A NUMERICAL TECHNIQUE FOR 2D COMPRESSIBLE MULTIPHASE FLOW

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PURPOPSE OF THE MULTIPHASE FLOW MODEL

We wish to assess the effect of turbulent mixing at fluid interfaces due to Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz instabilities in problems for which the mean flow is either 1D or 2D.

We use a turbulence model based on the equations of multiphase flow to calculate mixing in 1D/2D real applications.

High-resolution 3D Large Eddy Simulation is applied to simpler problems and helps to validate the 2D turbulence model.

THE 2D TURBULENCE MODEL

Need to model:

mixing due to a pressure gradient or shock acting on density differences.

mixing due to turbulent diffusion

fluid inter-penetration + decay of concentration fluctuations

Choice of model:

Multiphase flow equations with mass exchange between the phases + turbulent diffusion terms.

Equations for Mass, Momentum, Internal energy (each phase)

Turbulence KE, Turbulence length scale

See: Laser and Particle Beams, vol12, p725(1994) - more recent developments, mass exchange terms, initial conditions model.

MODEL EQUATIONS(1)

Variables:-

f_r : phase r volume fraction
ρ_r : phase r density
e_r : phase r internal energy
u_r : phase r velocity
m_{rs} : fraction by mass of fluid s in phase r
L : turbulence length scale
k : turbulence KE

Mass transport:

$$\frac{\partial}{\partial t}\left(f_r\ \rho_r\ m_{rs}\right)+\frac{\partial}{\partial x_j}\left(f_r\ \rho_r\ m_{rs}\ u_{rj}\right)=\frac{\partial}{\partial x_j}\left(f_r\ \rho_r\ D\,\frac{\partial m_{rs}}{\partial x_j}\right)+\sum_p\left(m_{ps}\ \Delta M_{pr}-m_{rs}\ \Delta M_{rp}\right)$$

$D =$ diffusion coefficient $\sim \sqrt{k}\,L$

$\Delta M_{rs} =$ mass transferred from phase r to phase s $\sim \dfrac{\sqrt{k}}{L}$

MODEL EQUATIONS(2)

Momentum:

$$\frac{\partial}{\partial t}(f_r\ \rho_r\ u_{ri})+\frac{\partial}{\partial x_j}(f_r\ \rho_r\ u_{ri}\ u_{rj})=-\,f_r\frac{\partial p}{\partial x_i}+\text{Reynolds stress, drag, mass exchange, added mass, gravity}$$

Drag on phase r due to phase s:

$$D_{rs}=-C_1\frac{\rho_{rs}\ f_r\ f_s}{L}\left|W\right|W_i$$

where $W_i=u_{ri}-u_{si}-u_{ri}^d+u_{si}^d$ and $u_{ri}^d=-\dfrac{D}{f_r\ \rho_r}\dfrac{\partial\left(f_r\ \rho_r\right)}{\partial x_i}$, diffusive velocity.

Internal energy:-

$$\frac{\partial}{\partial t}(f_r\ \rho_r\ e_r)+\frac{\partial}{\partial x_j}(f_r\ \rho_r\ e_r\ u_{rj})=-h_r\ f_r\ p_r\frac{\partial\overline{u}_j}{\partial x_j}+\text{diffusion, mass exchange, source}$$

h_r: compressibility factor.

The turbulence model has been implemented in an existing 2D Eulerian hydrocode (Youngs, in Numerical Methods for Fluid Dynamics, eds Morton and Baines 1982).

Main features of the method

• Lagrangian step

• followed by rezone or advection step. Monotonic advection method of van Leer used. XY splitting.

• can have several Lagrange steps per advection step.

• semi-Lagrangian option - mesh stays rectangular but moves with the mean fluid velocity in one direction.

• interface tracking method used

• separate density, internal energy, pressure for components in a mixed cell

Implementation of the turbulent mixing model

- mixing step (transport due to u_r - u, advection + turbulent diffusion)

  XY splitting used

- mass exchange step

- Lagrange step (extend for multifluid acceleration)

- Rezone step

At an appropriate stage in the calculation interface tracking is switched of and the turbulent mix model is switched on. A key numerical issue is the reduction of mixing due to numerical diffusion after the turbulent mixing model has been activated :—

- use of van Leer method in the mixing step

- initial conditions model (ODE's used to estimate growth of mixing zone up to the time when width ~ 2 Δx)

THE MIXING STEP(1)

Transport of fluid variables with velocity $\mathbf{u}_r - \overline{\mathbf{u}}$.
Where $\overline{\mathbf{u}}$ = volume weighted mean velocity.
XY splitting used.

Advection with velocity $\mathbf{u}_r - \mathbf{u}_r^d - \overline{\mathbf{u}}$, + diffusion
Advection :-

(a) volume fractions (f_r)
(b) quantities defined per unit volume eg density ρ_r
(c) quantities defined per unit mass eg internal energy e_r

at cell boundaries :-

Volume fluxes δV_r
Mass fluxes $\delta M_r = \hat{\rho}_r \delta V_r$
Internal energy fluxes $\delta E_r = \hat{e}_r \delta M_r$

$\hat{\rho}_r$ and $\hat{e}_r$ set by using van Leer formulae $\Rightarrow$ monotonic behaviour for density and internal energy.

Some extra care needed for the calculatio n of the volume fluxes δV_r.

Diffusion : fully implicit in time. ADI method.

THE MIXING STEP(2)

Advection - incompressible process. For cell $j+1/2$ (in 1D)

$$f^1_{rj+1/2}\, V_{j+1/2} = f^0_{rj+1/2}\, V_{j+1/2} + \delta V_{rj} - \delta V_{rj+1}$$

Need $\sum_r \delta V_{rj} = 0$ - no net volume flux across a cell boundary

$$\delta V_{rj} = \hat{f}_{rj} \left(u_{rj} - u^d_{rj} - \overline{u} + \Delta u \right) A$$

$\hat{f}_{rj}$ calculated by using a van Leer formula. Note that the upwind direction is not the same for all phases

Velocity correction Δu included

By iteration Δu is chosen to give

$$\sum_r \delta V_{rj} = 0$$

Then monotonic behaviour for $f^1_{rj+1/2}$ and $\sum_r f^1_{rj+1/2} = 1$

Mass exchange step:

•Relative straightforward (no coupling between cells)

•Exchange of volume → exchange of mass → exchange of mass fractions, internal energy etc

Lagrangian step:

•Extend to calculate multifluid acceleration. Implicit treatment for drag terms.

•Multifluid internal energy update used previously

•Reynolds stresses, turbulence KE equation, length scale equation includes as separate steps.

THE LAGRANGE STEP(1)

Multifluid acceleration (x - direction)
Implicit drag formulation

$$\rho_r \frac{u_r^1 - u_r^x}{\Delta t} = -f_r \frac{\partial p}{\partial x} + \sum_s D_{rs} + \sum_s A_{rs} + \text{mass exchange terms}$$

u_r^x = x - velocity at end of mixing/mass exchange steps
u_r^1 = x - velocity at end of acceleration step.

Drag: $$D_{rs} = -\frac{C_1 \rho_{rs} f_r f_s}{L} |W| W_x$$

$$W_x = u_r^1 - u_r^d - u_s^1 + u_s^d, W_y = v_r^1 - v_r^d - v_s^1 + v_s^d, |W| = \sqrt{W_x^2 + W_y^2}$$

Added mass: $$A_{rs} = -C_a \rho_{rs} f_r f_s \left[\frac{u_r^1 - u_r^x}{\Delta t} - \frac{u_s^1 - u_s^x}{\Delta t}\right] \sim -C_a \rho_{rs} f_r f_s \left[\frac{D_r u_r}{Dt} - \frac{D_s u_s}{Dt}\right]$$

Two fluids present (most of problem) $\Rightarrow$ quadratic equation for $|W|$
More than two fluids present $\Rightarrow$ Neutron - Raphson iteration
(Note: each node calculated separately)

THE LAGRANGE STEP(2)

Internal Energy Equations

$$f_r \, \rho_r \frac{\partial e_r}{\partial t} = -h_r \, f_r \, p_r \, \text{div} \, \bar{\mathbf{u}}$$

$$h_r = \text{compressibility factor} = \frac{1/\left(\rho_r \, c_r^2\right)}{\sum_s f_s/\left(\rho_s \, c_s^2\right)}$$

mean pressure used in acceleration step: $p = \sum h_r \, f_r \, p_r$

differential compressibility $(h_r \neq 1)$ implies volume fractions should change during the Lagrange step:

$$f_r^1 \, V^1 = f_r^o \, V^o + f_r^o \, h_r \, \delta V$$

$$\text{where } \delta V = V^o . \text{div} \, \bar{\mathbf{u}} \, . \Delta t$$

(cut-offs needed to prevent non-physical results)

Pressure relaxation also essential - time scale related to sound speeds c_r.

