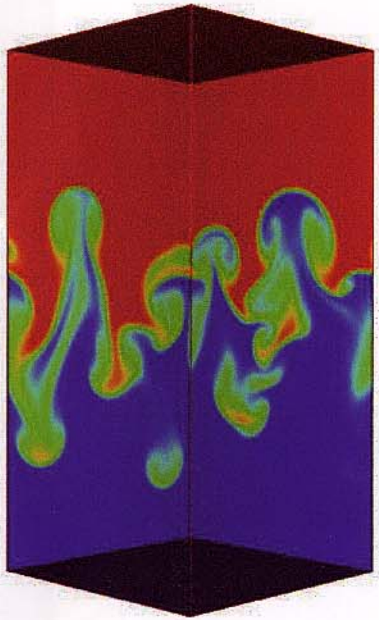
Transition Stages of Rayleigh-Taylor Instability between Miscible Fluids



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Overview

- Three 256x256x1024-point and one 512x512x2040-point Direct Numerical Simulations (DNS) were performed of Rayleigh-Taylor instability with different initial conditions.
- The smaller jobs executed on 128 CPU's of ASCI Blue-Pacific (IBM SP2) at LLNL. Simulation times varied from 200 to 300 machine hours.
- The larger job executed on 1024 CPU's and took roughly 50 machine days.
- Small and large simulations attained outer-scale Reynolds numbers of 3000 and 5500, respectively.
- **Mixing-zone growth exhibits an initial diffusion stage, followed by a nonlinear stage.**
- **Growth and mixing are sensitive to initial conditions for duration of simulations.**
- **For many statistics, height of mixing zone (h) is a better progress variable than time (t).**

Governing equations

$$\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = -\rho \frac{\partial u_j}{\partial x_j} = \frac{\rho}{\mathrm{Re}\, Sc} \frac{\partial}{\partial x_j}\left(\frac{1}{\rho}\frac{\partial \rho}{\partial x_j}\right)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\rho \delta_{i3}}{Fr^2}$$

$$\tau_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}$$

$$\frac{\partial \rho Y}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_j Y\right) = \frac{1}{\mathrm{Re}\, Sc} + \frac{\partial}{\partial x_j}\left(\rho \frac{\partial Y}{\partial x_j}\right)$$

