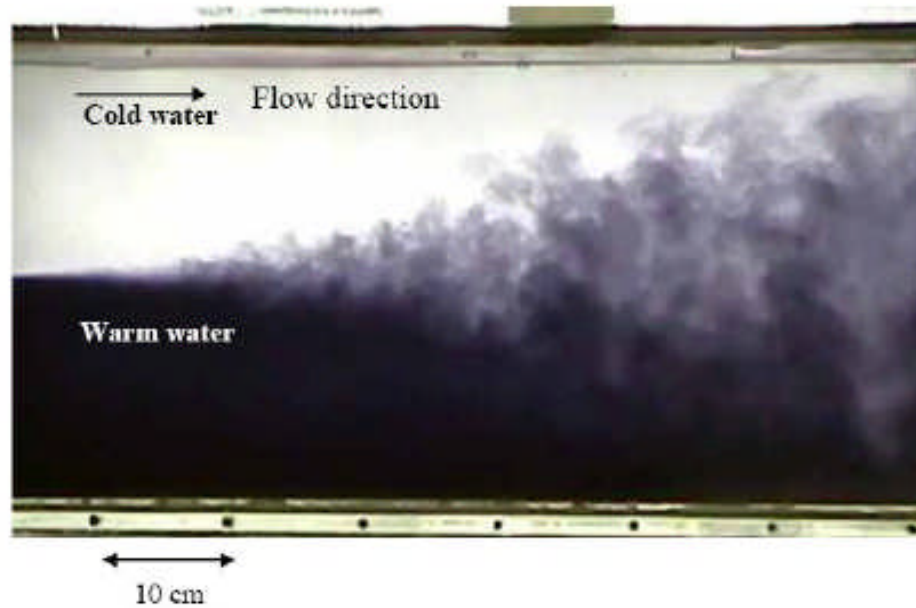
3D simulation is greatly enhancing our understanding of RT mixing



DNS: Direct Numerical Simulation – needed to understand the effect of Reynolds No.

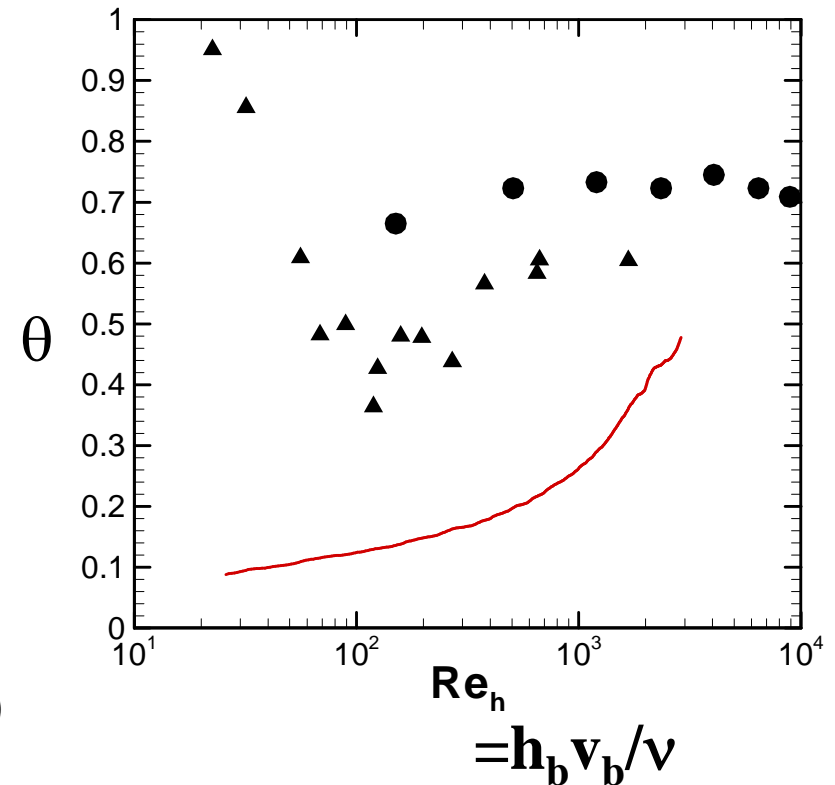
LES: Large Eddy Simulation – best approximation to high-Reynolds No. mixing in more complex flows (explicit “sub-grid-scale” dissipation model or high-wavenumber dissipation Implicit in the numerical scheme: ILES)

Measurements of molecular mixing parameter: Malcolm Andrews group at Texas A&M



$$Sc = \frac{\nu}{D} = \left[\frac{L_{vis}}{L_{diff}} \right]^2$$

- $Sc=700$ (brine/water)
- ▲ $Pr=Sc=7$ (cold/hot water)
- $Sc=0.7$ (gases)



- Experiments using a pH indicator (phenolphthalein) at multiple equivalence ratios give a measure of the volume fraction variance, Meuschke et al (J.Fluid.Mech. 2009)
- Measurement of molecular mixing demonstrates a large influence of Schmidt number at small Re , but tending toward saturation at high $Re \sim 10^4$
- Note similarity to jet mixing, Dimotakis (2000)
 - “mixing transition” at $Re = U\delta/\nu = 1-2 \times 10^4$
- LES should capture the high – Re behaviour (post mixing transition), $Re > 10^4$, $\bar{\theta} \sim 0.7$

DNS for simple
problems



High resolution 3D
simulation (LES) for
more complex problems

As computer power increases
the LES should get closer and
closer to the full scale
applications

calibration / validation



Engineering models



Applications

The case considered in
this talk, self-similar RT
mixing is a key test-case
for model calibration

Historical Comments

1950 – 1980s

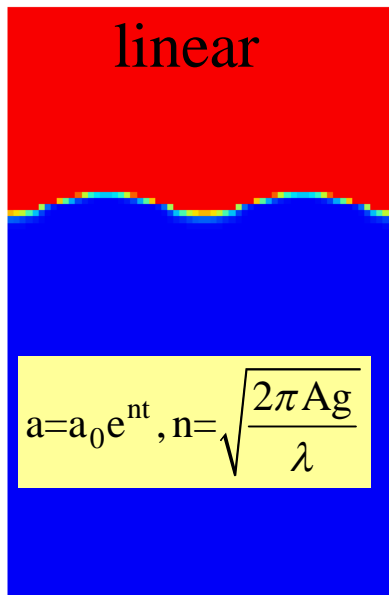
Main focus, in The West, was on the evolution of a single sinusoidal mode (small amplitude linear growth → large amplitude non-linear growth) [see review papers by David Sharp, PhysicaD (1984) and Snezhana Abarzhzi (2008)]

However, the single mode theory was applied to ‘ random initial perturbations’ by Garret Birkoff at Los Alamos in the 1950s by assuming a range of initial perturbations with amplitude = a small fraction (~ 0.01) of the wavelength and then calculating the dominant scale as a function of time. (*Fermi was also working on RT at this time*)

Single mode Rayleigh-Taylor instability

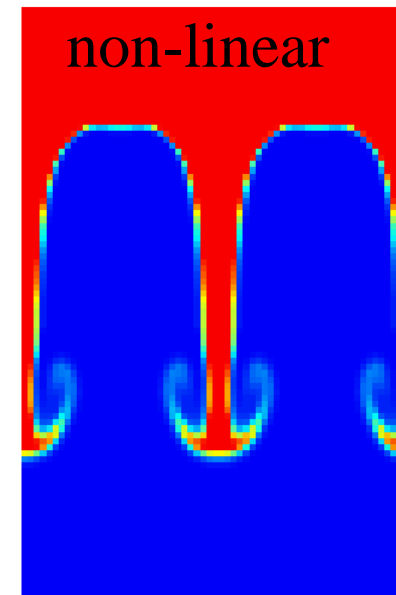
2D simulation at density ratio $\rho_1 / \rho_2 = 20$

Atwood number: $A = \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}$



$$a = a_0 e^{nt}, n = \sqrt{\frac{2\pi Ag}{\lambda}}$$

early time: exponential growth
(19th C theory for interfacial waves
with sign of $\rho_1 - \rho_2$ reversed)



late-time: bubbles rise
with velocity: $V \sim \sqrt{Ag\lambda}$

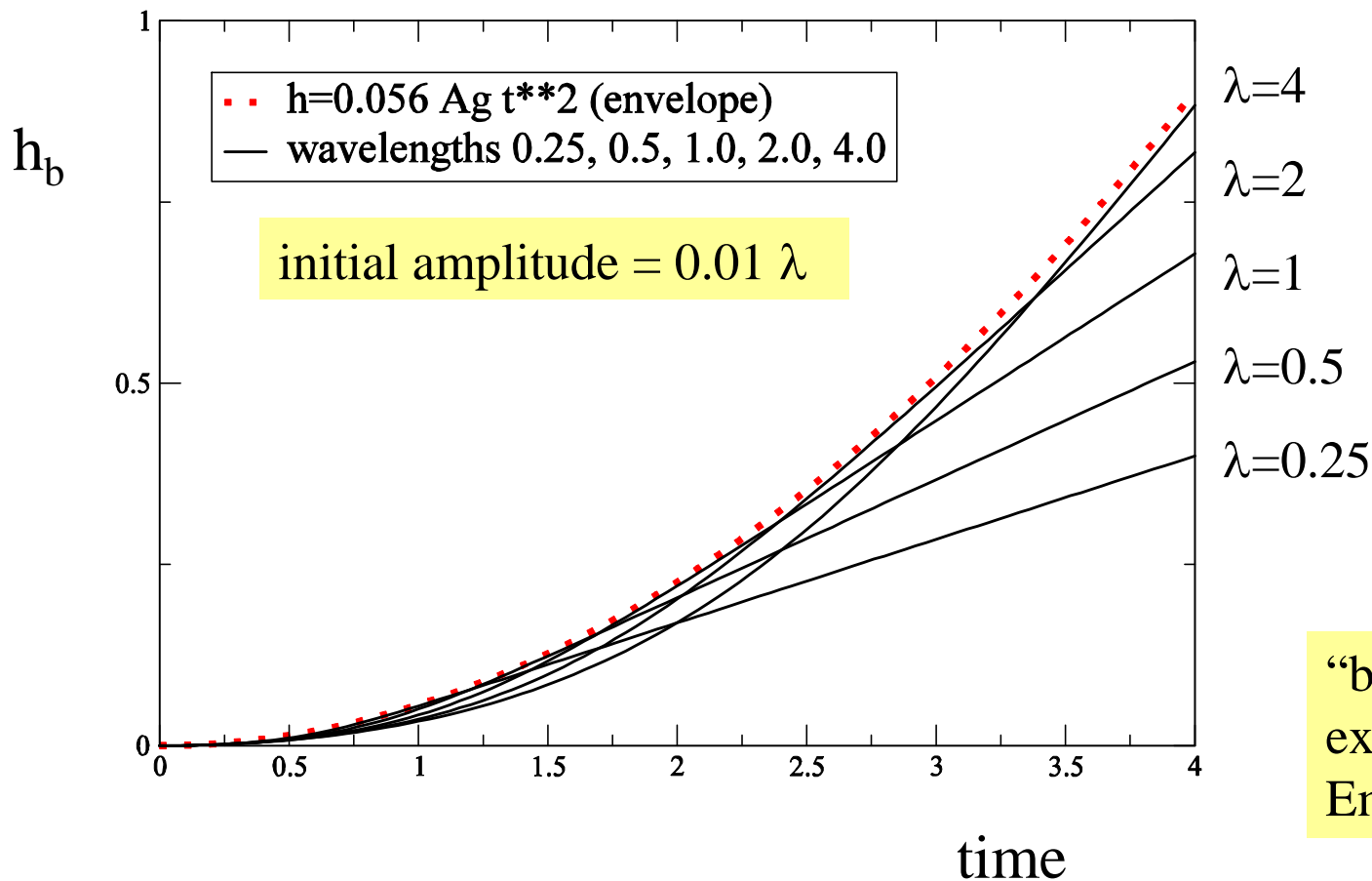
Atwood No. close to 1 : Equation due to Layzer (1955) gives a good approximation to the

bubble velocity $V = \frac{dh_b}{dt}$: $(2 + E) \frac{dV}{dt} = (1 - E) Ag - \frac{6\pi V^2}{\lambda}$ where $E = \exp\left(-\frac{6\pi h_b}{\lambda}\right)$

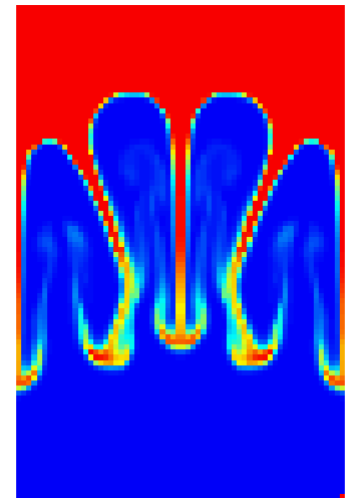
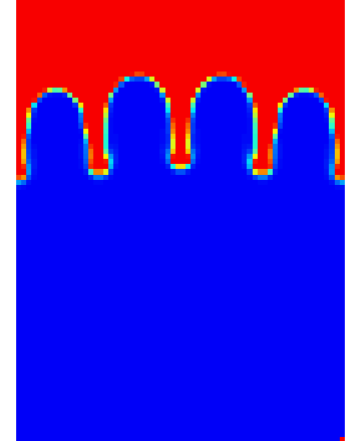
The Layzer equation was use at AWRE in the 1960s and 70s as the basis of a non-linear model for bubble and spike growth – Cameron & Pike (1965), Pizer (1978)

Multimode initial perturbations

Apply Layzer equation to a range of wavelengths
(similar technique used by G. Birkhoff, Los Alamos report, 1954)



2D simulation



“bubble competition”
experiments of
Emmons et al. 1960.