- volume transfer (δV_{rs})
- internal energy transfer $(p \, \delta V_{rs})$

THE REZONE (ADVECTION) STEP

Calculated transport across cell boundaries due to mean velocity $\overline{\mathbf{u}}$.
3rd order van Leer used for all variables.
Straightforward extension of previous technique except for two issues

(a) Volume fraction advection

Phase r volume fraction for advection across cell boundary $x = x_j$

$$\hat{f}_{rj} = f_{rb} + \frac{1}{2}(1-\varepsilon) S D_{rj}$$

b: donor cell, $\varepsilon = |\delta V|/V_b$, D_{rj} : unlimited volume fraction gradient in donor cell.

$S =$ van Leer limiting factor

need to use $S = \min_r S_r$ to ensure $\sum_r \hat{f}_{rj} = 1$

(b) Momentum advection

advect mass-weighted mean velocity : $\tilde{\mathbf{u}}$ (van Leer advection)
advect velocity differences : $\mathbf{u}_r - \tilde{\mathbf{u}}$ (first order)

INITIAL CONDITIONS MODEL(1)

Simple estimate of the mix width from acceleration vs time behaviour - solve ODE's at interface nodes. Does not affect the hydro.

Used to calculate the early time growth of the mixing zone when it is too small to be resolved by the multiphase flow model -> improved accuracy.

Also models, in a very approximate way, the effect of initial perturbation level on the early-stage mixing zone growth.

Sets the initial conditions for the turbulent mix model calculation when the mixing zone is a few meshes wide. (The turbulent mix model can be switched on at different interfaces at different times).

INITIAL CONDITIONS MODEL(2)

Solves ODE's for mix penetrations (h_1, h_2) and mix velocities (V_1, V_2) at interface nodes.

$$(\rho_1+\rho_2)(1+E_i)\frac{DV_i}{Dt}=(\rho_1-\rho_2)(1-E_i)\,g_n-C_D\frac{F_i\rho_i}{R}V_i|V_i|$$

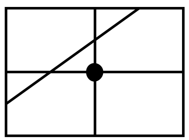
$$\frac{Dh_i}{Dt}=V_i+e_n h_i$$

$$E_i=\exp\left(\frac{-4\,\beta_1 h_i}{\lambda_o}\right) \qquad R=\max\left\{\min(h_1,h_2),\frac{C_D\,\lambda_o}{2\beta_1}\right\}$$

a_o = initial amplitude

λ_o = initial dominant length scale

- $\underline{n}$ = interface normal calculated from the interface reconstruction
- $g_n=\underline{g}\bullet\underline{n}$
- e_n = strain rate in the direction of $\underline{n}$
- for shock acceleration in the non-linear regime use $|(\rho_1-\rho_2)g_n|$ instead of $(\rho_1-\rho_2)g_n$
- Solve at each 'interface' node



- Special technique needed to advect

  $h_1, h_2, \quad V_1, V_2$

INITIAL CONDITIONS MODEL(3)

Use values of h_1, h_2, V_1, V_2 to set initial conditions for turbulent mix model calculation

Diffuse fluids into each other:

$$\frac{\partial f_1}{\partial \tau} = \mathrm{div}\left(D \nabla f_1\right) , \quad D \sim h^2 \sqrt{f_1 f_2}$$

Integrate from $\tau = 0$ to 1

V_1, V_2 used to set fluid velocity separation and turbulence KE.

h_1, h_2 used to set length scale

mass exchanged between fluids in a cell to set initial concentration fluctuation

VALIDATION STRATEGY

Various terms in the mix model require a total of 11 model constants to be set.

Earlier turbulence models (eg the widely used k-ε model) relied on experimental date to determine the model coefficients.

It is now feasible to use 3D simulation results (LES code TURMOIL3D) + experimental data in simple situations to set the model coefficients.

Experiments considered here

1D Rayleigh-Taylor mixing (Rocket-Rig, LEM)

AWE linear shock tube experiments (2D on average)

The simple incompressible RT problem $(\rho_1, \rho_2, \mathbf{g\ constant})$ is the key problem for fixing the turbulence model coefficients.

Loss of memory tends to occur $\rightarrow$ self-similar mixing with length scale gt^2:

Bubble penetration $h_1 = \alpha \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2} gt^2$

α ~ 0.05 to 0.06
(AWRE Foulness, LLNL (LEM), Chelyabinsk 70)

TURMOIL3D calculations with short-wavelength initial perturbations (growth purely by mode coupling) give α ~ 0.03, less than observed.

Need to add long wavelength initial perturbations:-

$$\sigma^2 = \int_0^\infty P(k)\, dk$$

where $\left\{ \int_{2\pi/\lambda}^{\infty} P(k)\, dk \right\}^{\frac{1}{2}} = \varepsilon \lambda$

ε = 0.0005 gives self-similar growth with α ~ 0.05. It is assumed that this corresponds to a typical experimental situation.

Model coefficients are chosen to fit the key quantities.

α **: growth rate coefficient**

$$\frac{D}{P} : \frac{\text{turbulence KE dissipated}}{\text{Loss of potential energy}}$$

θ **: molecular mixing fraction**

$$\frac{\int \overline{f_1 f_2}\, dz}{\int \bar{f}_1 . \bar{f}_2\, dz}$$

Values used are based on TURMOIL3D calculations (800 x 400 x 400 zones, ε = 0.0005): -

α	=	**0.05**
D/P	=	**0.4 (no experimental data)**
θ	=	**0.7 (some experimental confirmation)**

Still leaves one key degree of freedom

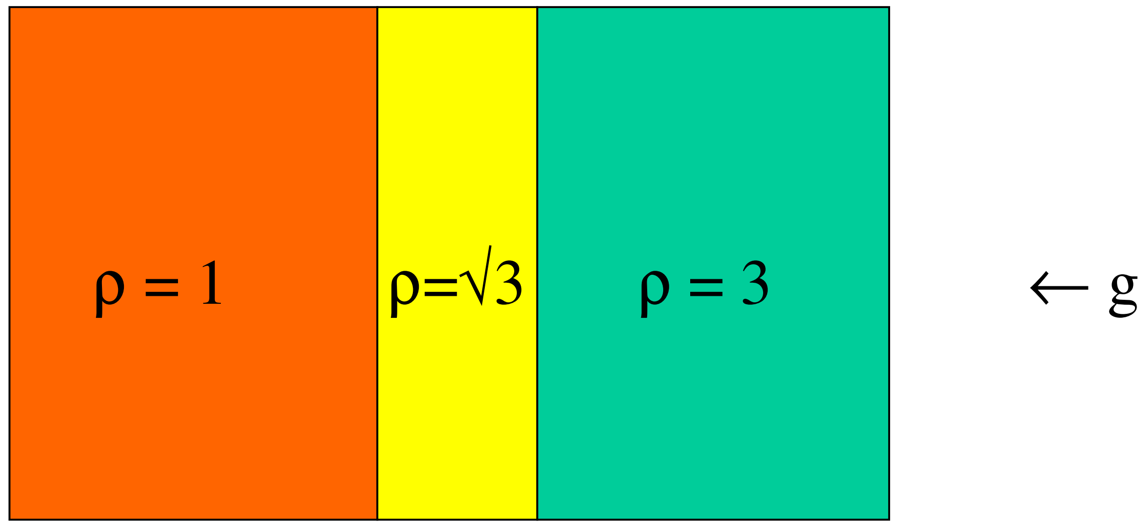
$$\Delta = \frac{\Delta u_D}{\Delta u_D + \Delta u_P}$$