$$X = \frac{\rho - \rho_1}{\rho_2 - \rho_1}$$

$$\rho Y = \rho_2 X$$

ρ = density

u_j = velocity vector

p = pressure

τ_{ij} = viscous stress tensor

Y = heavy fluid mass-fraction

X = heavy fluid mole-fraction

ρ_1 = density of light fluid

ρ_2 = density of heavy fluid

$\mathrm{Re} = \rho_1 l U / \mu = (2\pi l/N)^{-4/3}$

$Sc = \mu / \rho_1 D = 1$

$Fr = U/(gl)^{1/2} = 1$

N = number of x grid points

l = scaling length

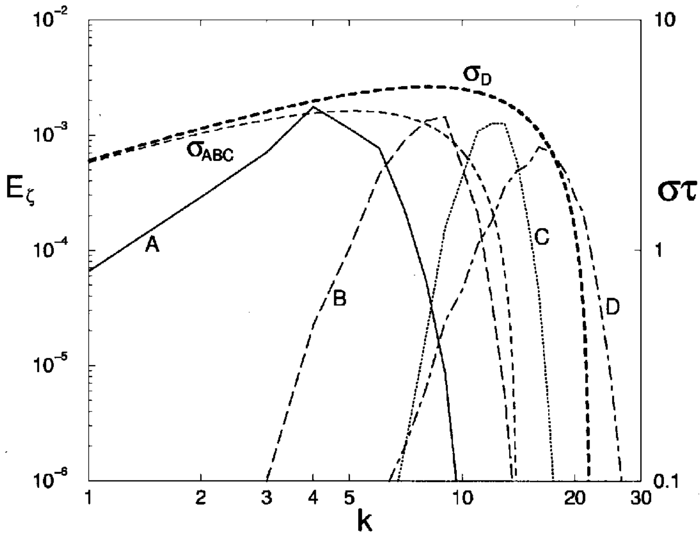
U = scaling velocity

g = acceleration

Numerical method

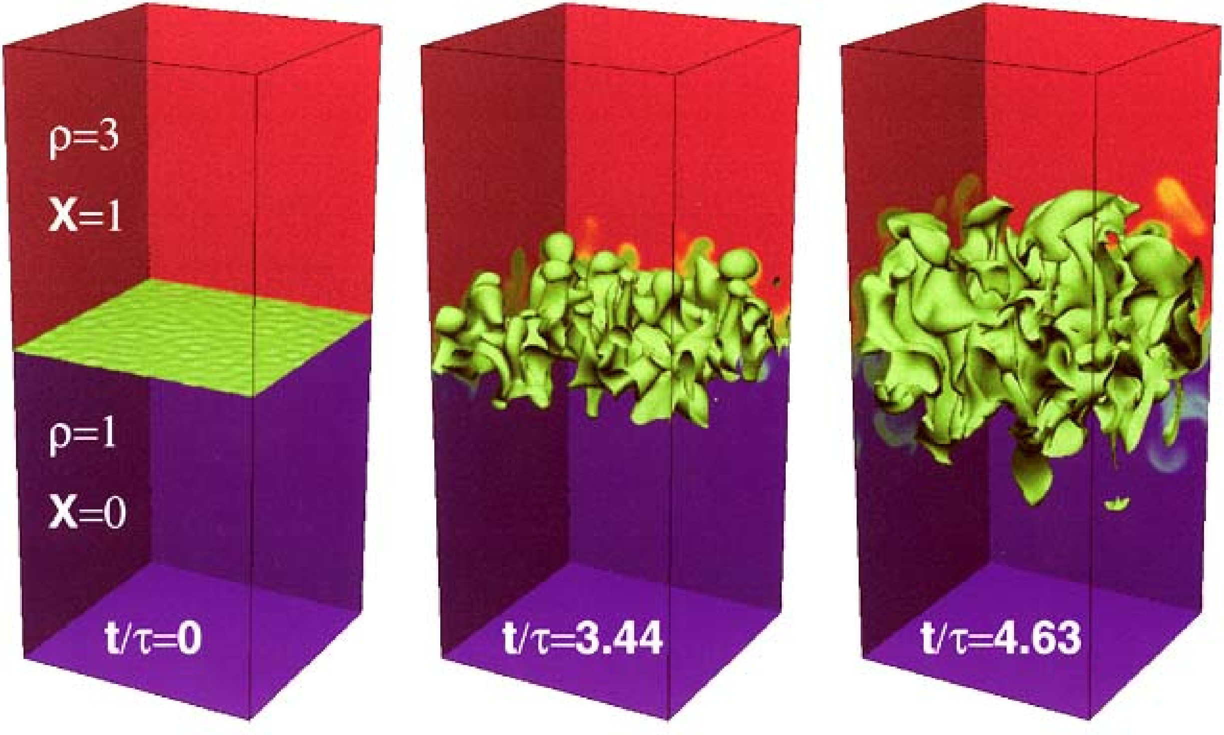
- **Spatial derivatives:**
  - Spectral in x and y
  - Eighth-order compact in z
- **Time integration of density equation:**
  - 3rd-order, Adams-Bashforth-Moulton method
- **Time integration of momentum equation:**
  - (1) account for advection and diffusion
  - (2) solve Poisson equation for pressure
  - (3) add pressure and acceleration effects
- **Boundary conditions:**
  - periodic in x and y
  - walls in z (Neumann pressure, no through flow)