Research in the Soviet Union

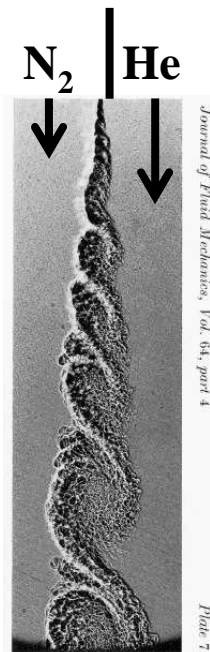
Belen'kii and Fradkin (1965) - Lebedev Institute 1950s?

Treat RT mixing as a turbulent diffusion process. Use single-equation turbulence model (length scale, L =mixing zone width), similar to that used for turbulent shear flow. Includes dissipation, $\varepsilon = k^{3/2} / \ell_t$

$$L = 270\alpha^4 \log \frac{\rho_1}{\rho_2} \left(\int \sqrt{g} dt \right)^2 \quad \text{where } \ell_t = \alpha L$$

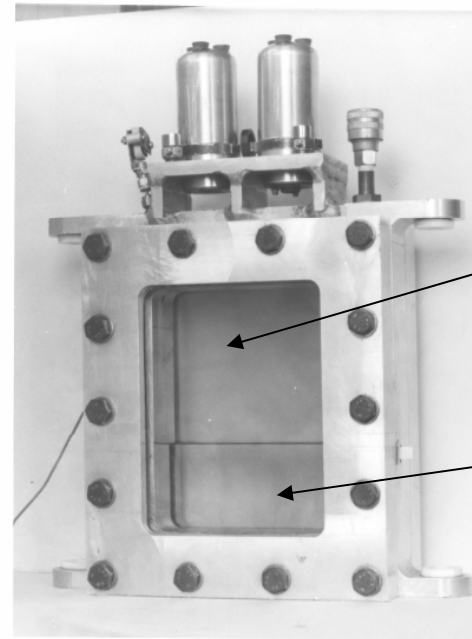
Current understanding is based on a combination of the two approaches – influence of initial conditions, large-scale coherent structures (bubbles and spikes), approximate self-similar behaviour, turbulent diffusion, Richardson(Kolmogorov) cascades for kinetic energy and concentration fluctuations (\Rightarrow molecular mixing)

Rocket-Rig RT experiment - AWRE Foulness ,1980s, (see, Read ,1984; Smeeton & Youngs, 1988; Youngs, 1989)



mixing layer:
Brown and Rosko,
JFM, (1974)

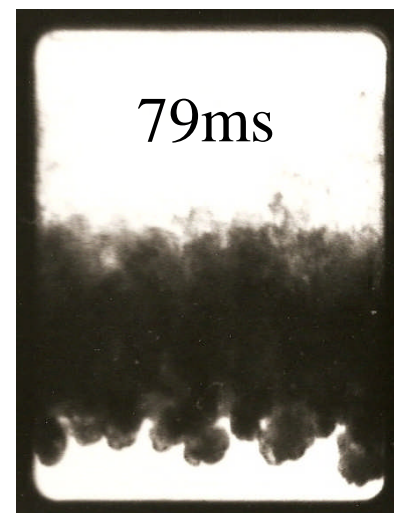
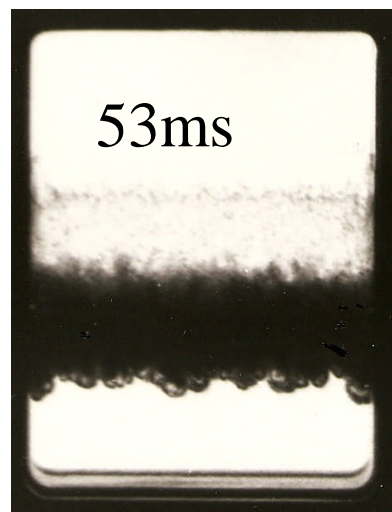
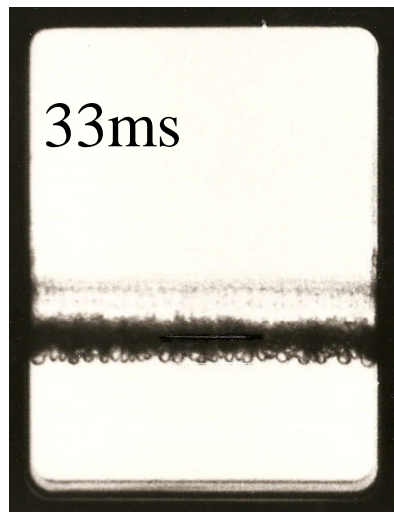
length scale
increases by
vortex pairing



Compressed SF₆

Pentane

$$\frac{\rho_1}{\rho_2} = 8.5$$



h_s (spike)

h_b (bubble)

length scale increases by bubble competition

Experiments show increase in length scale as mixing evolves – if mixing is self-similar, dimensional analysis suggests

mixing zone width

$$W = f\left(\frac{\rho_1}{\rho_2}\right) g t^2$$

The Rocket-rig experiments showed

$$h_b = \alpha A g t^2 \quad \text{where } \alpha \simeq 0.06 \text{ and } A = \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}$$

and h_s/h_b a slowly increasing function of ρ_1 / ρ_2

very simple pattern
for the amount of
mixing

h_b = penetration of dense fluid (bubble distance)

h_s = penetration of light fluid (spike distance)

More recent Linear Electric Motor experiments at LLNL, (Dimonte & Schnieder, 2000) gave $\alpha \sim 0.05$, Texas A&M $\alpha=0.07$

Also similar results from experiments performed by Kucherenko's group at Chelyabinsk-70 (Kucherenko et al., 1991)

LOSS OF MEMORY OF INITIAL CONDITIONS (Youngs 1984)

If the initial surface consists of small random short wavelength perturbations then, after a short time:

dominant length scale \gg viscous scale

dominant length scale increases by mode coupling

\Rightarrow expect loss of memory of the initial conditions to occur (as assumed in turbulent shear flow, Townsend, 1976*)

\Rightarrow unique value of α

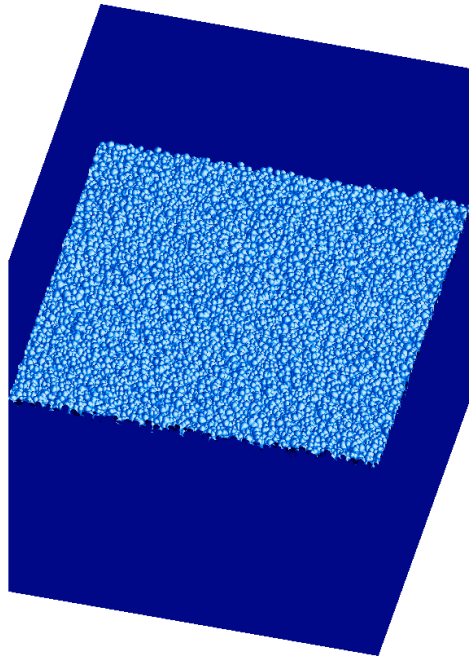
It was noted that mixing would be enhanced if long-wavelength initial perturbations with sufficiently high amplitudes were present.

However, before high-resolution 3D simulation was feasible it was thought that loss of memory of initial conditions would apply to low end of the observed range of α values (~ 0.05)

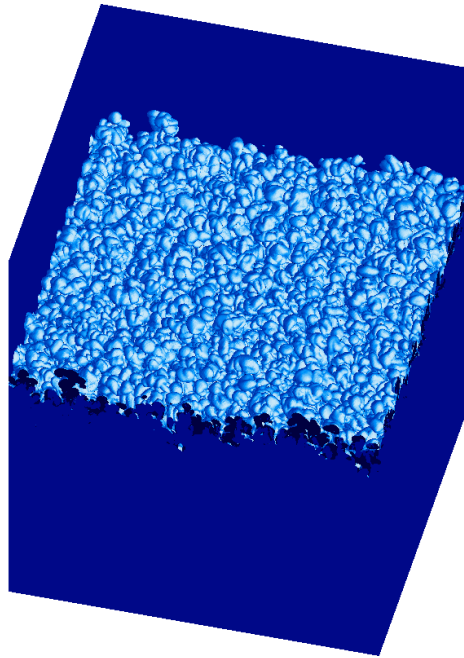
* was known at the time that shear layer growth varied from experiment to experiment

**TURMOIL MILES ($\rho_1 / \rho_3 = 3$) 720 x 600 x 600 meshes
(simple explicit compressible code run at low Mach no)**

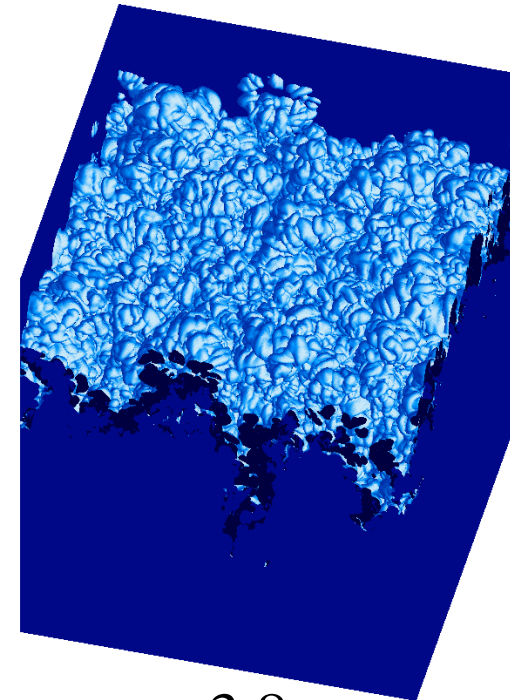
Short wavelength initial perturbations : random combination of Fourier
modes: wavelengths:- $4 \Delta x$ to $8 \Delta x$, amplitude s.d.:- $0.04 \Delta x$