$\Delta u_D =$ **mixing velocity due to turbulent diffusion**

$\Delta u_P =$ **mixing velocity induced by pressure gradient**

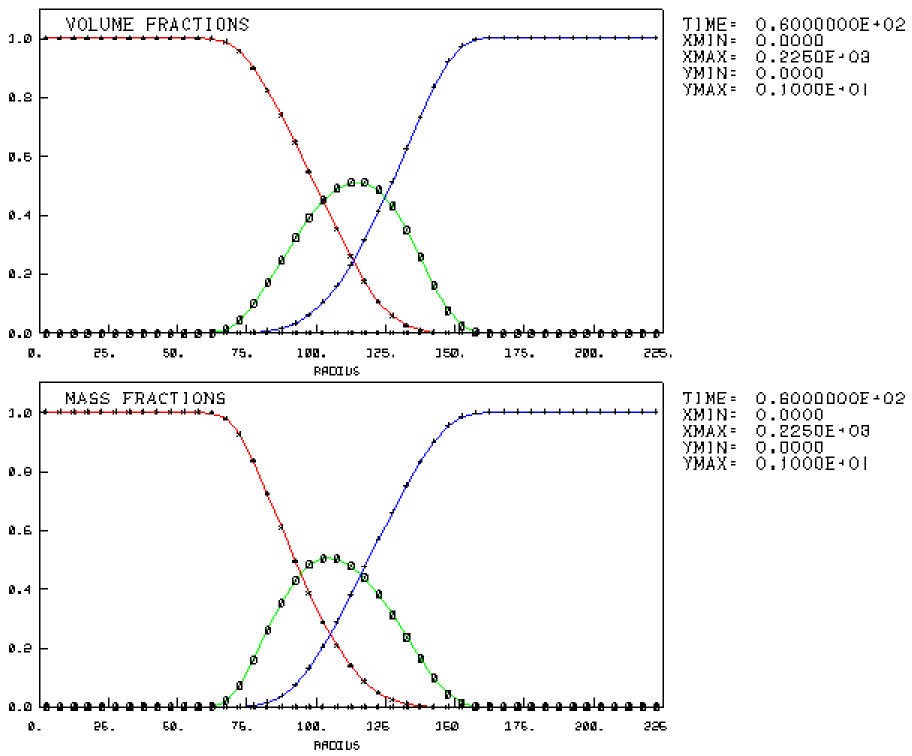
Results shown here for $\Delta = 0.4$ **- gives reasonably results for 2D problems**

Three-fluid test problem

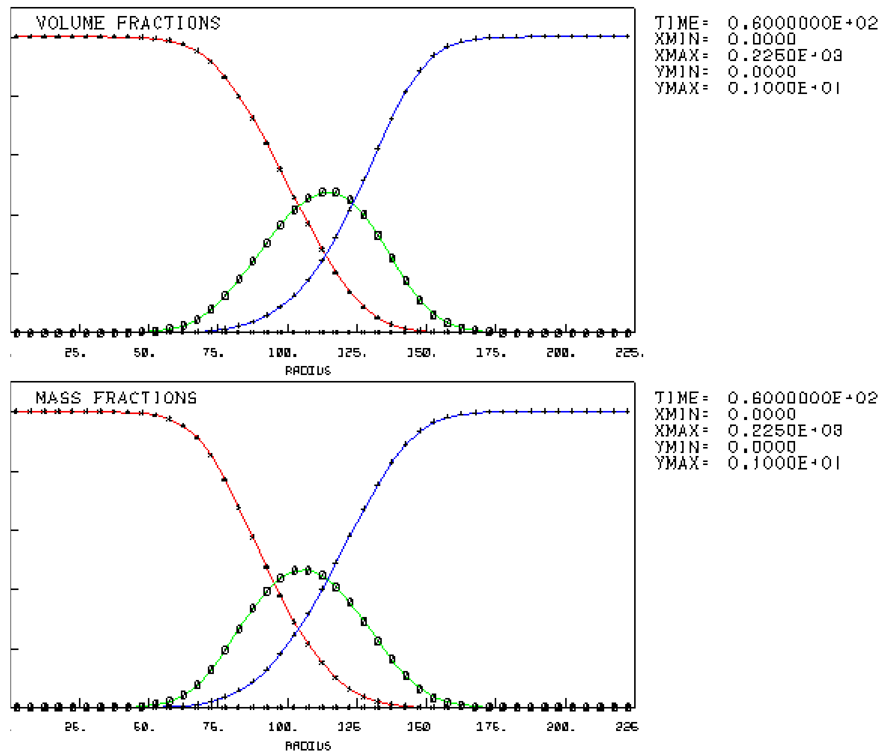


Zoning used: 45 zones (5 zones in middle layer)

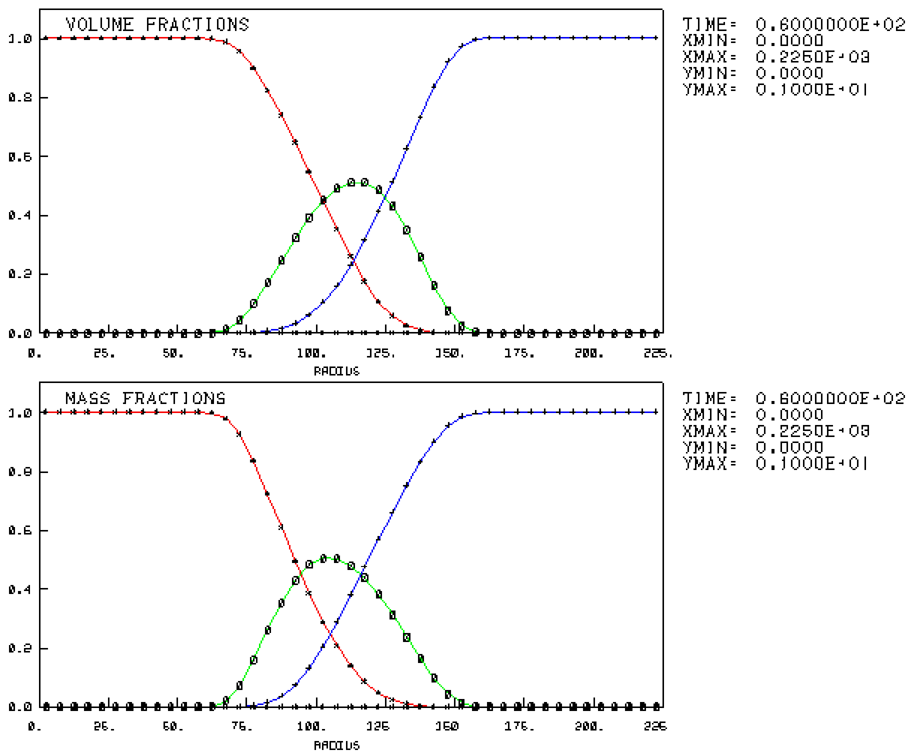
90 zones (10 zones in middle layer)