Initial conditions

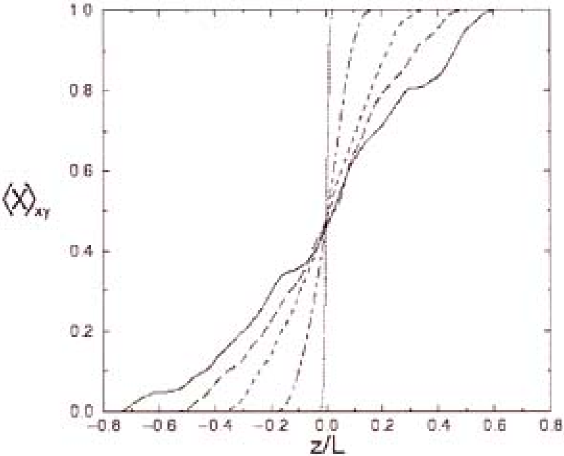


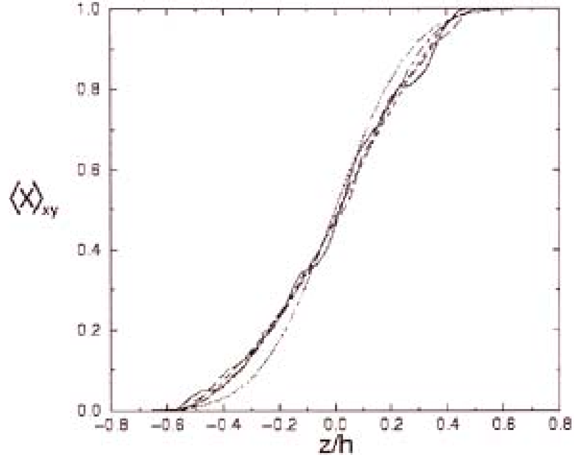
- E_ζ (k) = spectrum of initial interfacial perturbations
- k = 2-D (x-y) wavenumber
- $\sigma\tau$ = nondimensional growth rate from Linear Stability Theory (LST)
- High wavenumber perturbations are initially damped by diffusion

Time-evolution of R-T instability for DNS Case C



Time-evolution of horizontally-averaged mole-fraction profiles for Case C

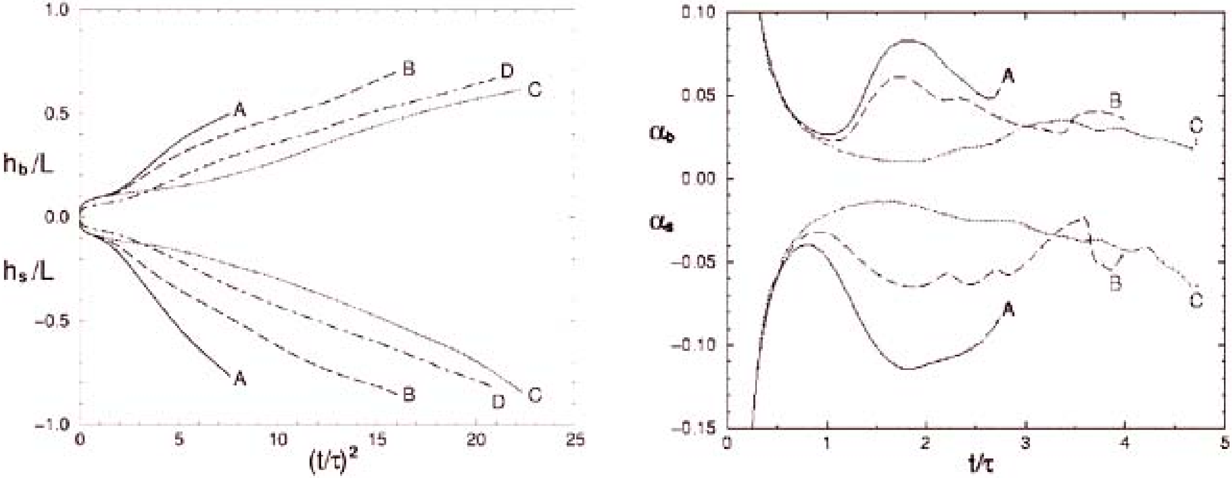




Dotted line: $t/\tau=0.0$, Short-long dashed line: $t/\tau=2.26$, Short dashed line: $t/\tau=3.40$, Long dashed line: $t/\tau=3.95$, Solid line: $t/\tau=4.52$