$t = 0.8$



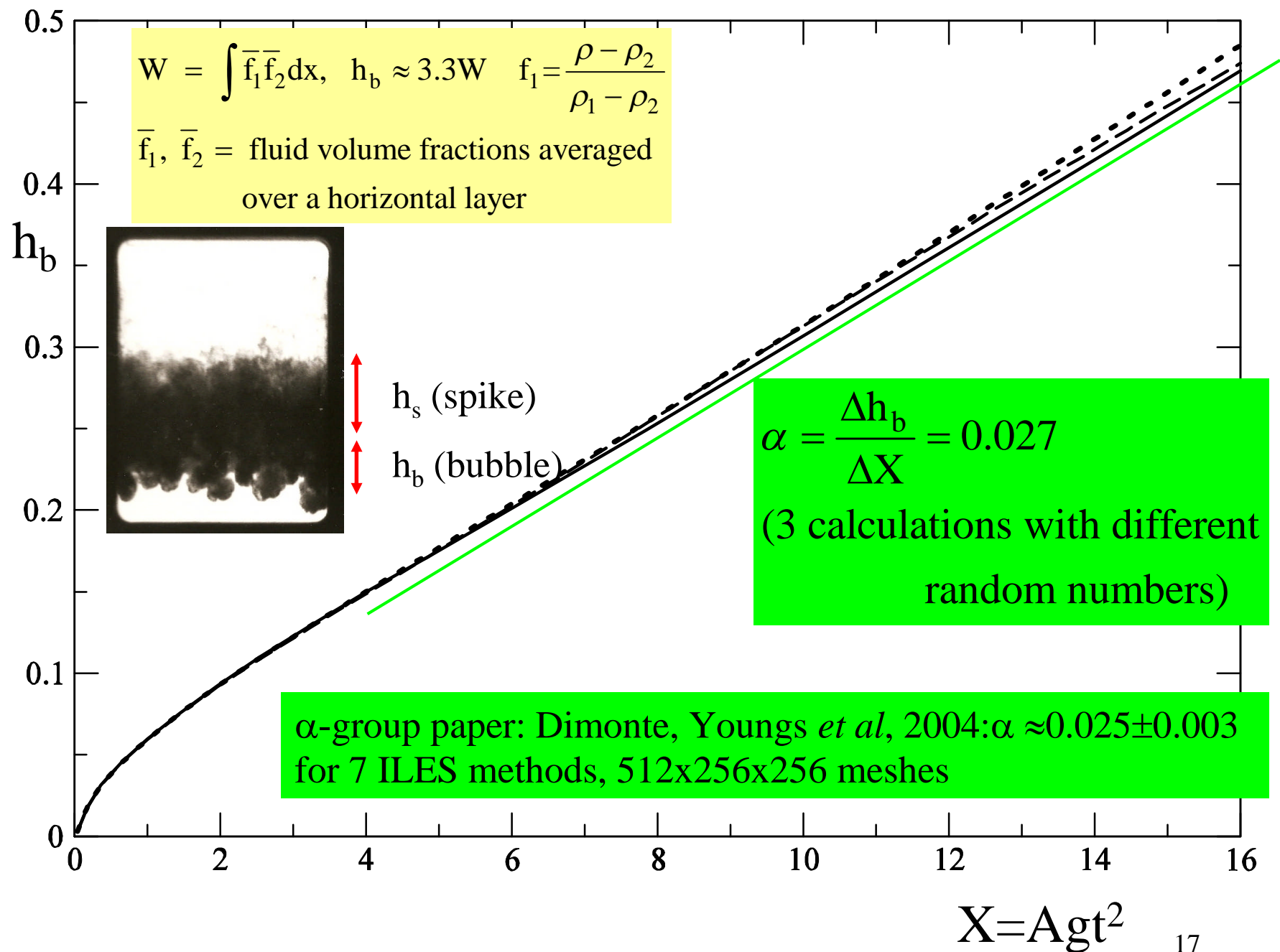
$t = 2.0$



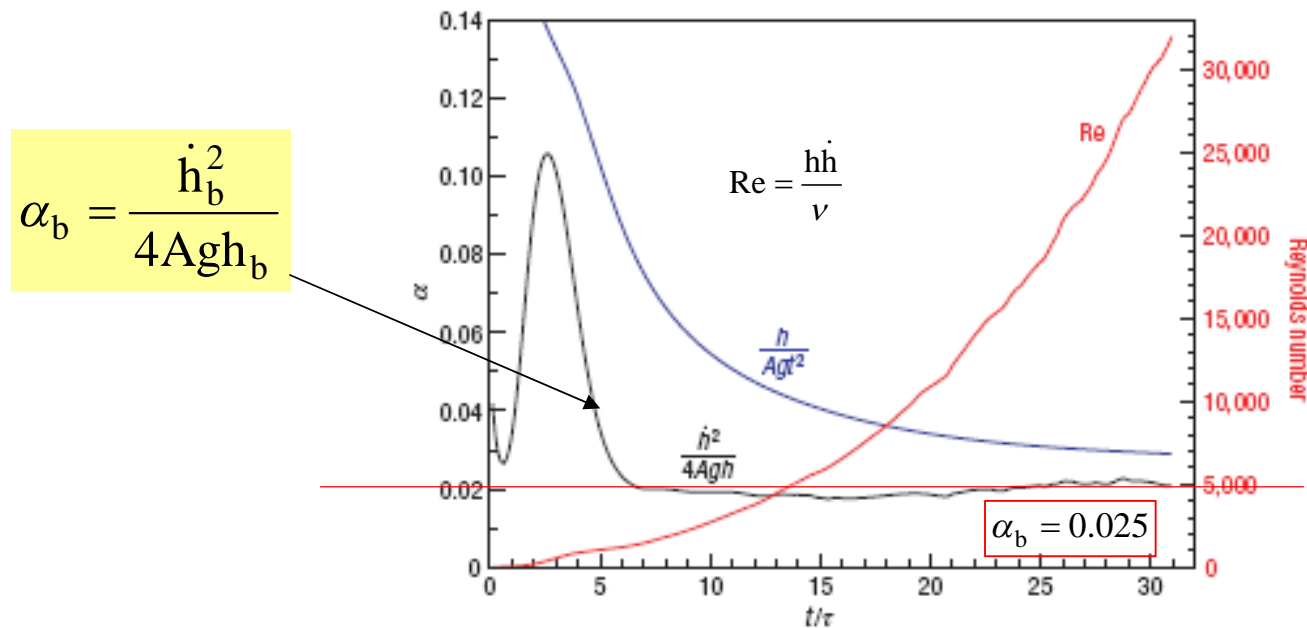
$t = 3.8$

Calculation performed on the AWE Cray XT3 (8000 processing elements). For these calculations: 360 processors for 24 hours

(repeat of calculation described in Youngs(2007) – in Grinstein et al. ILES book)



Cabot & Cook, LLNL, 2006: 3072³ DNS



DNS suggests that α may increase slowly with $Re \Rightarrow$ some uncertainty in high Re limit.

\Rightarrow need to repeat the TURMOIL simulations with as high a resolution as possible to be sure that the self-similar limit is reached.

For the ideal situation of “small random perturbations” a range of both LES and DNS results have all given values of α much less than observed \Rightarrow need to assume that in experiments low levels of initial long wavelength perturbations have enhanced mixing.

A model for enhanced self-similar growth was proposed by Inogamov(1999):

Long wavelength initial perturbations with amplitude \propto wavelength, up to size of experiment.

Note similarity to Birkhoff's argument

In mathematical terms

s.d of surface = σ , where $\sigma^2 = \int P(k)dk$ with $P(k) \sim 1/k^3$

have used here: wavelengths up to $\lambda_{\max} = \frac{1}{2}$ box width

and $\sigma = \varepsilon \times \lambda_{\max}$ (ε = a very small value)

used previously in Youngs (2003, 2007)

long wavelength perturbations,

$$\varepsilon=0.0005 \quad \alpha = \frac{\Delta h_b}{\Delta X} = 0.056$$

0.4

h_b

0.3

0.2

0.1

0

0

2

4

6

8

10

12

14

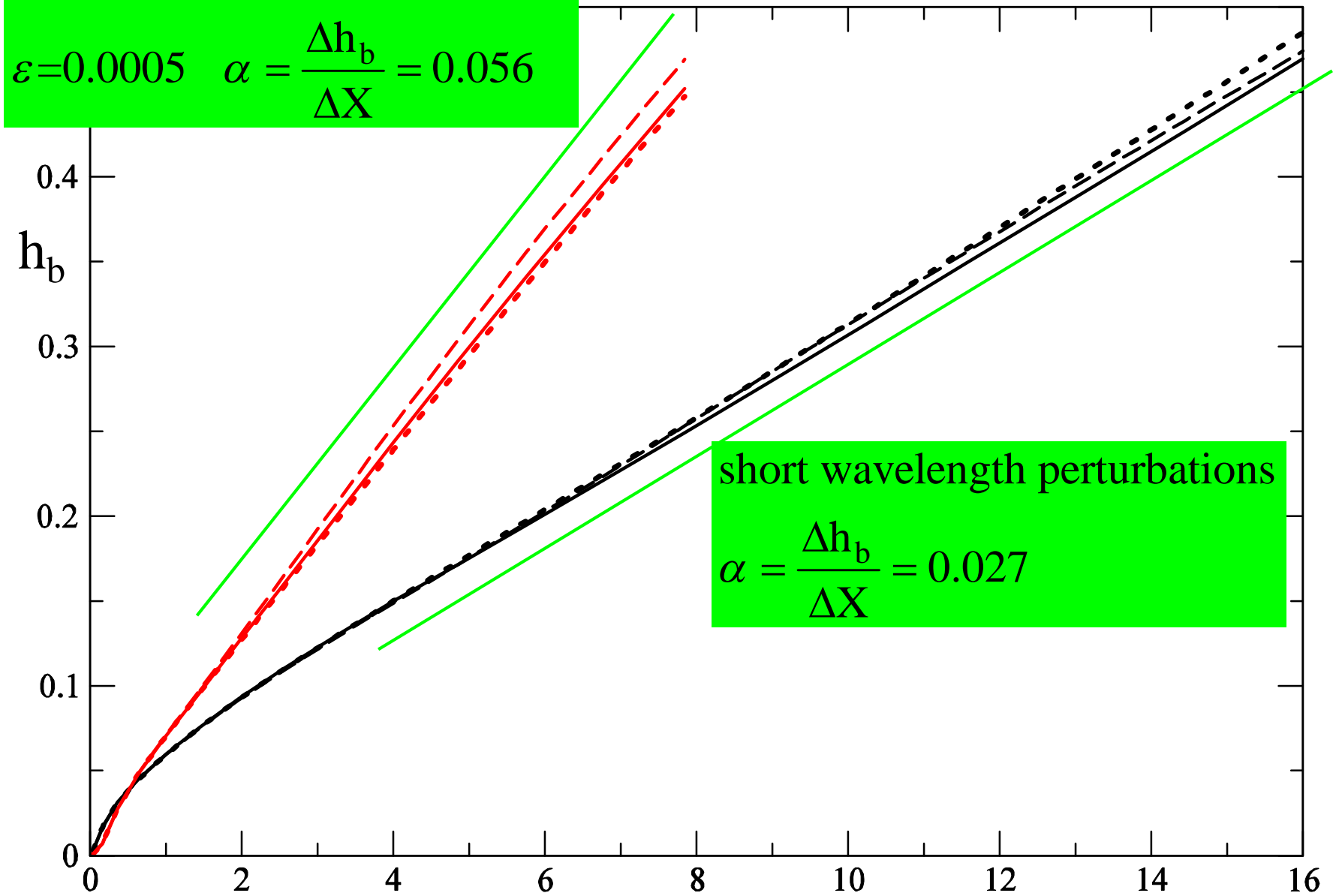
16

$X=Agt^2$

20

short wavelength perturbations

$$\alpha = \frac{\Delta h_b}{\Delta X} = 0.027$$



The current series of high-resolution TURMOIL simulations (in progress)

$\frac{\rho_1}{\rho_2} = 1.5$ 630 x 600 x 600, 1050 x 1000 x 1000 meshes

$\frac{\rho_1}{\rho_2} = 3.0$ 720 x 600 x 600*, 1200 x 1000 x 1000 meshes

1904 x 1600 x 1600 meshes (1 calculation planned)

$\frac{\rho_1}{\rho_2} = 20.0$ 930 x 600 x 600, 1550 x 1000 x 1000 meshes

Initial perturbations: (A) short wavelength perturbations only

$\lambda = 4\Delta x$ to $8\Delta x$, growth by mode coupling

(B) enhanced self-similar mixing, k^{-3} spectrum

(C) some calculations with spectra more typical
of experimental situations

* resolution used previously, Youngs(2007)

Results obtained from the simulations: key results needed for engineering model calibration.

Planar averages (as functions of x) of fluid volume fractions, $\overline{f_r}$,
 molecular mixing parameter, $\theta = \frac{\overline{f_1 f_2}}{\overline{f_1} \overline{f_2}}$
 turbulence KE, k

Different ways of defining k:

Single-fluid k: $k_1 = \frac{\overline{\frac{1}{2} \rho (\mathbf{u} - \tilde{\mathbf{u}})^2}}{\bar{\rho}}$ where $\tilde{\mathbf{u}} = \frac{\overline{\rho \mathbf{u}}}{\bar{\rho}}$

Two – fluid k: $k_2 = \frac{\overline{\frac{1}{2} \rho \mathbf{u}^2}}{\bar{\rho}} - \frac{1}{2} m_1 \tilde{\mathbf{u}}_1^2 - \frac{1}{2} m_2 \tilde{\mathbf{u}}_2^2$

(m_r = mass fraction)

Integral quantities

Bubble and spike distances, h_b and h_s , distances from the initial interface to the points where $\bar{f}_1=0.99$ and $\bar{f}_2=0.99$

Integral mix width, $W = \int \bar{f}_1 \bar{f}_2 dx$ - insensitive to statistical fluctuations.

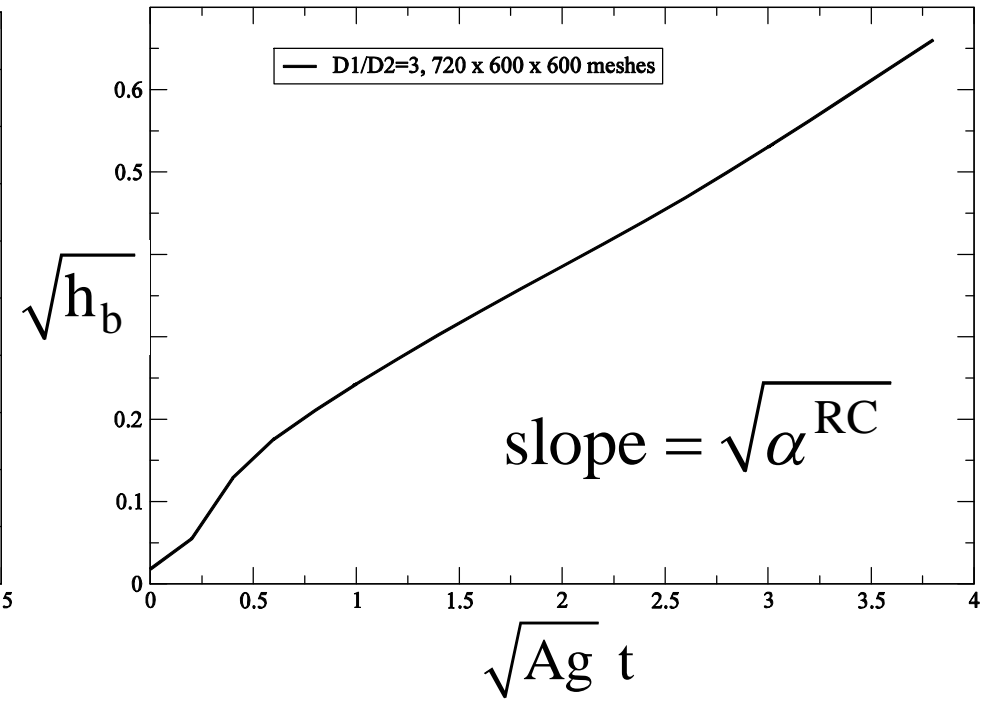
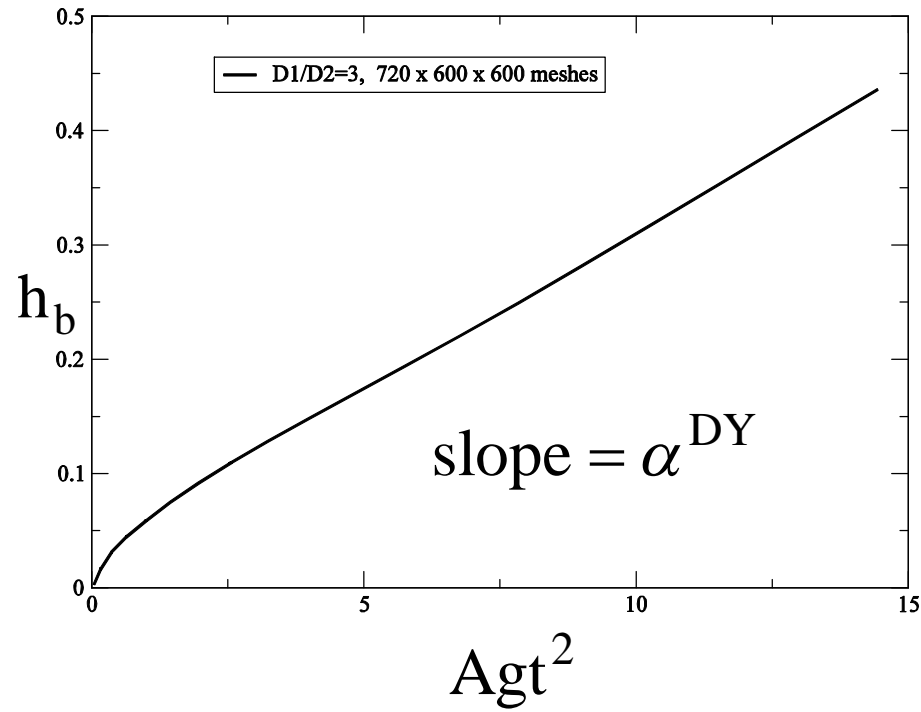
\Rightarrow alternative measure of bubble distance $h_b = \beta W$ ($\beta \sim 3$, estimated from the volume fraction profile) is used to calculate α_b as a function of time;

$$\alpha_b^{DY} = \frac{dh_b}{dX} \text{ (Dimonte, Youngs...2004)} \quad X = Agt^2$$

$$\alpha_b^{RC} = \frac{\dot{h}_b^2}{4Agh_b} \text{ (Ristorcelli \& Clark(2004), Cabot \& Cook(2006))}$$