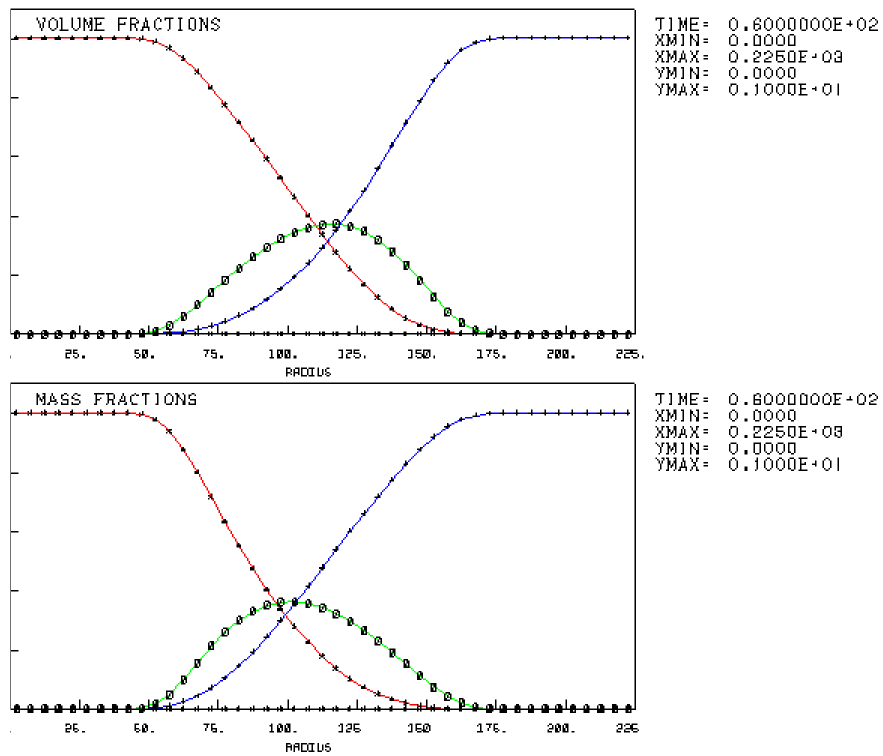
Van Leer advection



First order advection

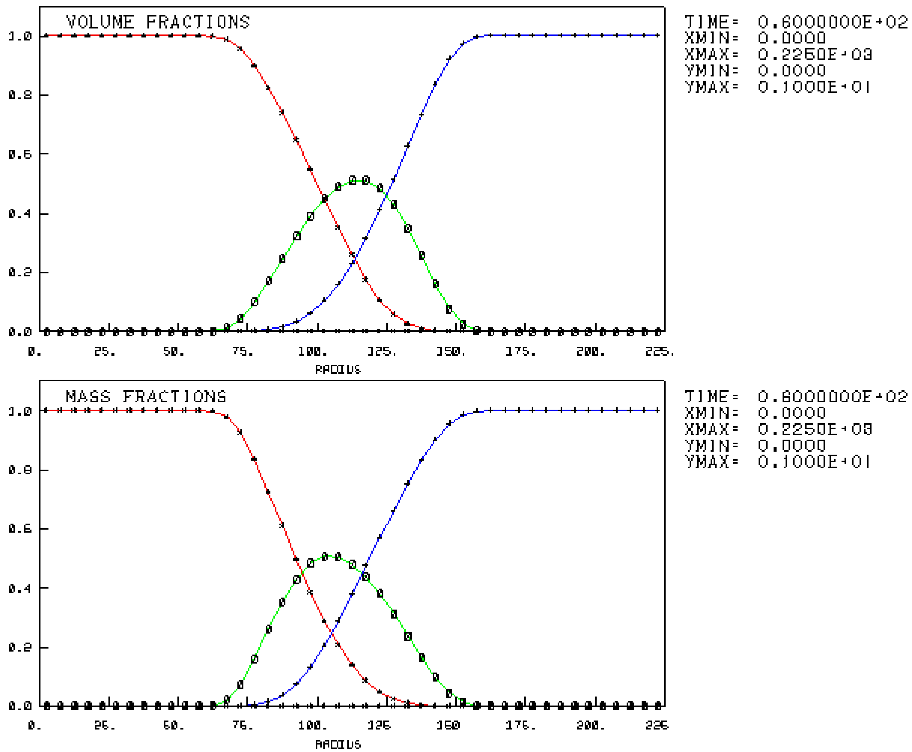


With initial conditions model

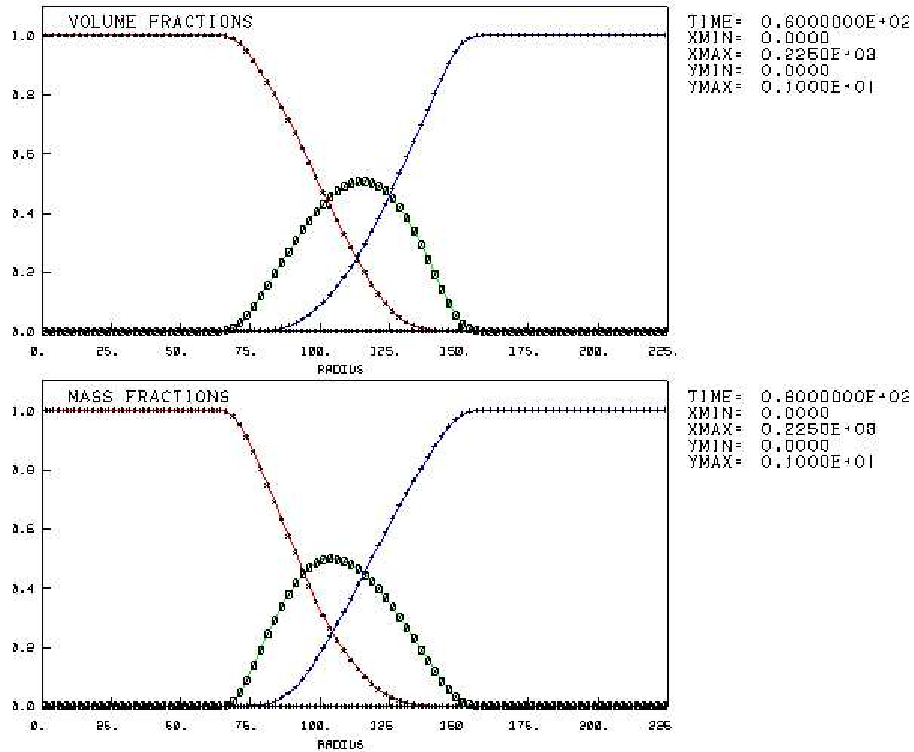


Without initial conditions model

van Leer advection + initial conditions model

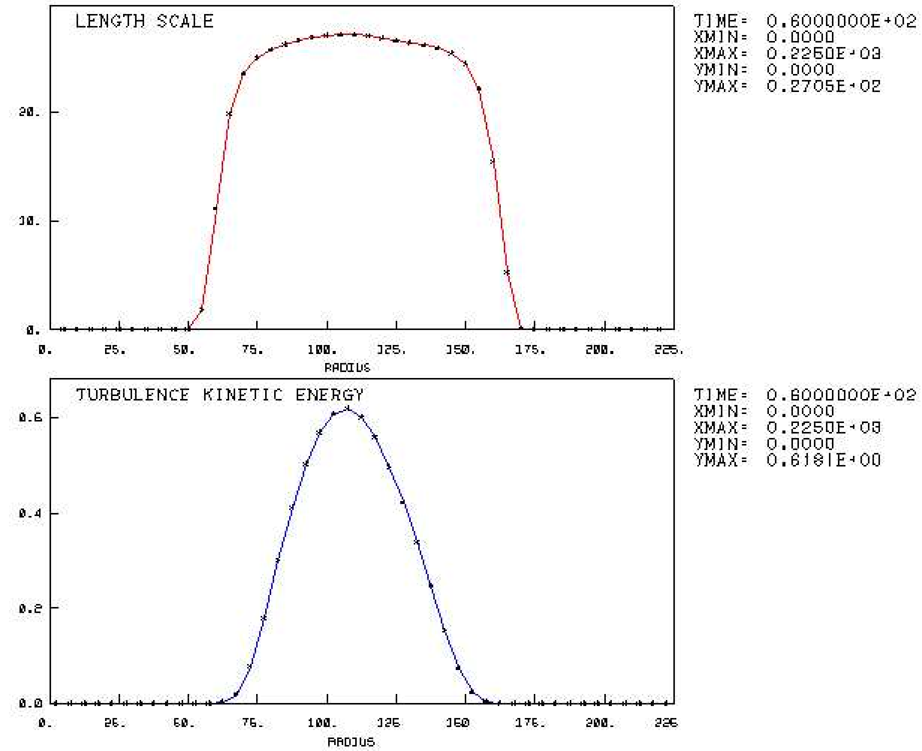


45 zones

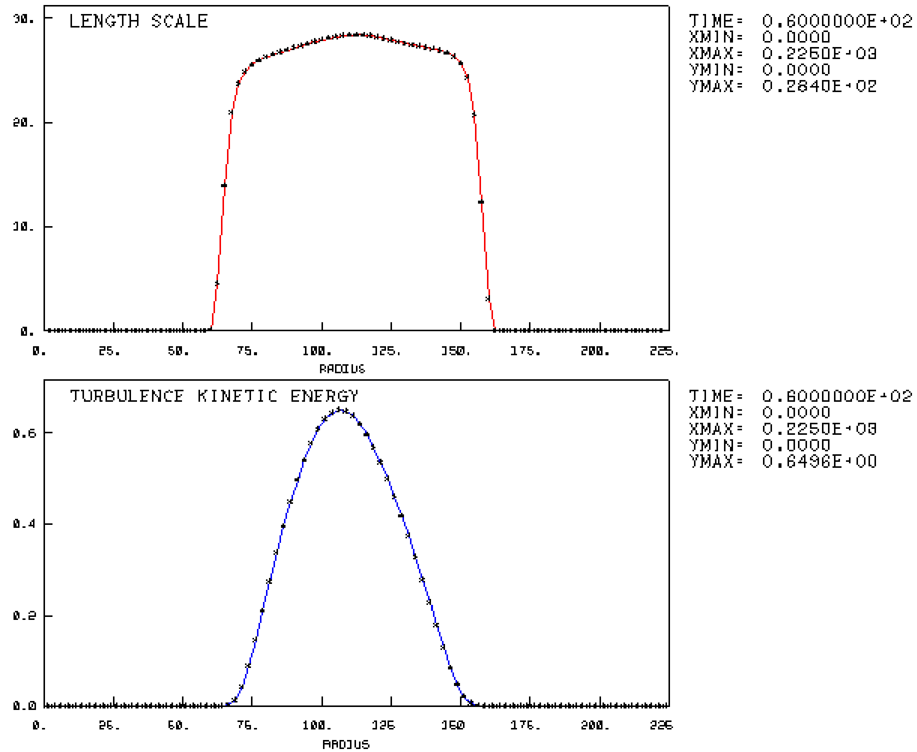


90 zones

van Leer advection + initial conditions model

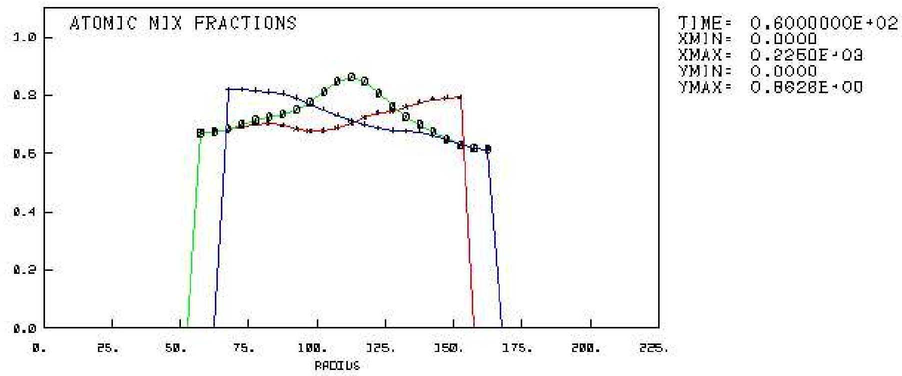