- Mix height h defined as range of z for which: $0.01 < X < 0.99$
- **Profiles collapse when plotted vs. z/h**

Growth rates of bubbles and spikes

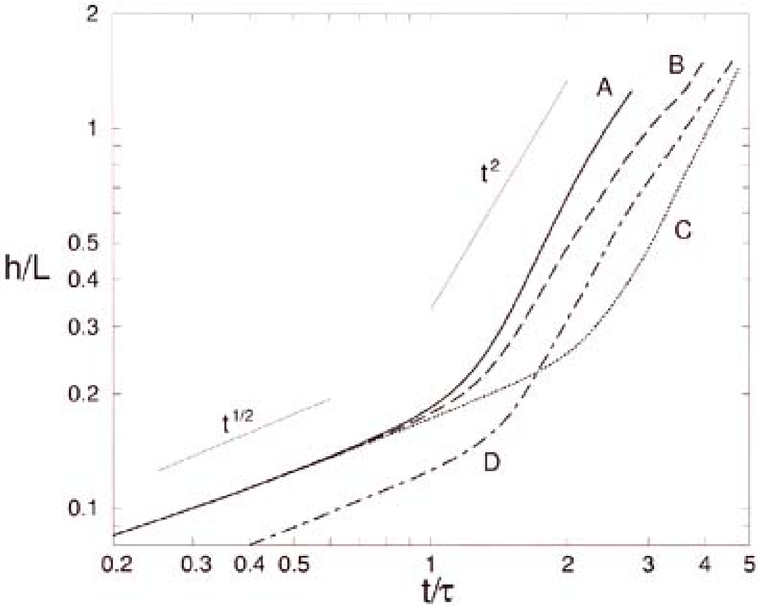


h_b = height of bubbles, h_s = height of spikes, i.e., $h = h_b - h_s$

α_b = growth coefficient of bubbles, α_s = growth coefficient of spikes, i.e., $h_i = \alpha_i A g t^2$

- **Growth rates can vary by factor of 2 depending on initial conditions**
- **α_b and α_s do not approach constant values**