Also calculate global molecular mixing parameter, $\Theta = \frac{\int \overline{f_1 f_2} dx}{\int \bar{f}_1 \bar{f}_2 dx}$,

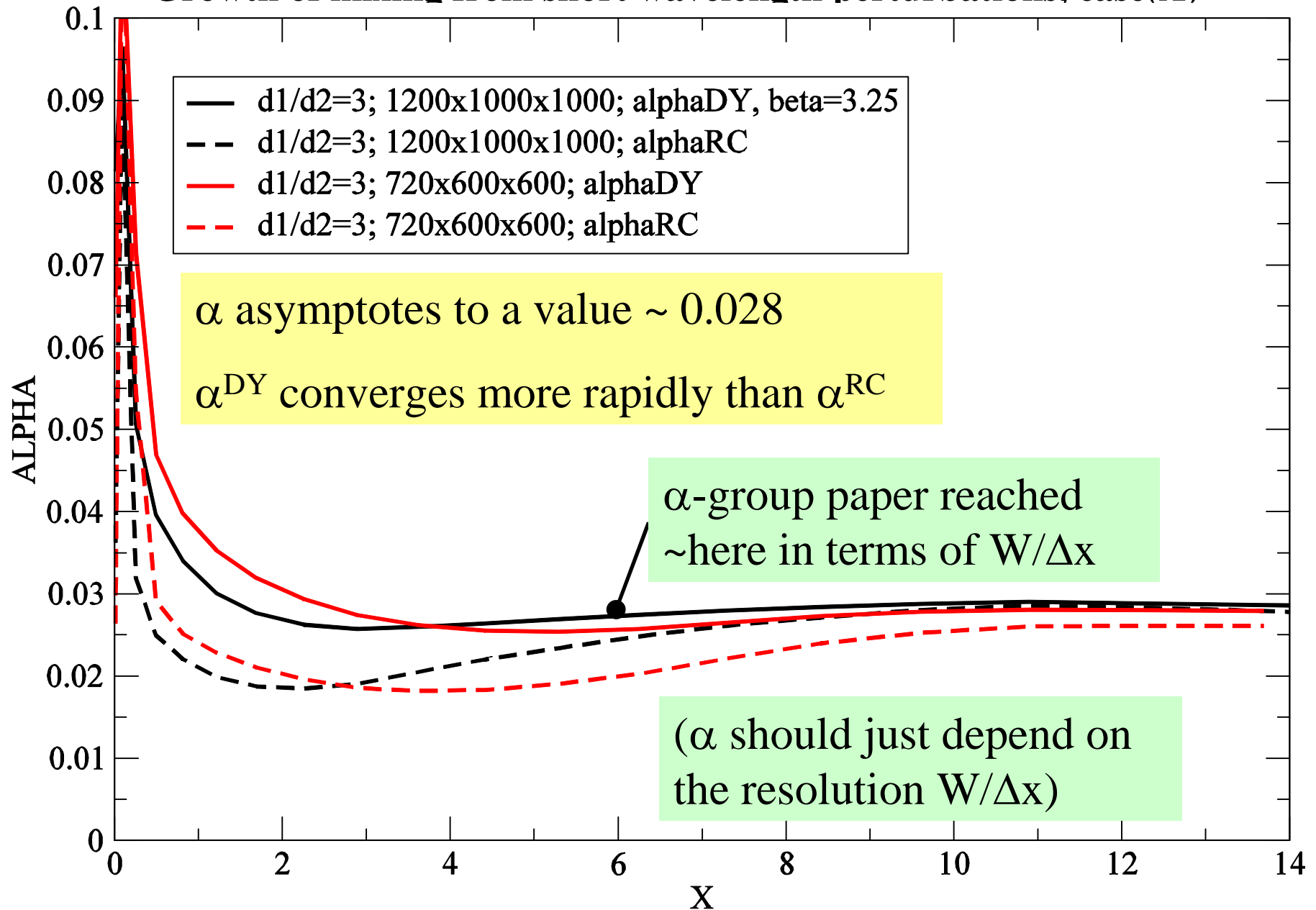
total KE (K), total loss of PE (P), and total sub-grid-scale dissipation (D) - giving $P=K+D$



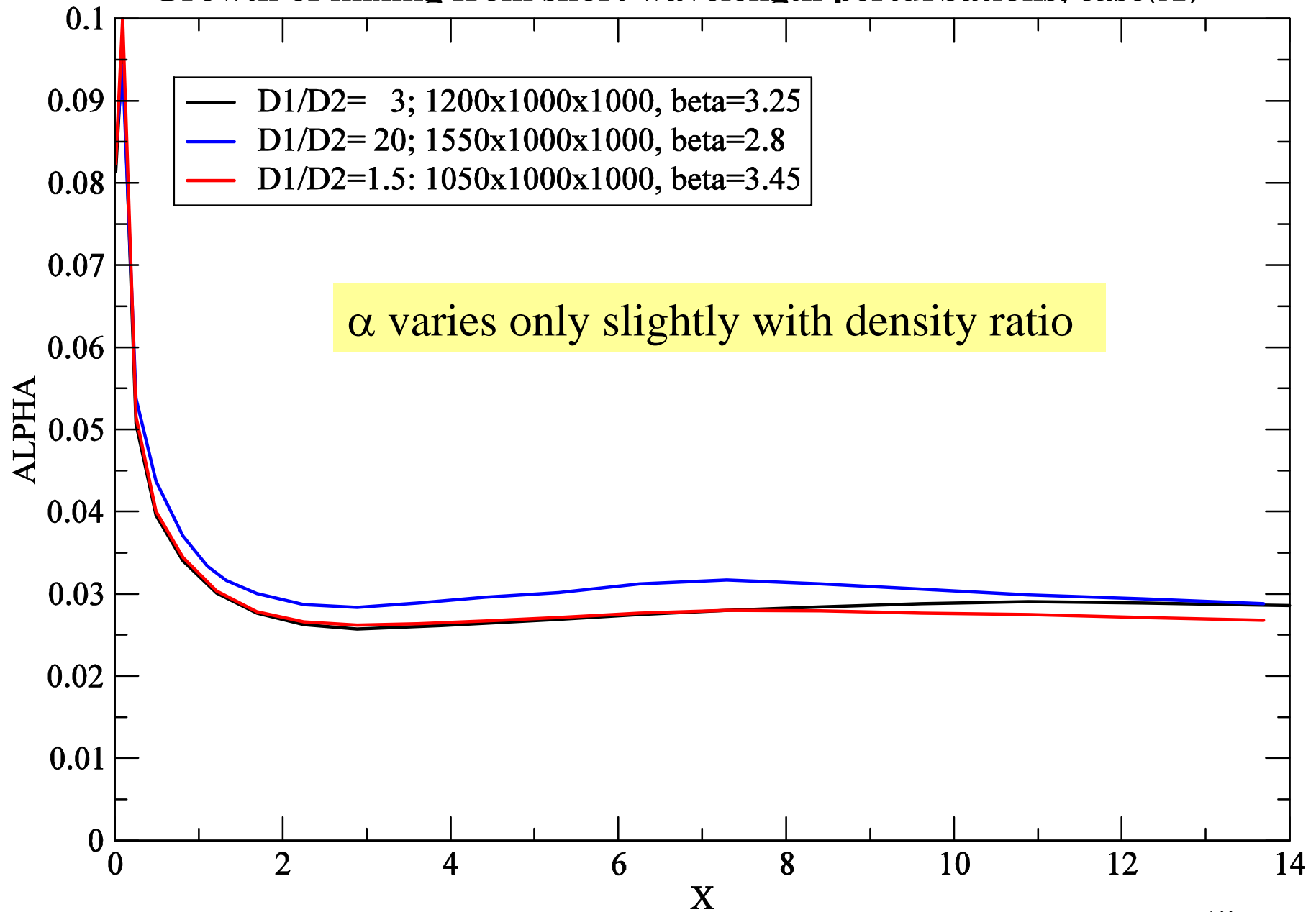
$$v_b = \dot{h}_b = Fr \sqrt{Agh_b}$$

$$\alpha^{\text{RC}} = \frac{Fr^2}{4}$$

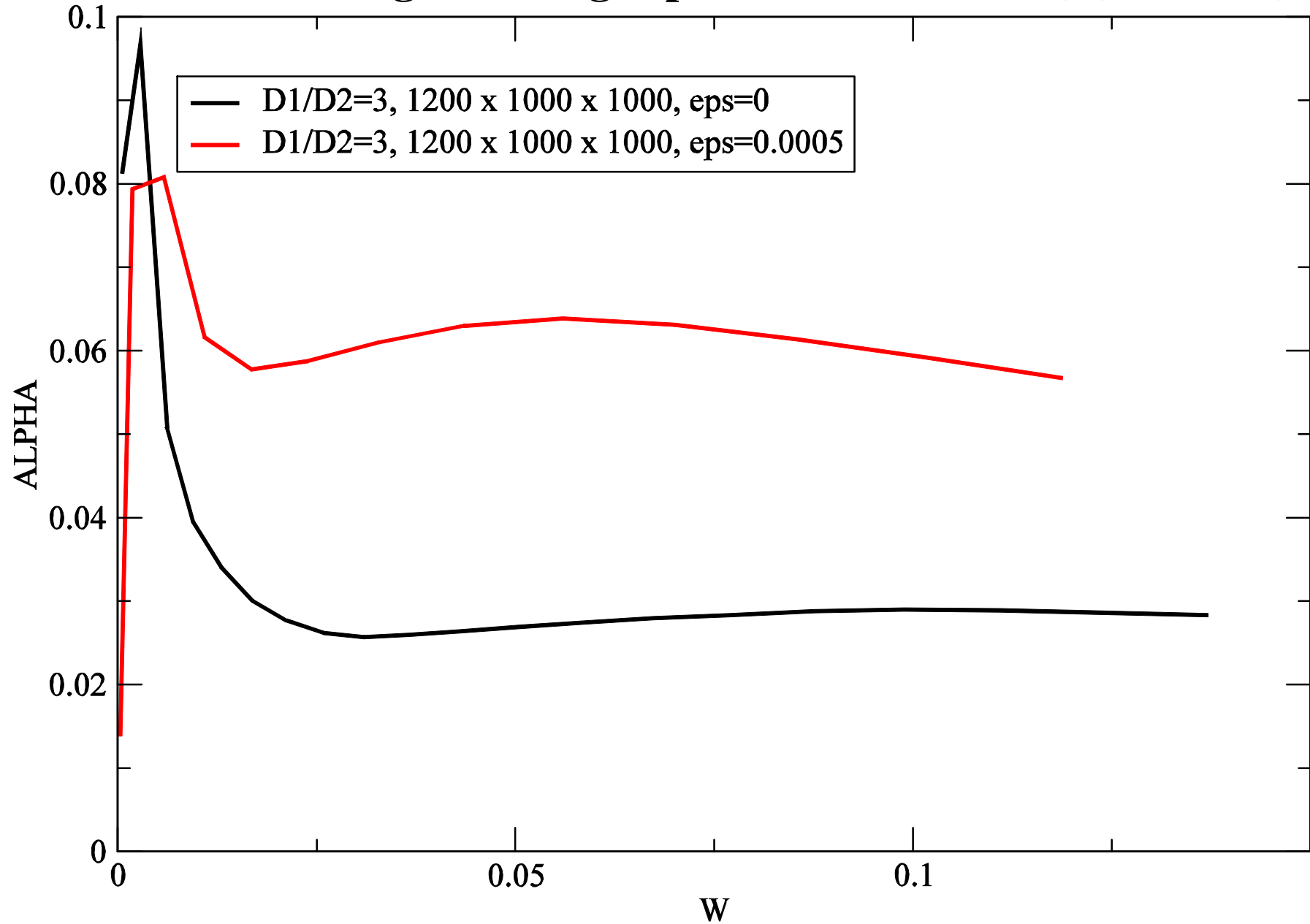
Growth of mixing from short wavelength perturbations, case(A)