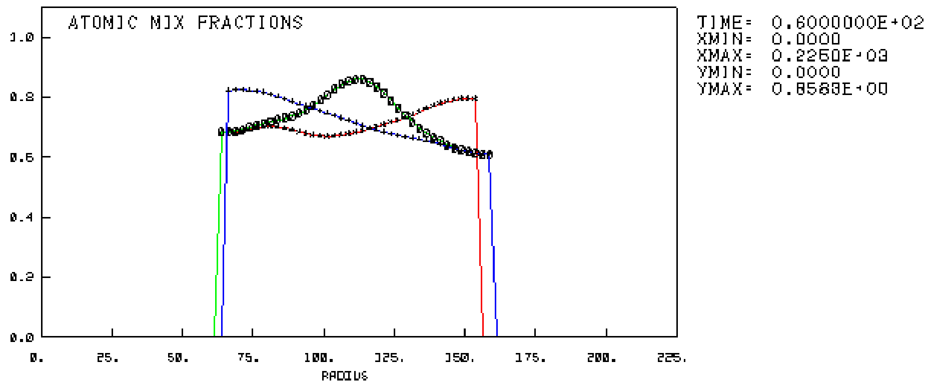
45 zones



90 zones

van Leer advection + initial conditions model

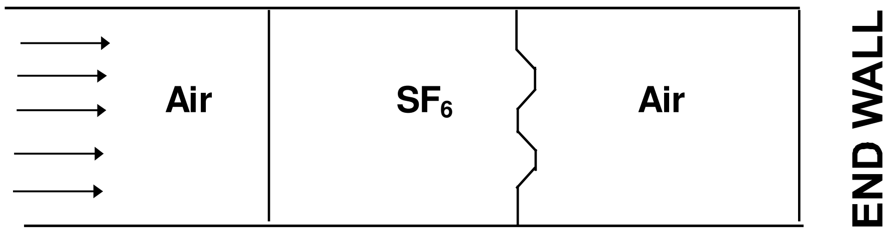




45 zones

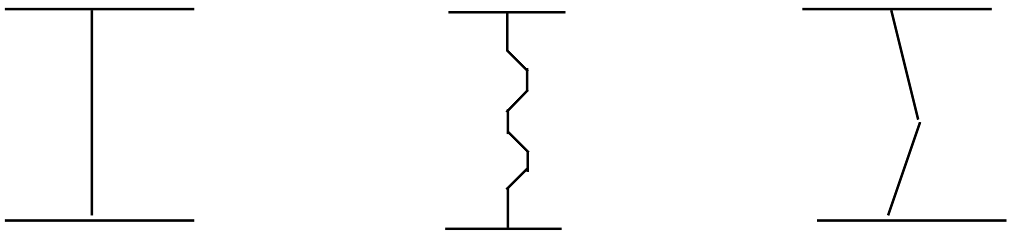
90 zones

SHOCK TUBE EXPERIMENT (AWE)



0.0 35.0 cm

Cross-section 20 x 10 cm



(a) flat (b) double bump (c) chevron

Moving mesh option used (semi-Lagrangian calculations)

3D LES:	400 x 320 x 160 zones	
	random interface perturbations	
	wavelengths	0.5 to 5 cm
	s.d	0.01 cm