Growth of mixing layer



h = height of mixing layer

L = $2\pi l$ = width of flow domain

t = time

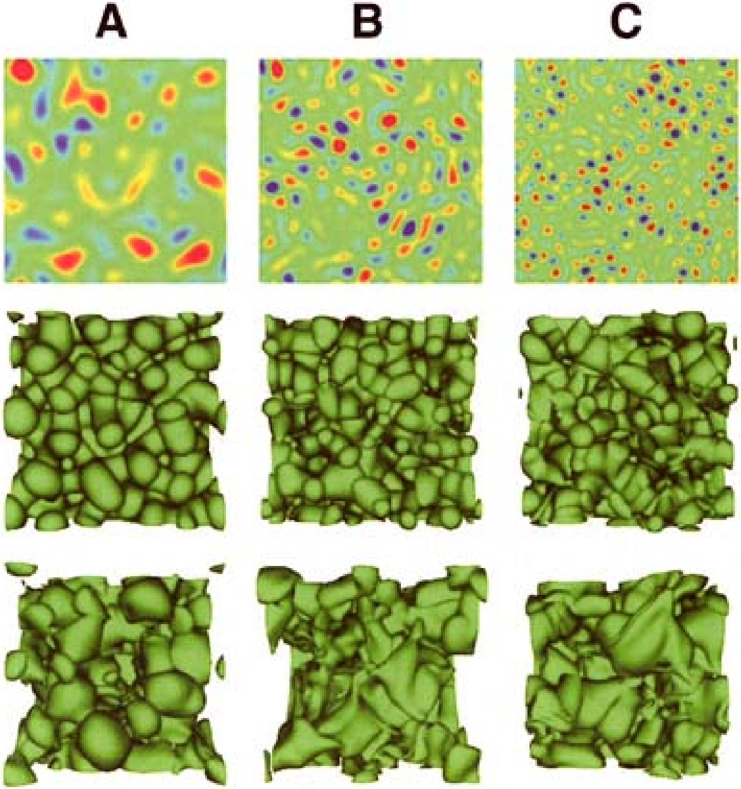
$\tau = (L/Ag)^{1/2}$

A = Atwood number

g = gravity

Early growth is diffusive, i.e., $t^{1/2}$; later, growth $\propto t^2$

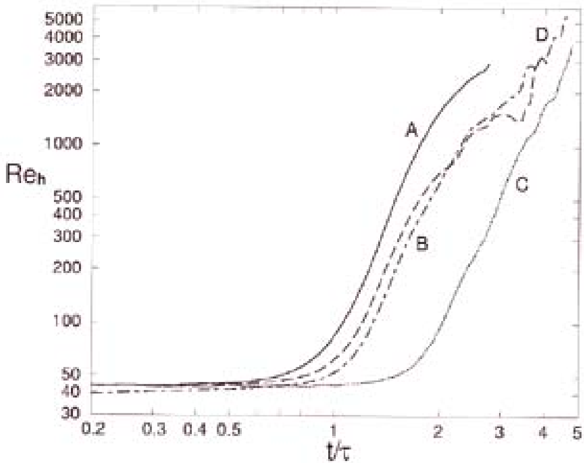
Bubble merger from initial perturbations

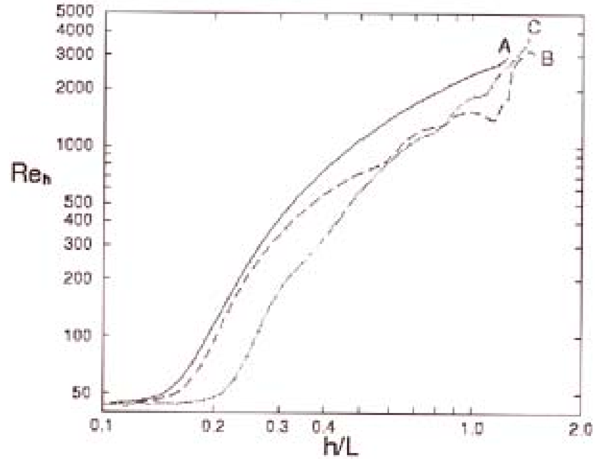


- Top Row: Initial perturbations at z = 0, blue: X = 0.35, green: X = 0.5 and red: X = 0.65
- Middle Row: X = 0.5 isosurface when h/L = 0.6
- Bottom Row: X = 0.5 isosurface when h/L = 1.25

- **Case A: bubbles rise more or less independently**
- **Case B: bubbles begin to merge when 0.6 < h/L < 1.25**
- **Case C: significant bubble merger for both h/L = 0.6 and h/L = 1.25**

Outer-scale Reynolds numbers

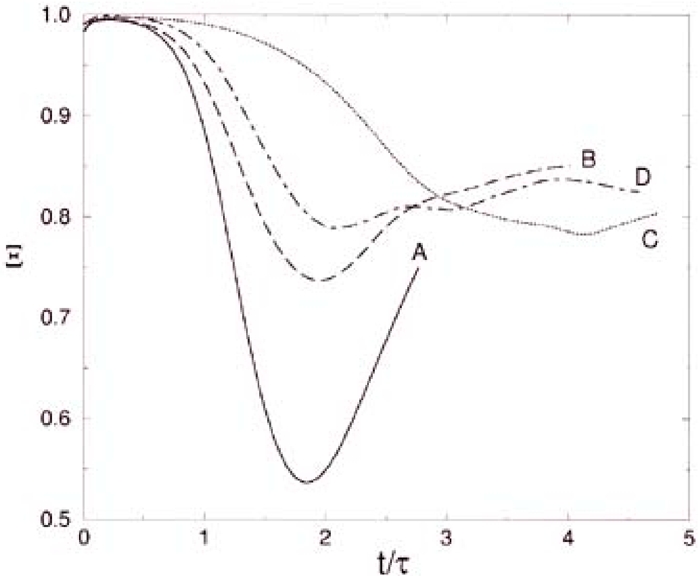




$$Re_h = \overline{\rho} h \dot{h} / \mu, \text{ where } \overline{\rho} = (\rho_1 + \rho_2)/2$$