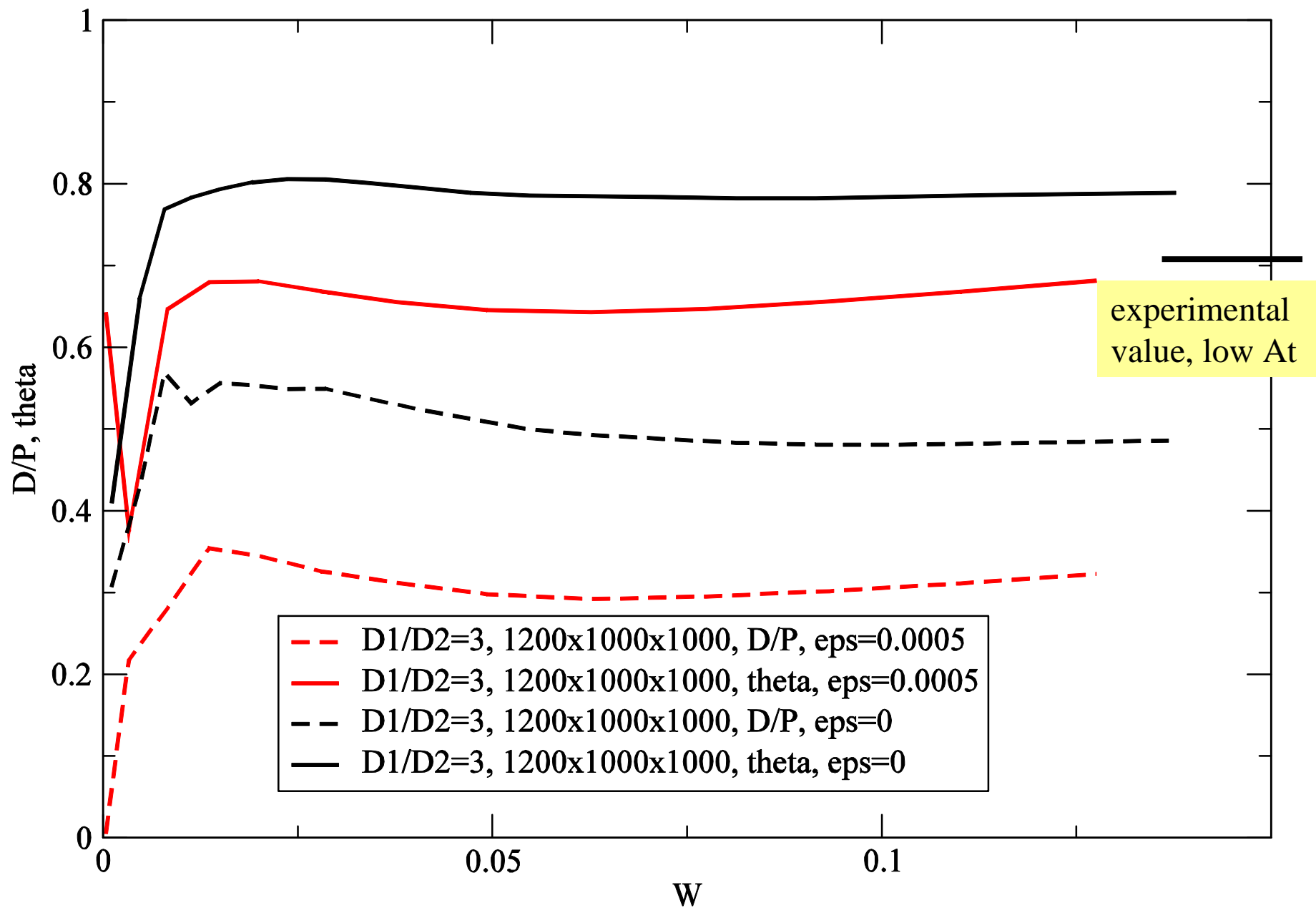
Growth of mixing from short wavelength perturbations, case(A)



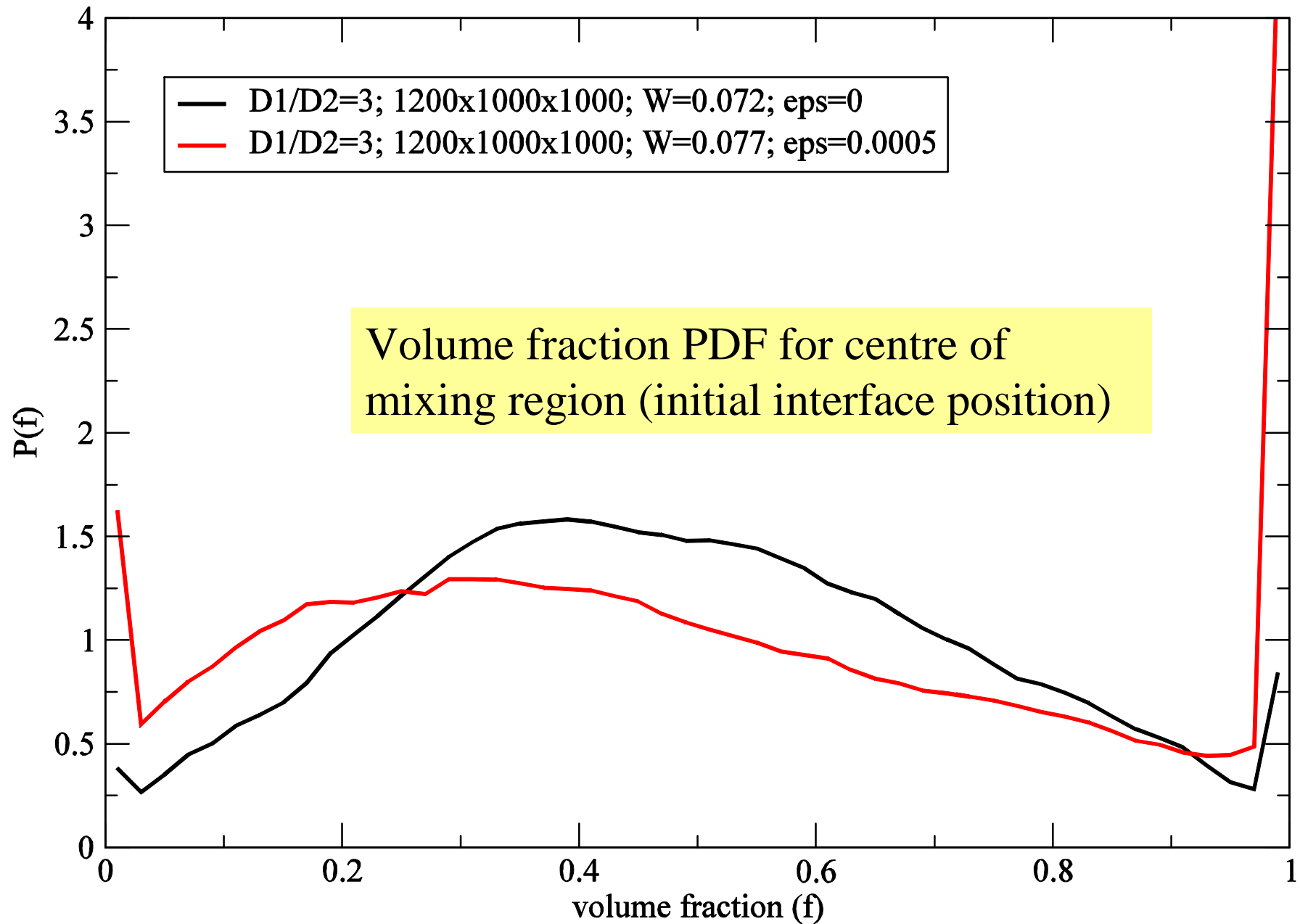
Influence of long wavelength perturbations: case(A) vs case(B)

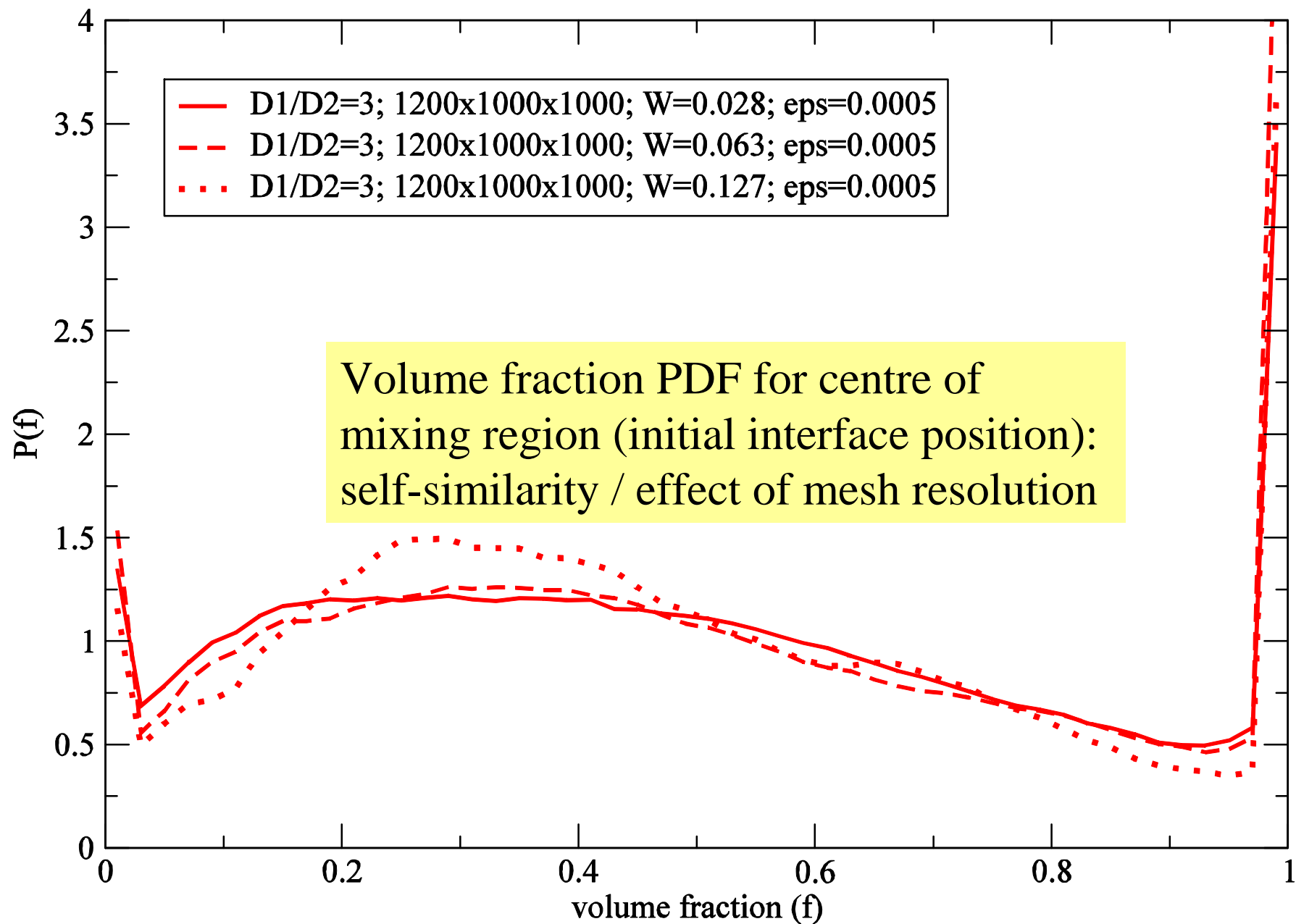


KE dissipation and molecular mixing parameter (Θ), case (A) vs case(B)