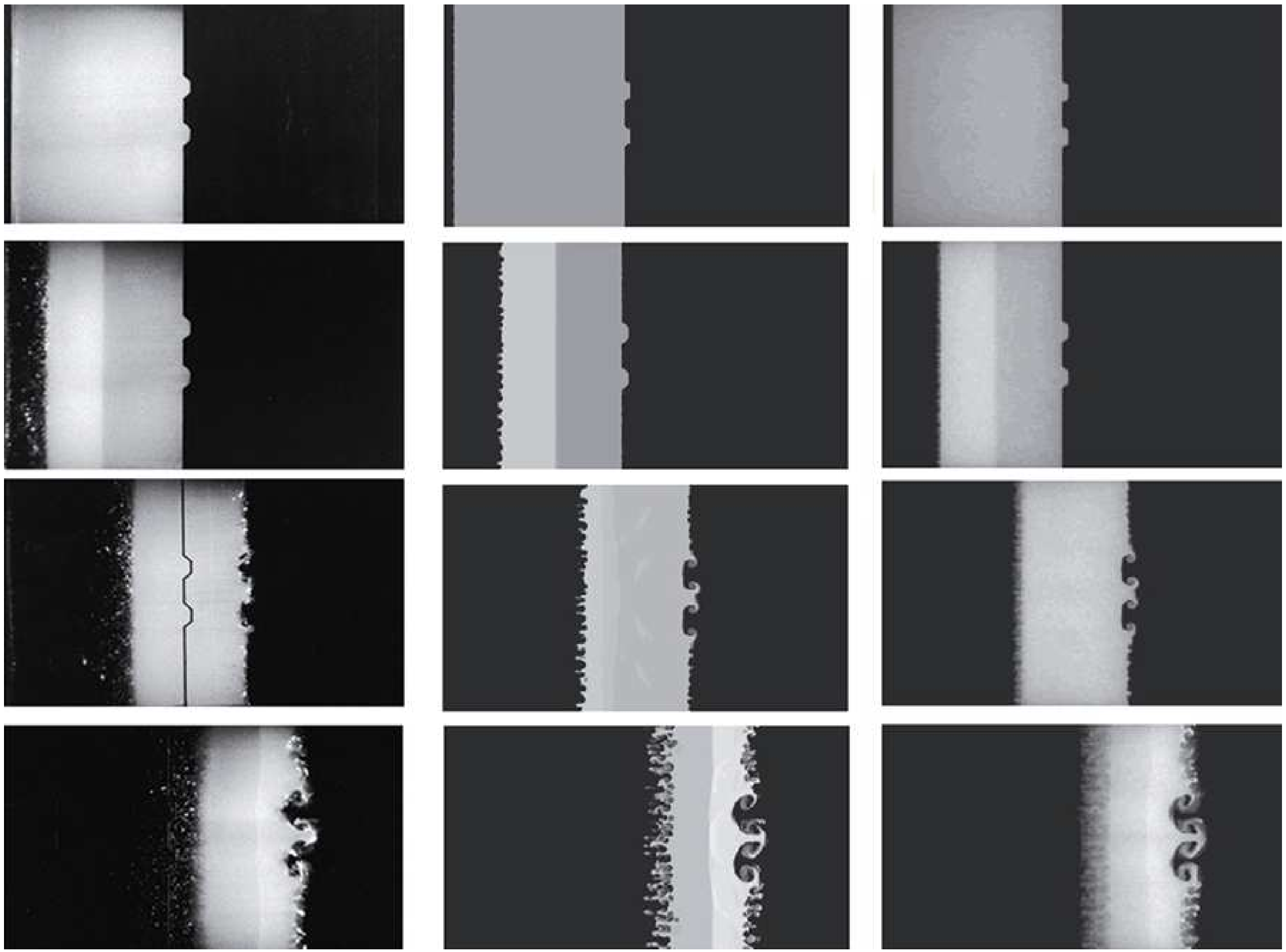
2D turbulence model calculation

200 x 160 zones

initial conditions model

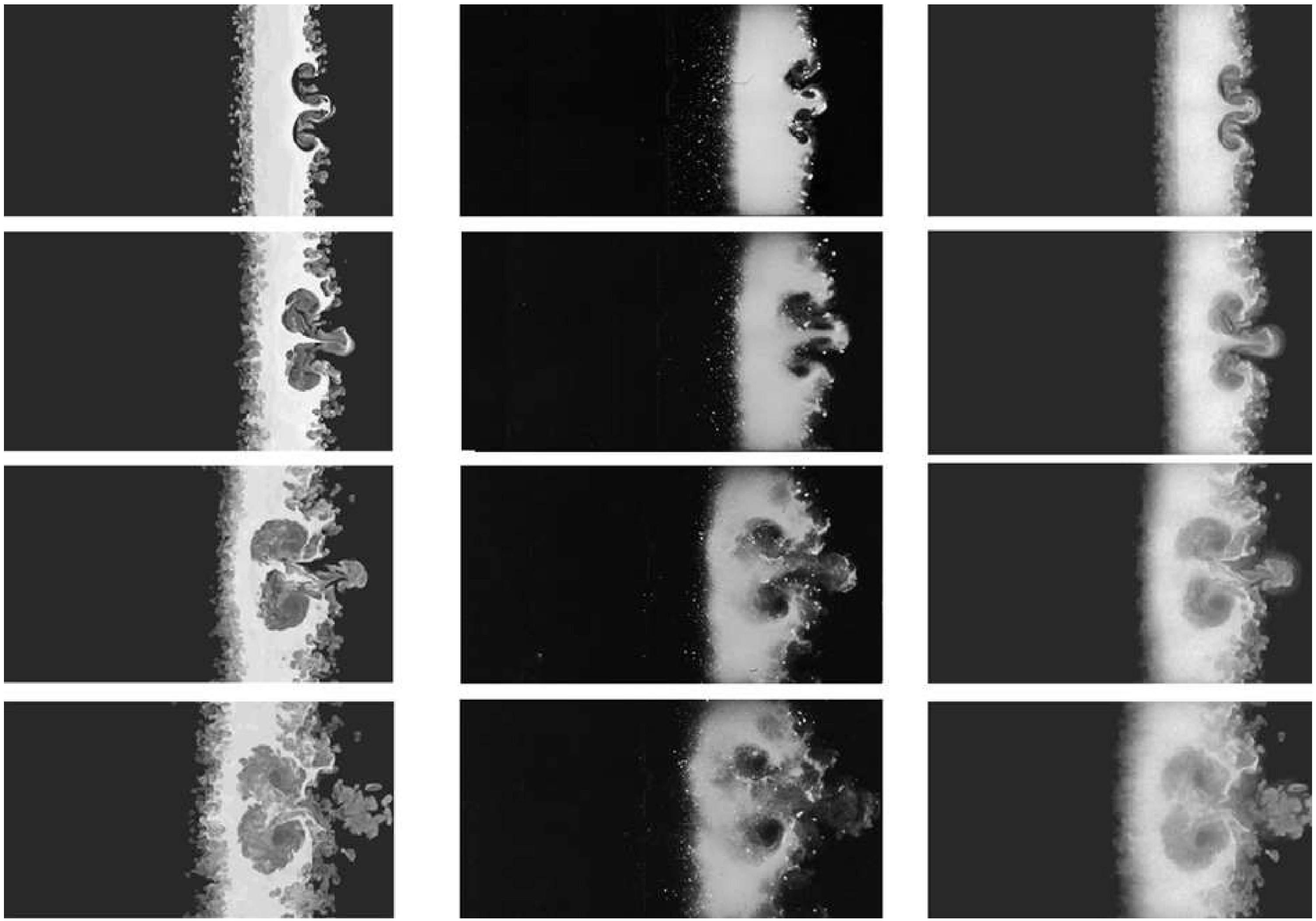
$a_o = 0.02$ cm, $\lambda_0 = 0.5$ cm

AWE SHOCK TUBE EXPERIMENT
Double Bump Results (0.0 - 1.9 ms)