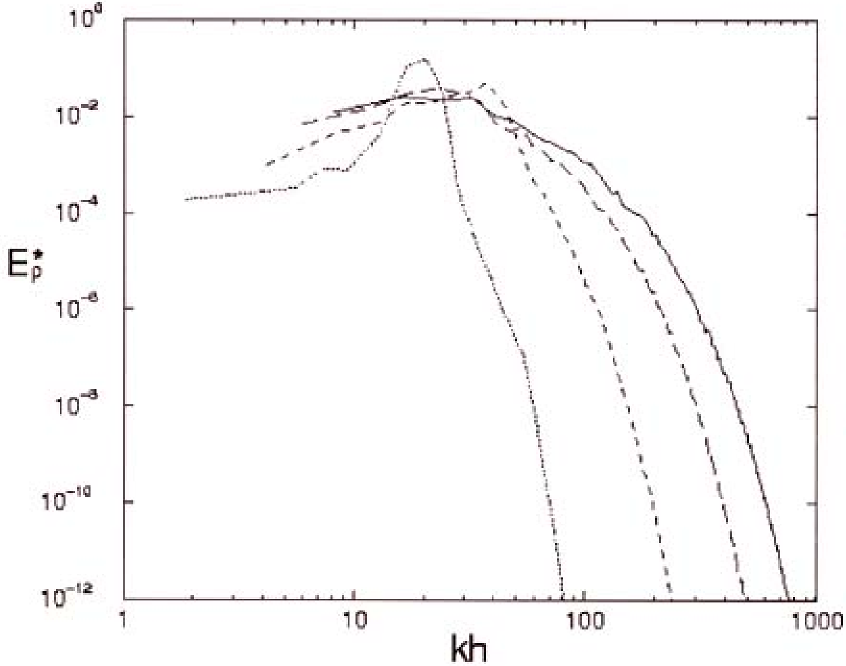
- Cases reach outer-scale Reynolds numbers of 3000-5500.
- Improved collapse achieved by replacing t with h as progress variable.

Mixing



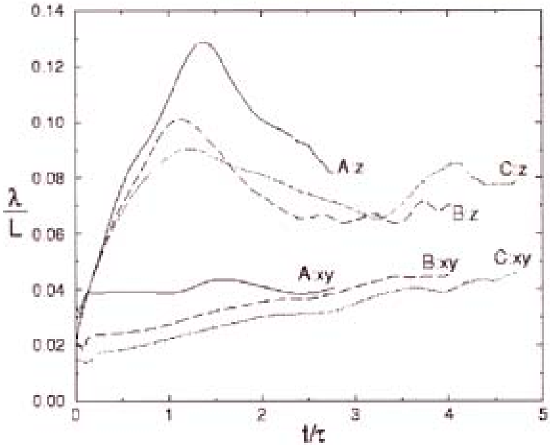
- Considering an equilibrium chemical reaction between fluids (stoichiometric mole ratio: $X_s = 1/2$), Ξ is the ratio of maximum possible product to actual product.
- $\Xi = 1$ corresponds to complete mixing within layer, whereas $\Xi = 0$ indicates no mixing (immiscible case).
- **Rates of mixing and entrainment do not come into balance within timespan of simulations.**