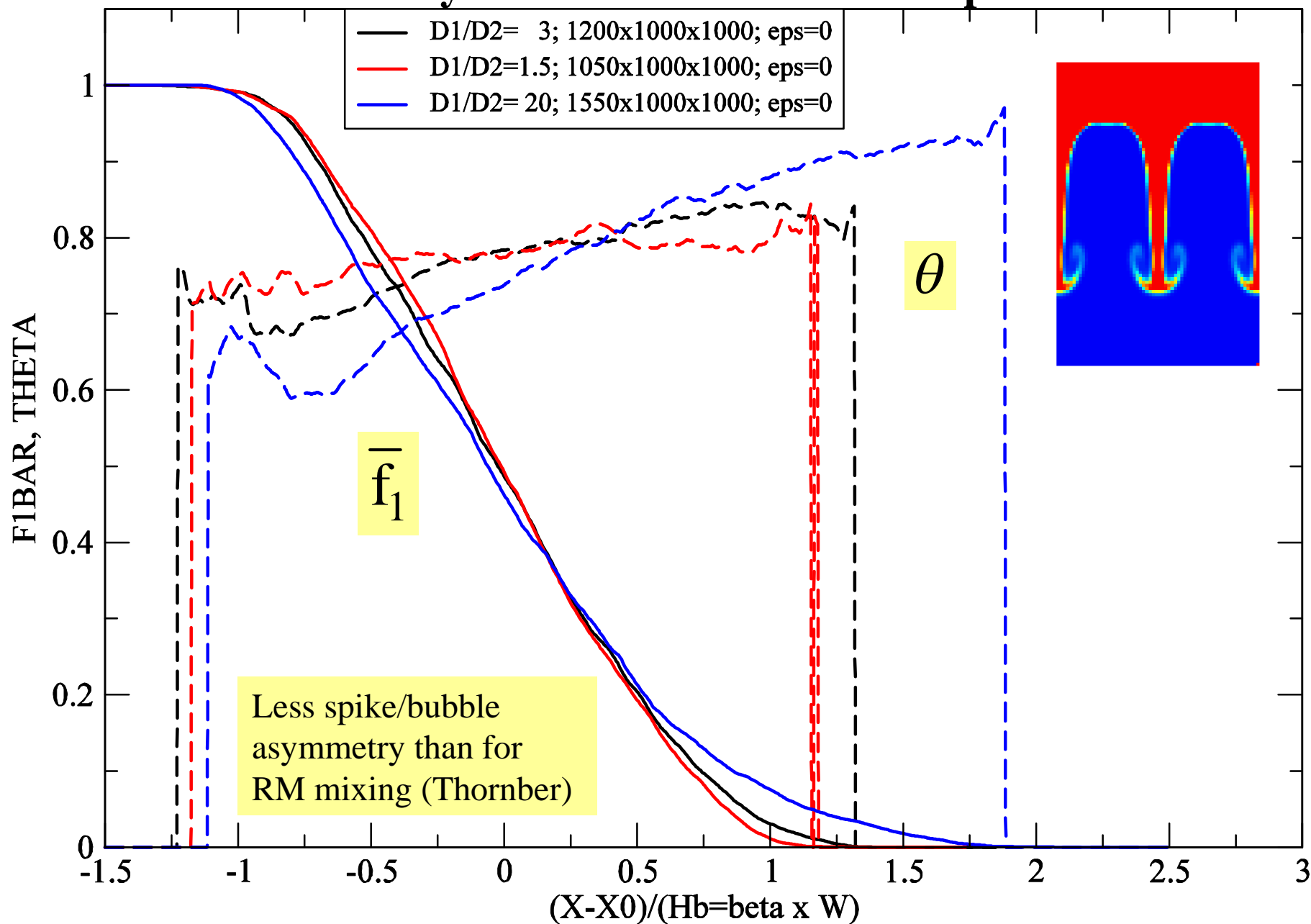


case(A) vs case(B), $\rho_1/\rho_2 = 3$

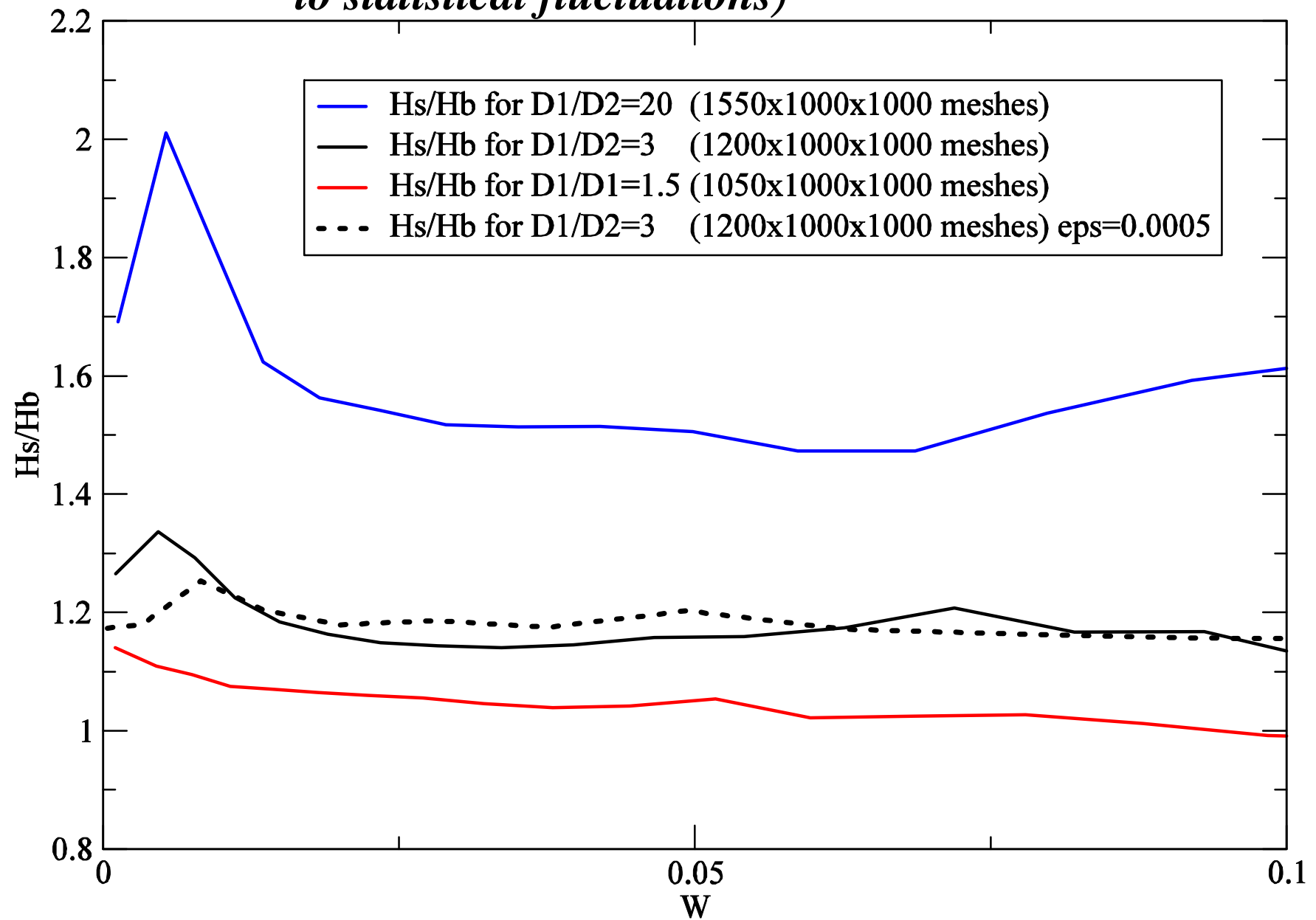


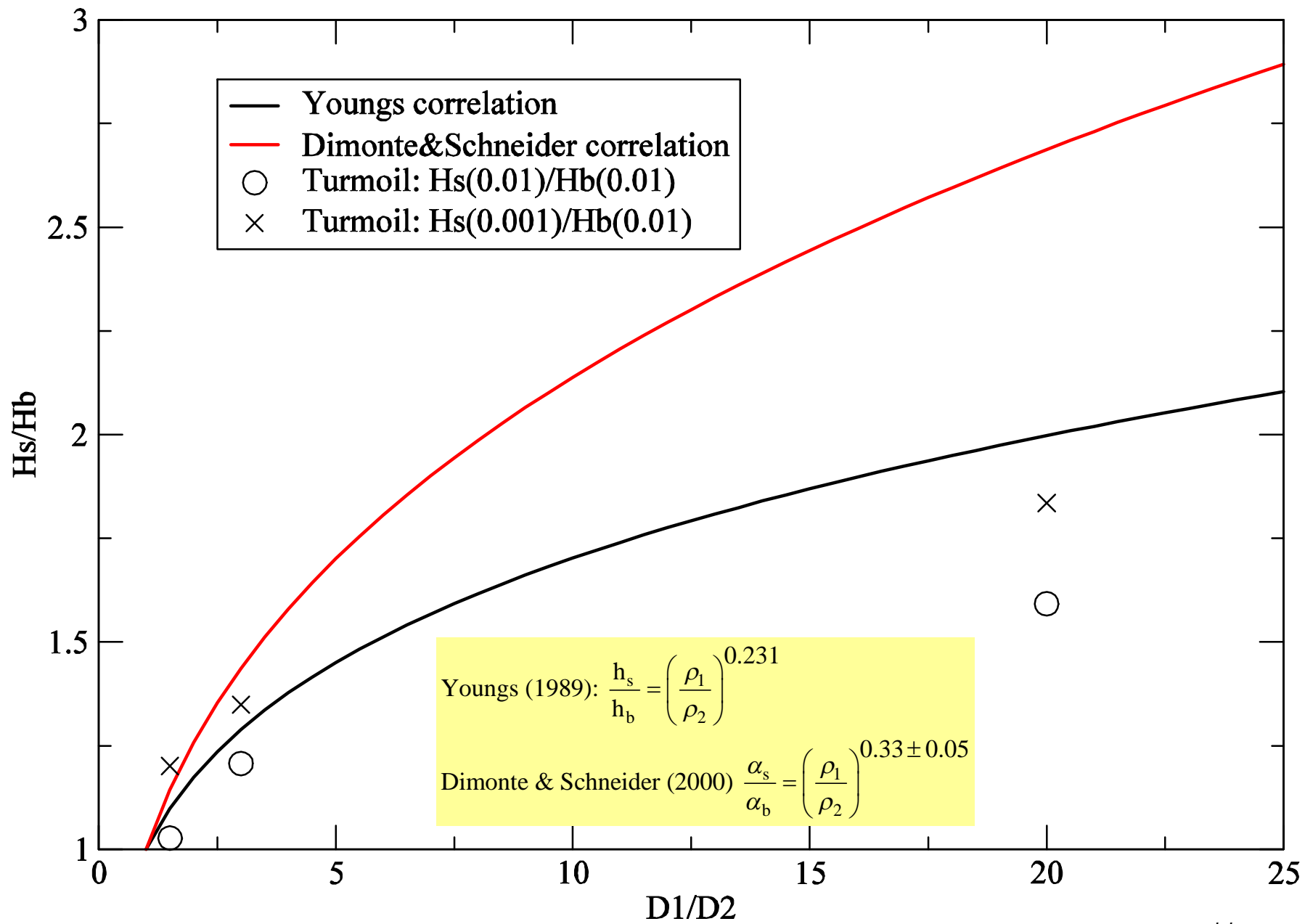


Effect of density ratio on volume fraction profiles

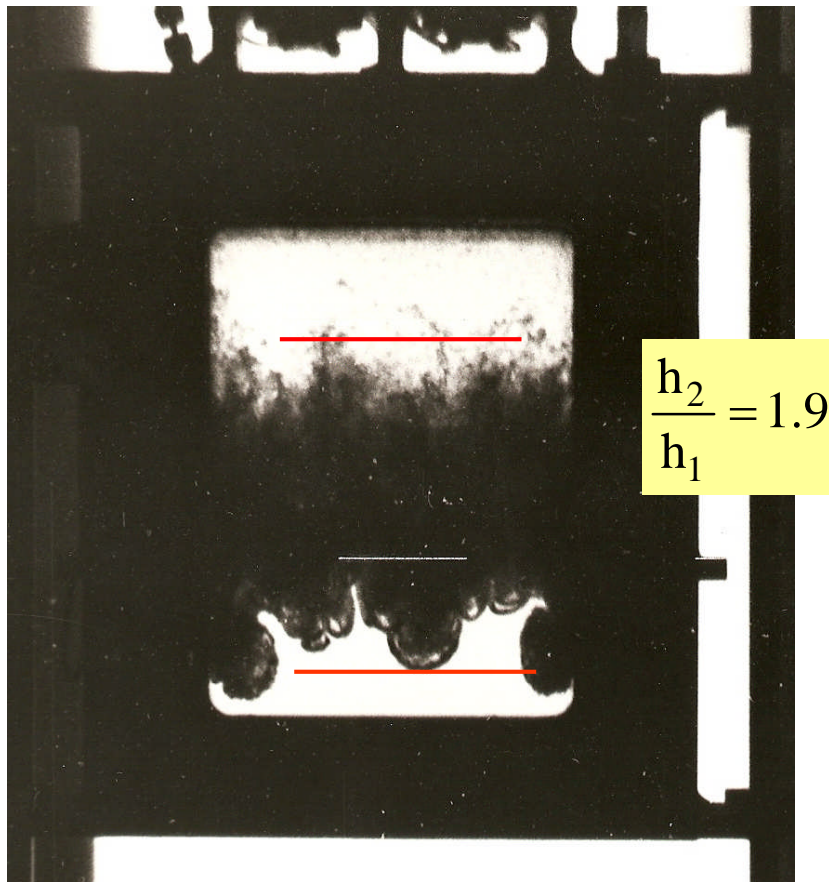


Spike/Bubble ratio, (*very susceptible to statistical fluctuations*)





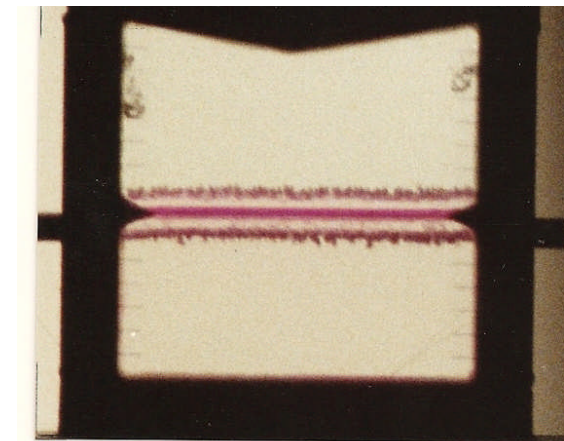
pentane / SF_6 : $\frac{\rho_1}{\rho_2} = 18.4$



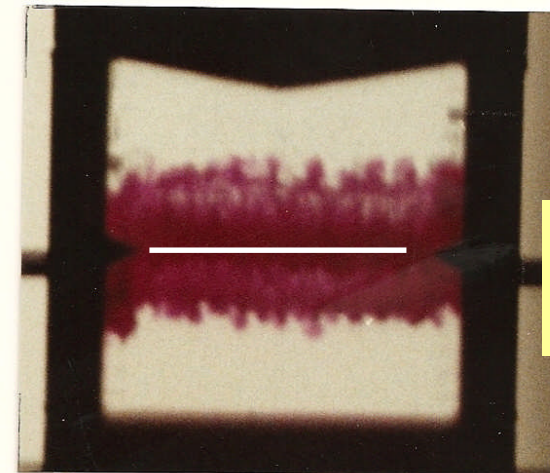
$$\frac{h_2}{h_1} = 1.96 \text{ (Rocket-Rig correlation)}$$