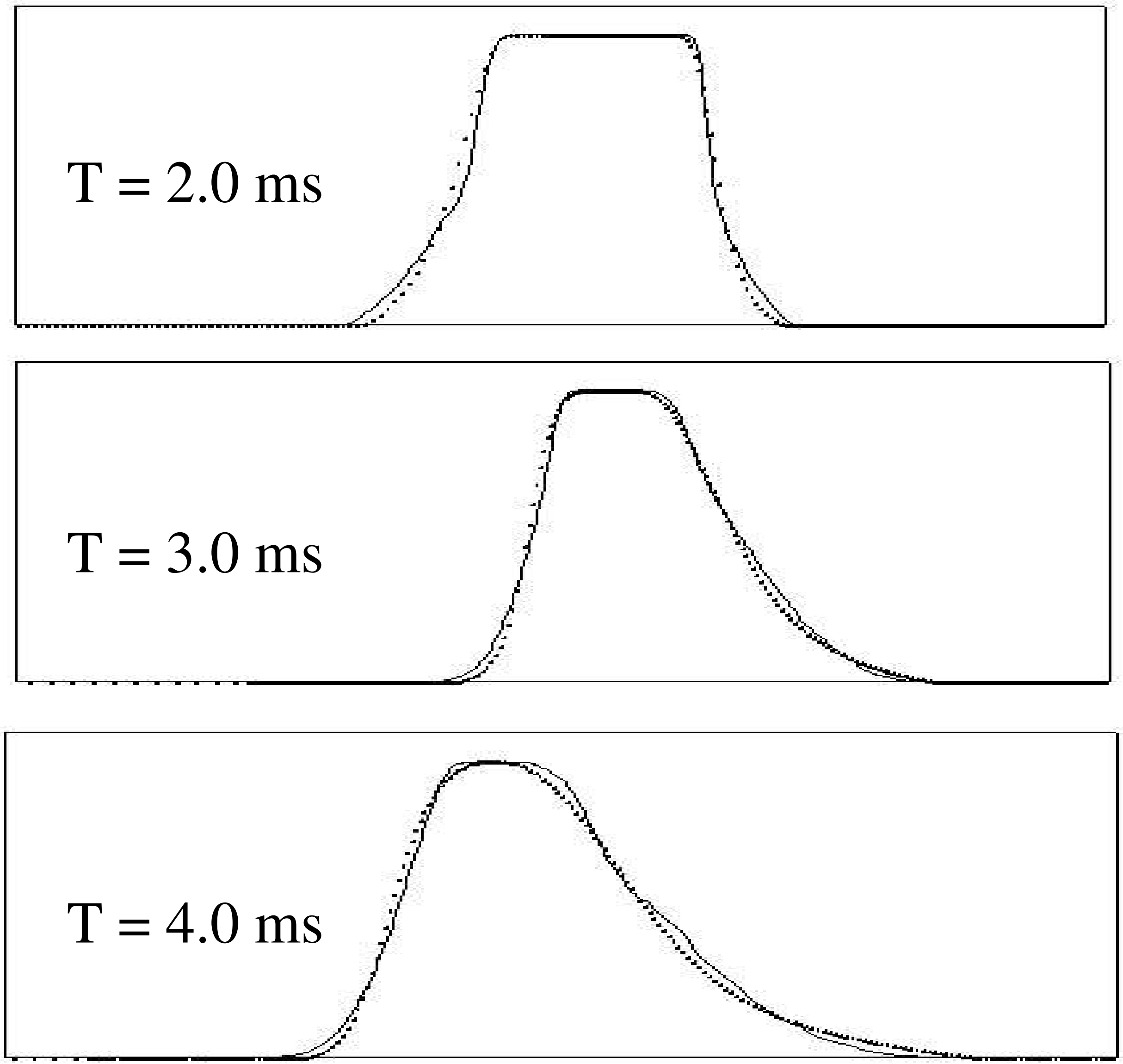


experiment 3D simulation 3D simulation + scattering

AWE SHOCK TUBE EXPERIMENT
Double Bump Results (2.2-3.9 ms)



3D simulation experiment 3D simulation+scattering



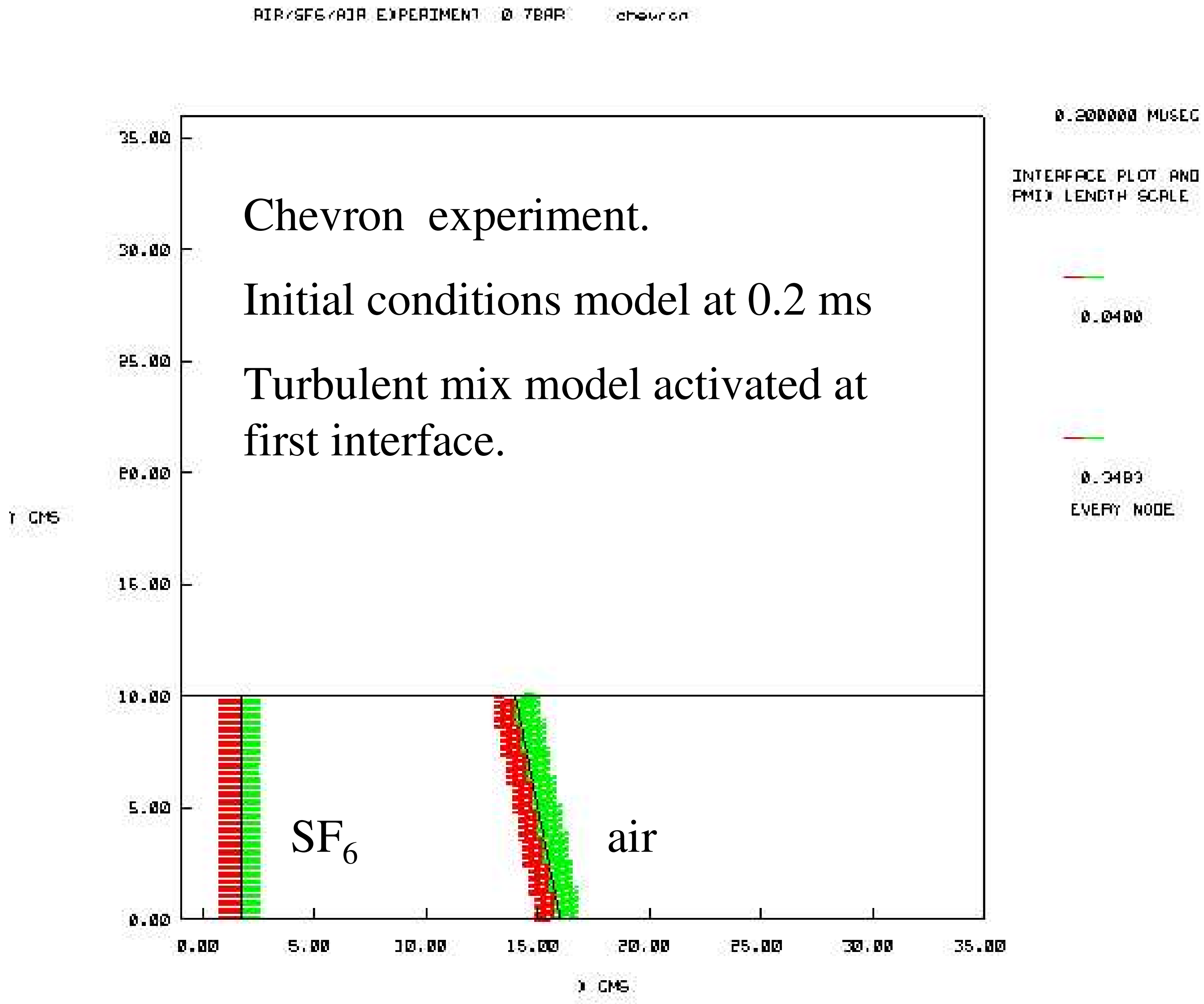
Flat interfaces: plane-averaged SF_6 volume fraction vs distance