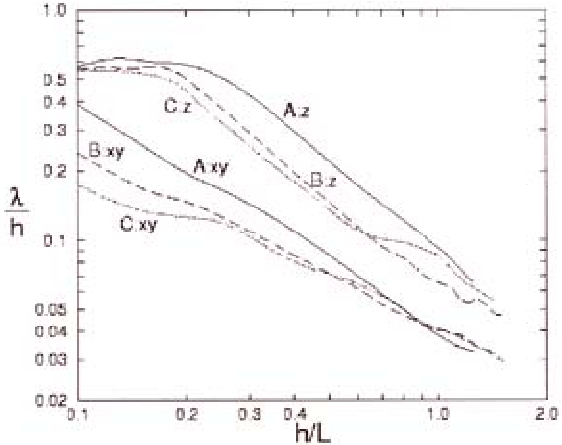
Spectra



- Normalized 2-D density spectra in z = 0 plane for Case C. Lines of increasing solidity denote increasing time.
- Beginning of a collapse at low wavenumber is evident towards end of simulation.
- Low-(kh) collapse indicates large-scale structures scale with mixing zone height.
- Full spectrum is still evolving, however, due to low Reynolds number.

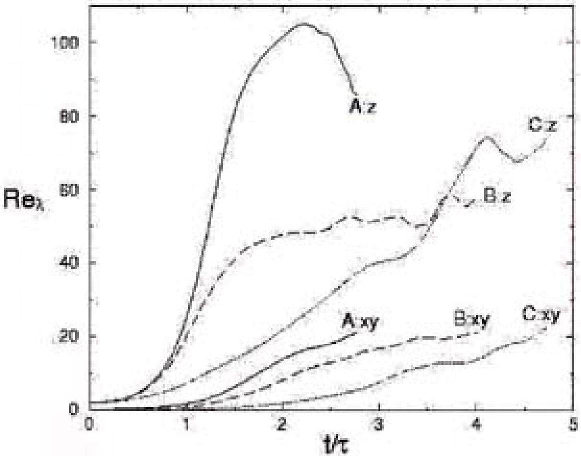
Taylor microscales

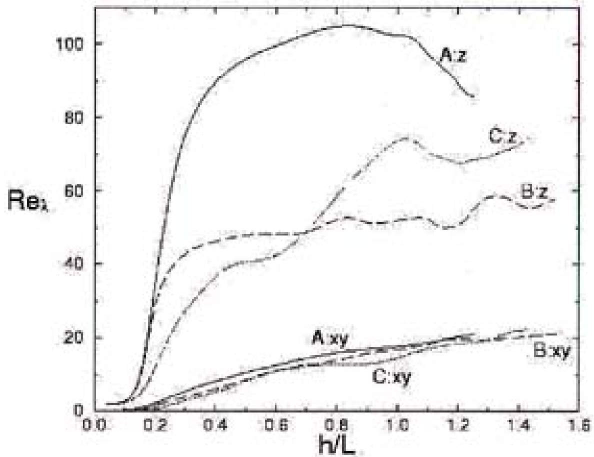




- Initial values for horizontal microscales are ranked in order of peaks of initial perturbation spectra.
- Vertical microscales grow much faster than horizontal scales due to directed body force.
- Flows exhibit strong anisotropy between horizontal and vertical microscales for duration of simulations.

Taylor Reynolds numbers





- Anisotropy in microscales also manifest in Taylor Reynolds numbers
- Vertical Taylor Reynolds numbers extremely sensitive to initial conditions with no collapse for either independent variable
- Near perfect collapse of horizontal Reynolds numbers when plotted vs. h/L

Conclusions

- Growth of R-T mixing layer depends sensitively on initial conditions.
- Ranking of growth rates is in same order as suggested by Linear Stability Theory.
- Mixing exhibits greater sensitivity to initial conditions than growth rates.
- Density-fluctuation spectra in interior of mixing zone indicate that imprint of the initial perturbation spectra is eventually lost; furthermore, the spectra exhibit good collapse at low wavenumbers by late simulation time.
- Taylor microscales and Reynolds numbers are also sensitive to initial conditions, nonmonotonic in their temporal evolution and reflect considerable and persistant anisotropy in the flow.
- Mixing zone height is a better progress variable than time, i.e., improved collapse occurs if statistics are compared at the same value of h and if spatial scales are nondimensionalized in terms of h.