$$= 2.61 \text{ (LEM correlation)}$$

NaI solution / water : $\frac{\rho_1}{\rho_2} = 1.89$, "2D" tank



(b) $t = 42.3 \text{ ms}$, $X = 203 \text{ mm}$

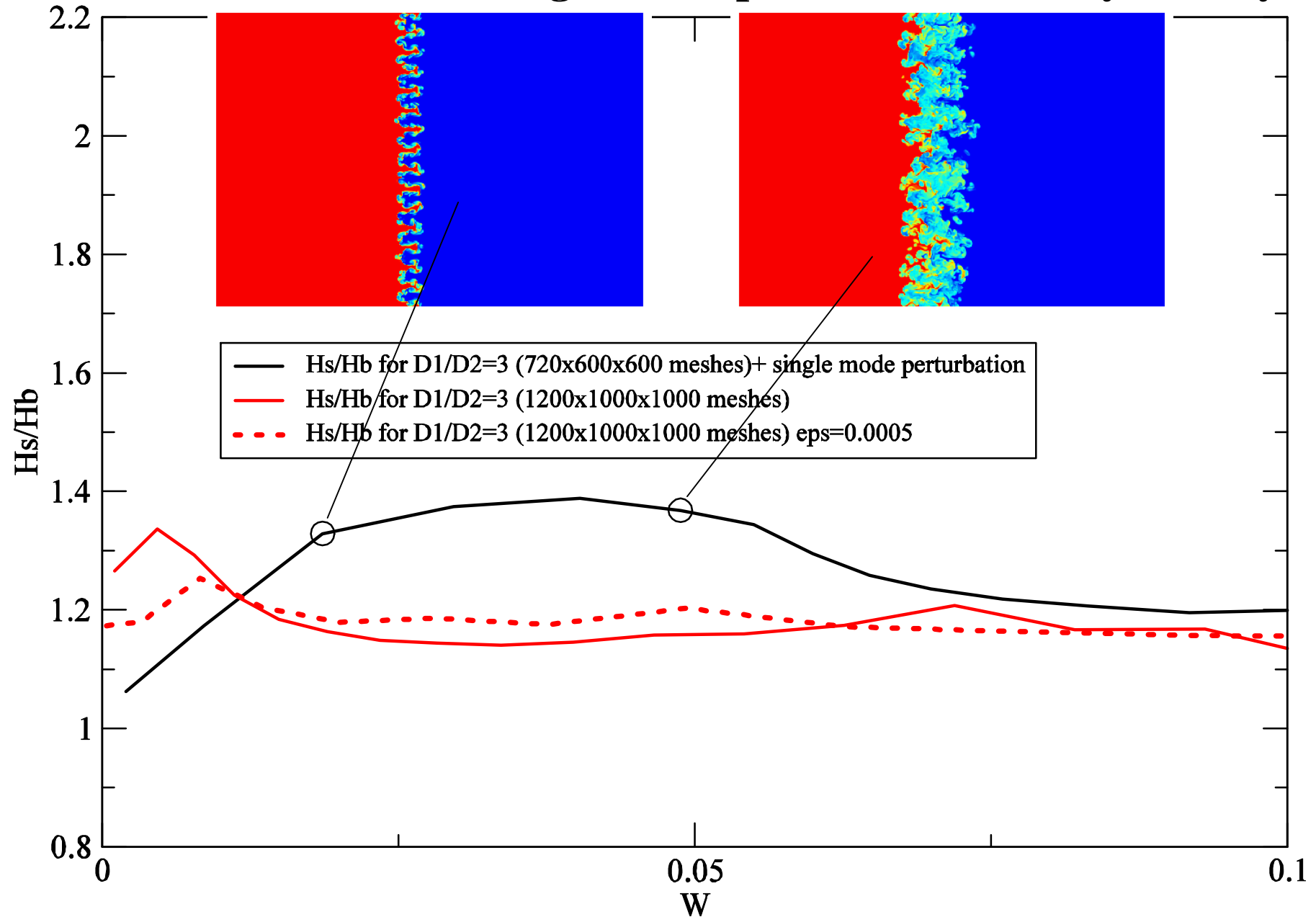


(f) $t = 78.7 \text{ ms}$, $X = 725 \text{ mm}$

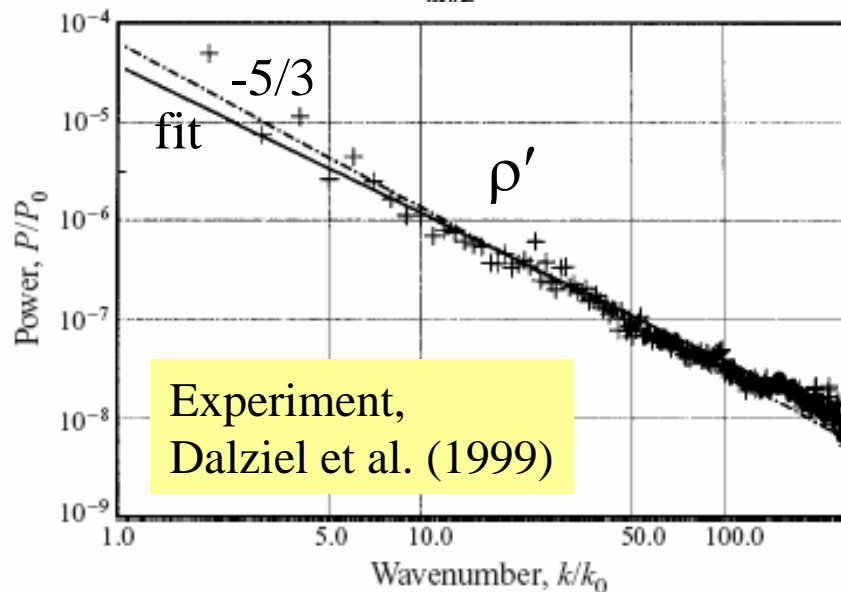
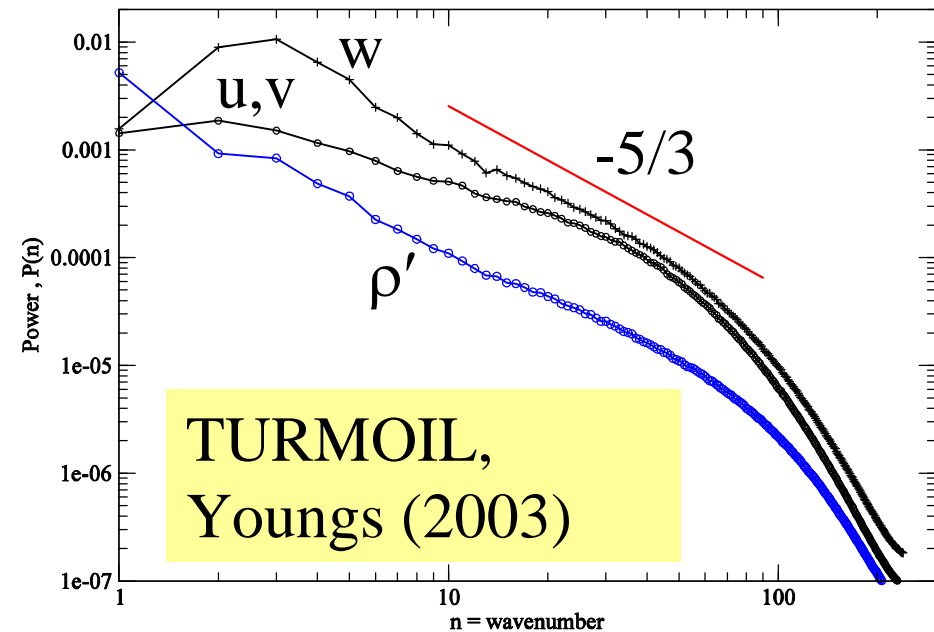
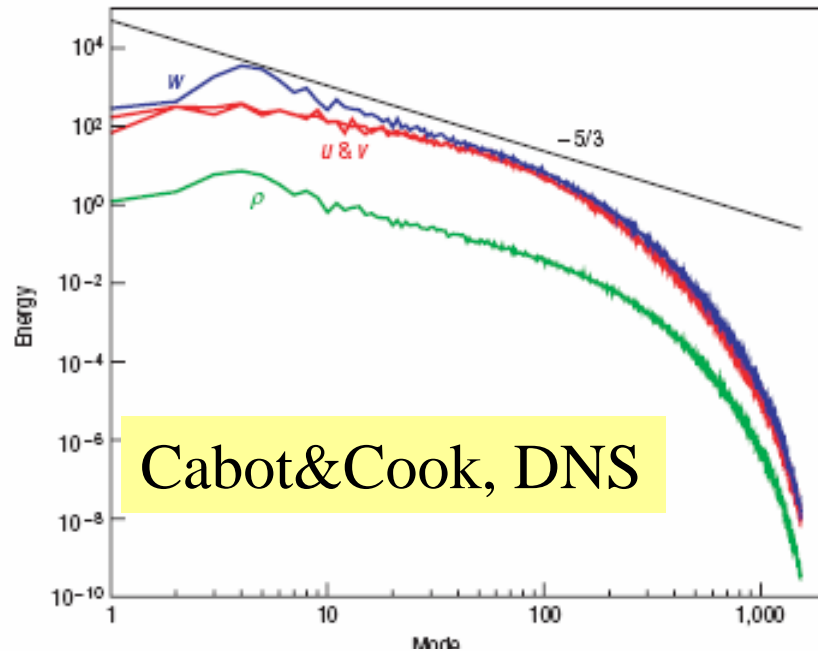
$$\frac{h_2}{h_1} = 1.16 \text{ (Rocket-Rig correlation)}$$

$$= 1.23 \text{ (LEM correlation)}$$

Effect of additional single mode perturbation on asymmetry



Power spectra: w (vertical velocity), u & v (horizontal velocity) and ρ (density)



DNS and ILES show similar behaviour for velocity spectra at low wavenumber.

DNS/ILES/Experiment all show spectra for ρ' slightly flatter than $k^{-5/3}$

Important Implications for Engineering Modelling

The results suggest that low levels of long-wavelength initial perturbations are the most probable explanation of the higher observed growth rates.

Experiments are finite:

The basic problem is not mixing at an infinite plane boundary with finite s.d. (this should asymptote to $\alpha \sim 0.03$) but mixing in a finite domain of size L , with low levels of perturbations with wavelengths up to size L . Then expect influence of initial conditions to persist throughout the duration of the experiment.

Similar conclusion apply to turbulent shear flows (influence of upstream conditions) – W.K.George, Freeman Scholar Lecture , ASME Fluids Engineering Meeting, 2008.

RANS models

one-point closure models e.g. (k, ϵ) model

Given set of model coefficients \Rightarrow a given value of α - does not capture dependence on initial conditions.

Solution adopted here

- Note that , for a given experimental series, assuming $\alpha = \text{const.}$, works quite well (“logarithmic” dependence on initial conditions)
- Derive model coefficient sets for a range of values of α , using 3D LES results for enhanced self-similar mixing (Inogamov)
- Use LES for simplified versions of the real problems, with estimates of realistic initial conditions, to estimate the appropriate $\alpha_{\text{effective}}$ for a given application.

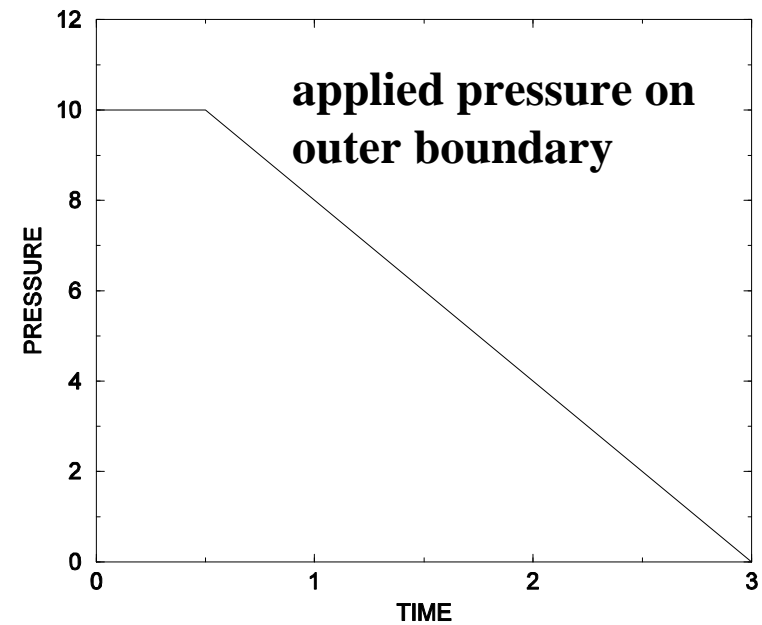
A simple spherical implosion (dimensionless units) – relevant to Inertial Confinement Fusion

Perturbation spectrum, $P(k) \sim \frac{1}{k^2}$, s.d.=0.0005
max. wavelength = shell thickness

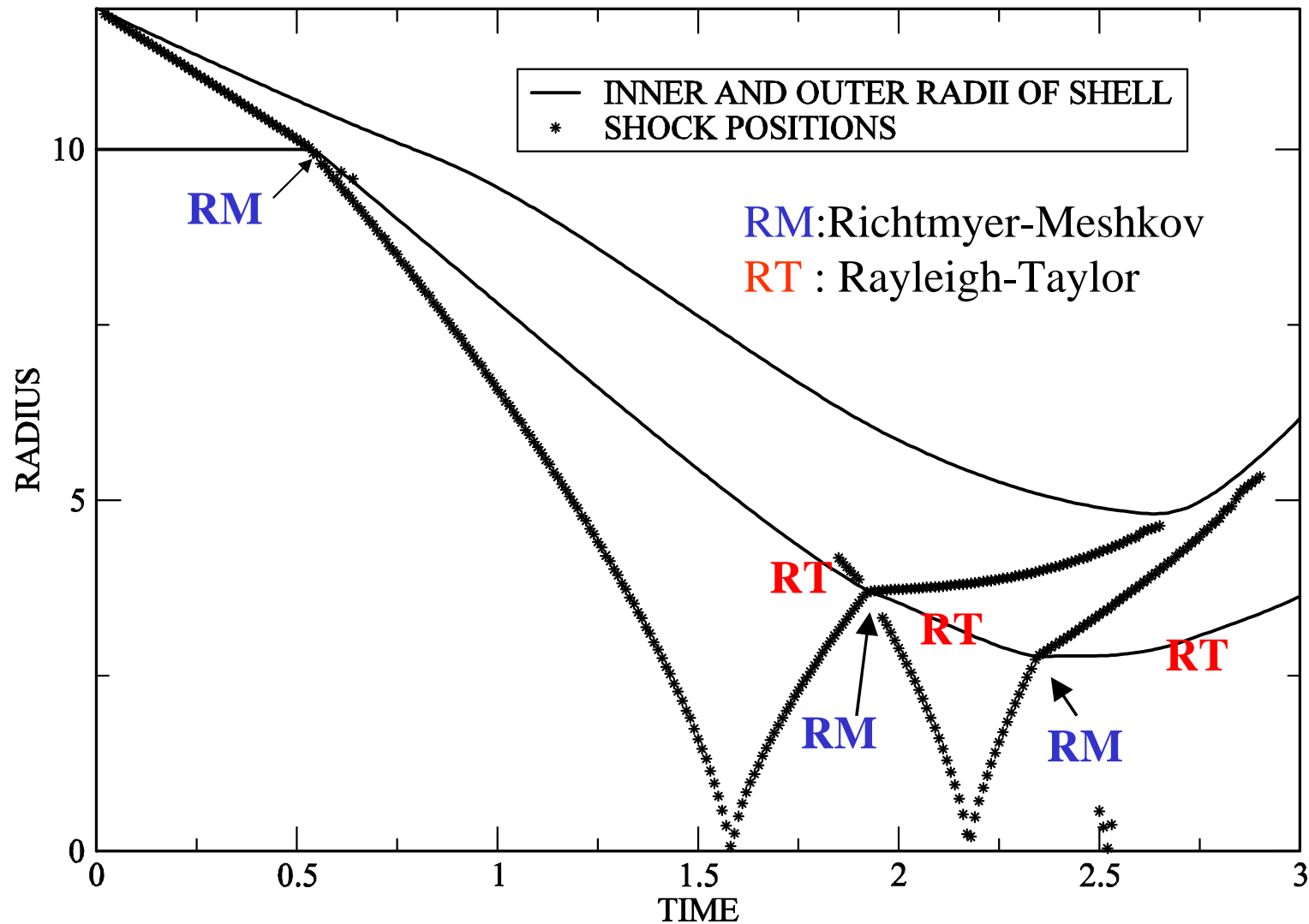
$\rho = 1.0$ $p = 0.1$
Outer radius = 12

$\rho = 0.05$, $p = 0.1$
Outer radius= 10

Perfect gas equations of
state $\gamma = 5/3$

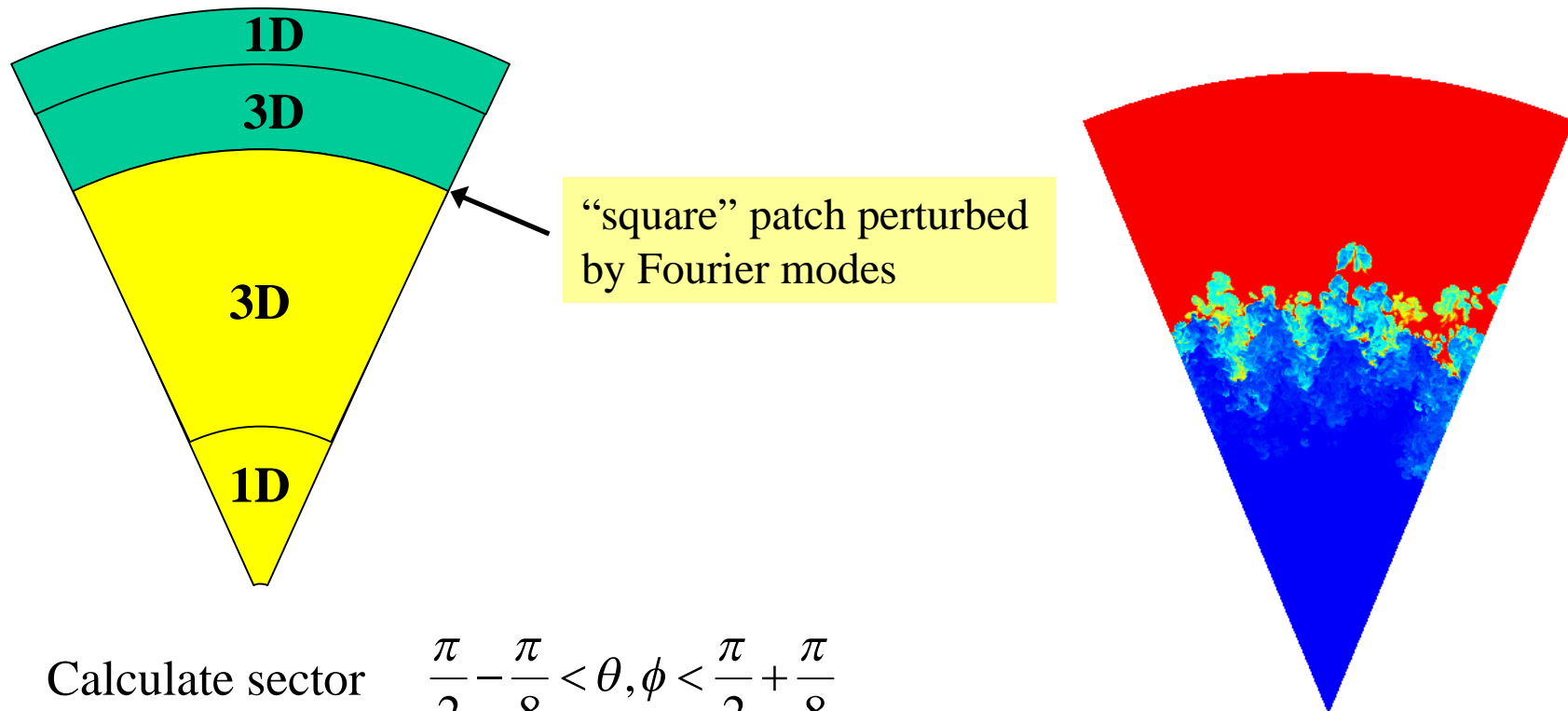


1D Lagrangian calculation



Note influence of initial conditions more complex: initial spectrum
+amplification due to first shock + spherical convergence – set initial
perturbations for late stage mixing

3D SIMULATION THE SPHERICAL IMPLOSION



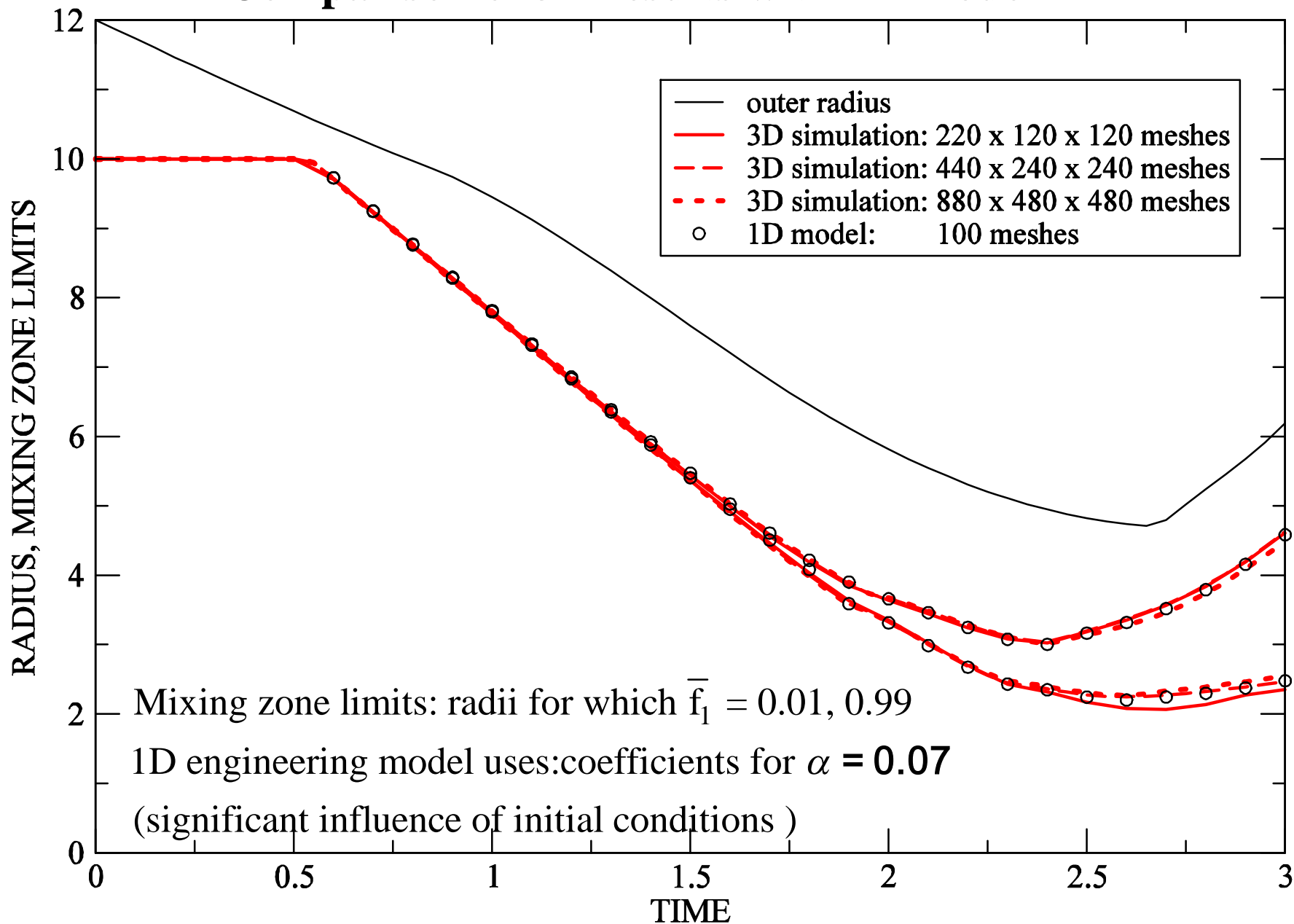
Calculate sector $\frac{\pi}{2} - \frac{\pi}{8} < \theta, \phi < \frac{\pi}{2} + \frac{\pi}{8}$

Spherical polar mesh, Lagrangian in r-direction,
1D Lagrangian regions at origin and at outer
boundary.

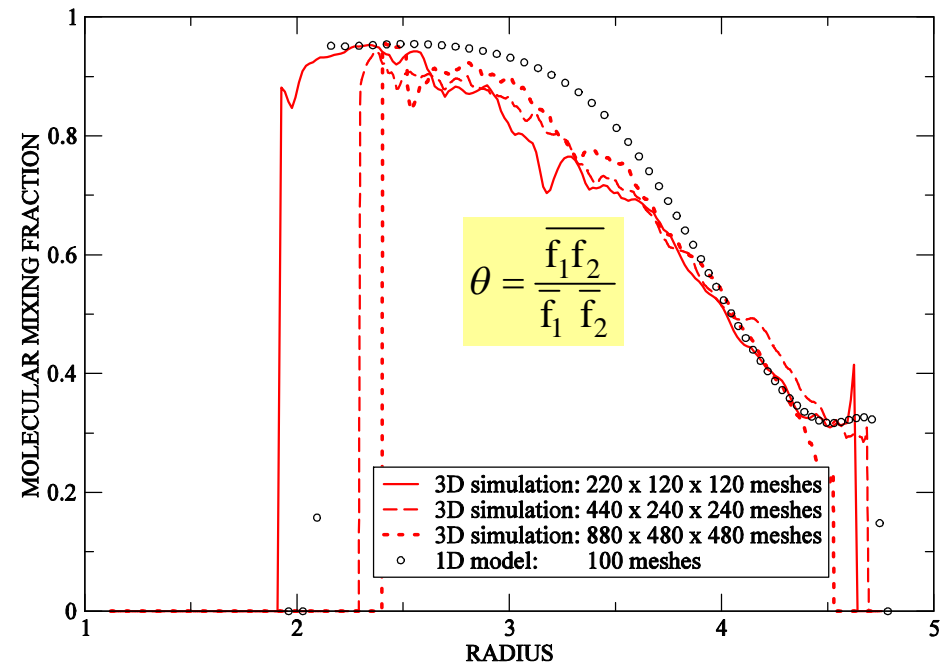
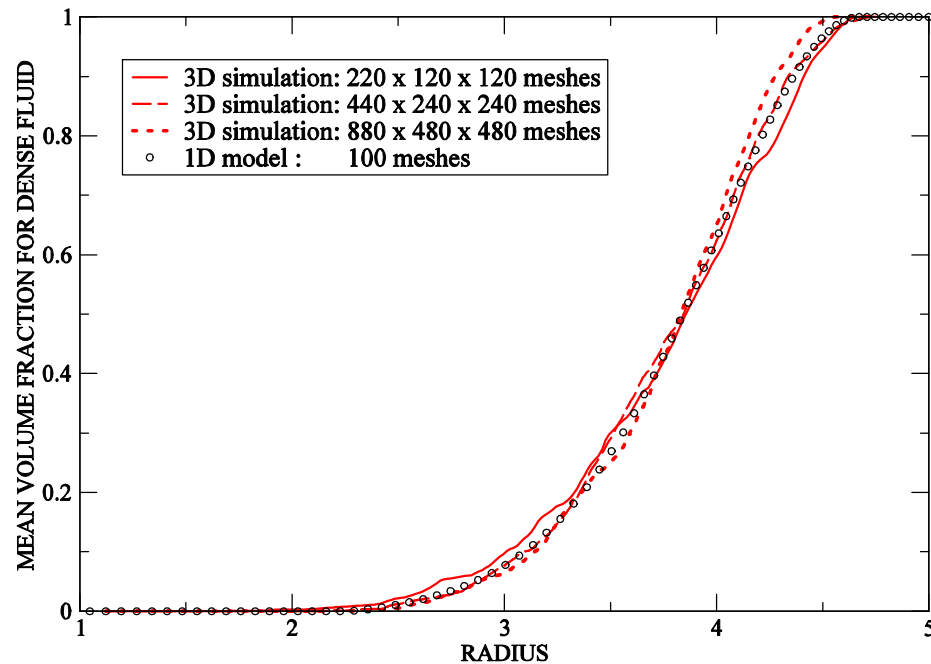
Perturbation spectrum $P(k) \sim k^{-2}$

Engineering model used here : multiphase flow equations
+turbulent diffusion terms + decay of concentration fluctuations
(a type of RANS model)

Comparison of 3D results with 1D model



Distributions at time=3



3D simulation for a simplified problem like this is used to “tune” the engineering model constants for a more complex application

CONCLUDING REMARKS

- A range of self-similar RT cases are currently being investigation using high-resolution MILES – enhanced growth due to long-wavelength perturbations and the effect of density ratio. The MILES approach should give accurate results for the high-Reynolds behaviour, using “modest” computer resources.
- The 3D simulations will provides much of the key data required for engineering model calibration.
- The influence of initial conditions is an extremely important issue. Needs to be allowed for both in the engineering modelling and comparison with experiment.

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