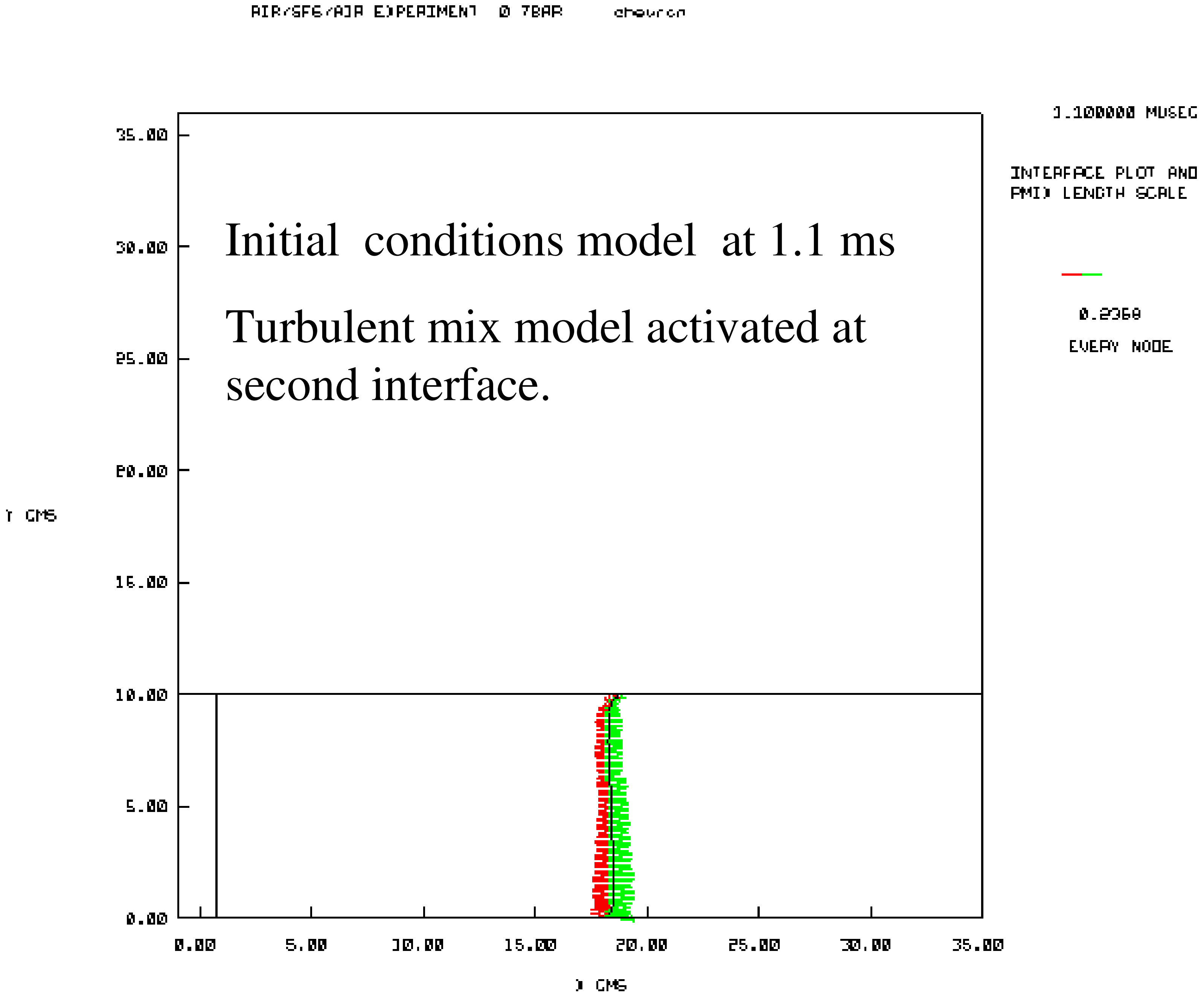
2D mix model •••• , 3D LES ——

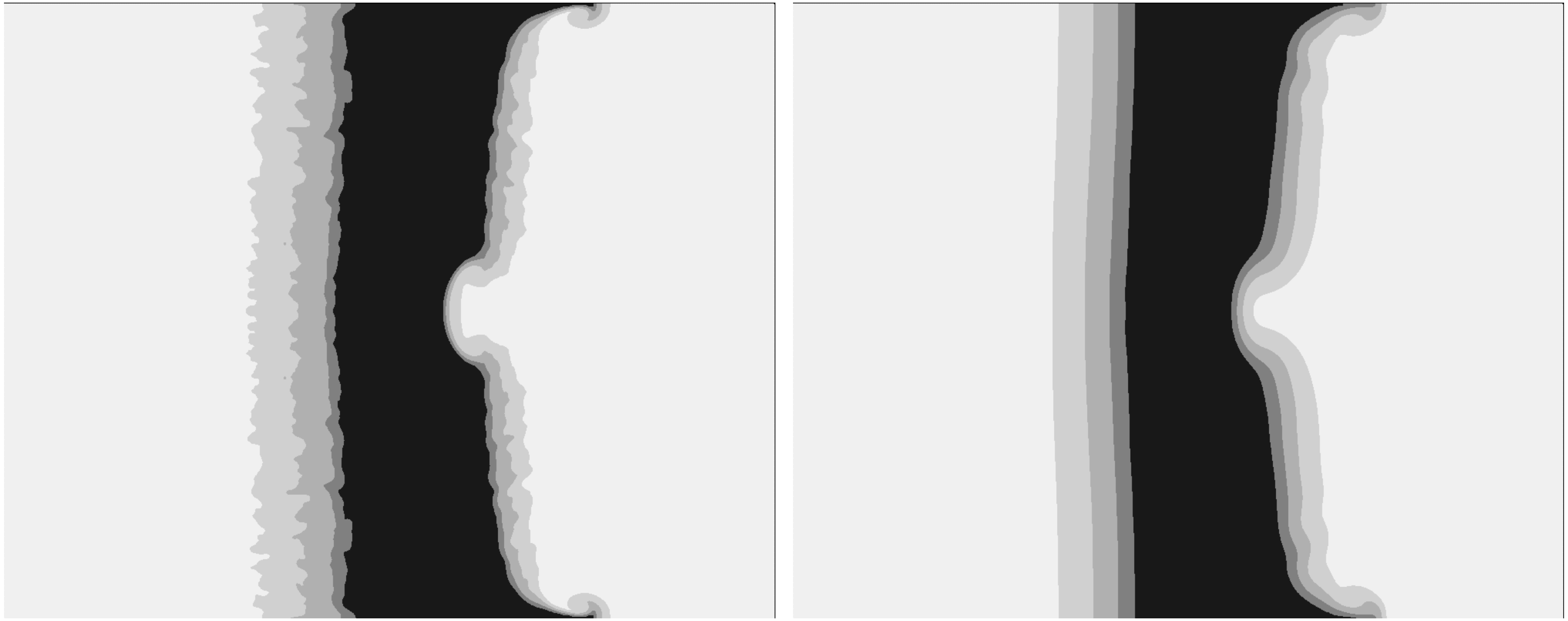
Chevron experiment.

Initial conditions model at 0.2 ms

Turbulent mix model activated at first interface.




AIR/SF6/AIR EXPERIMENT @ 7BAR chevron
1.100000 MUSEC
INTERFACE PLOT AND
RMIX LENGTH SCALE
0.2360
EVERY NODE
Initial conditions model at 1.1 ms
Turbulent mix model activated at second interface.
Y CMS
X CMS
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00

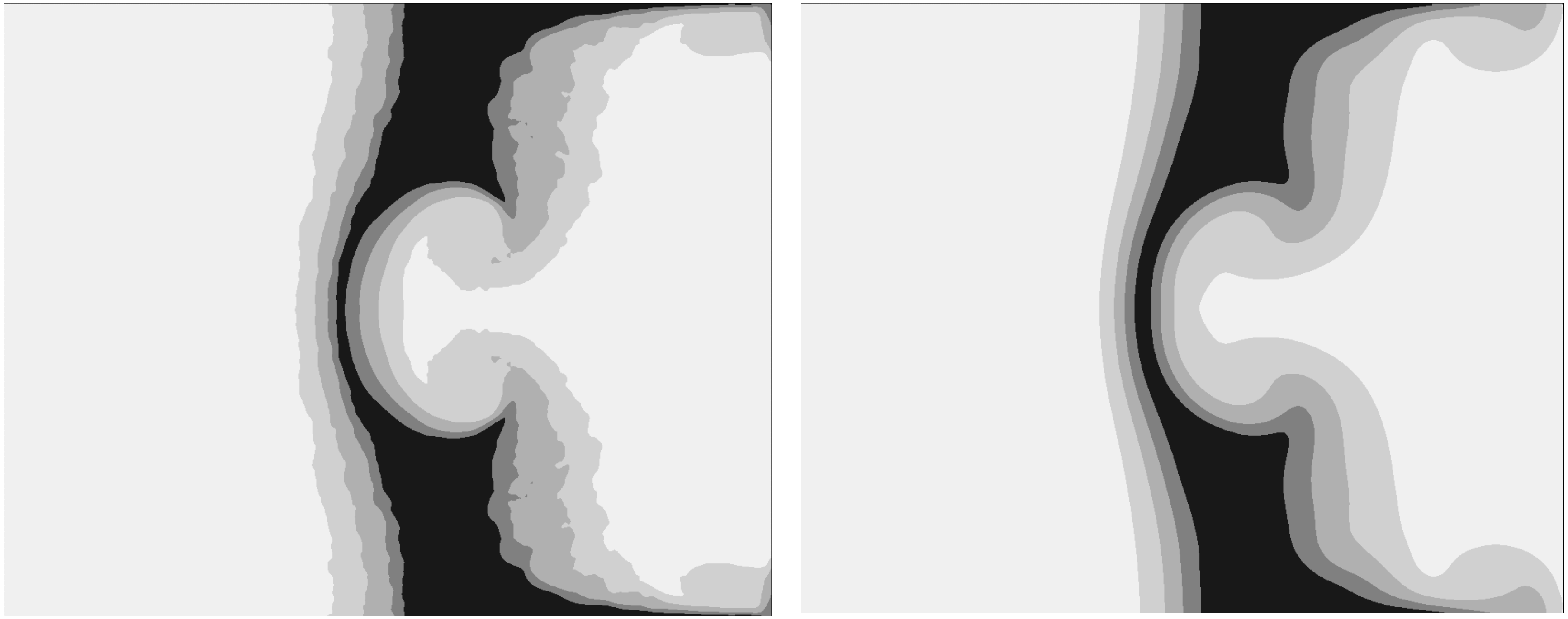


T=2.0ms

TURMOIL3D: 400x320x160 2D model: 160 zones vertical

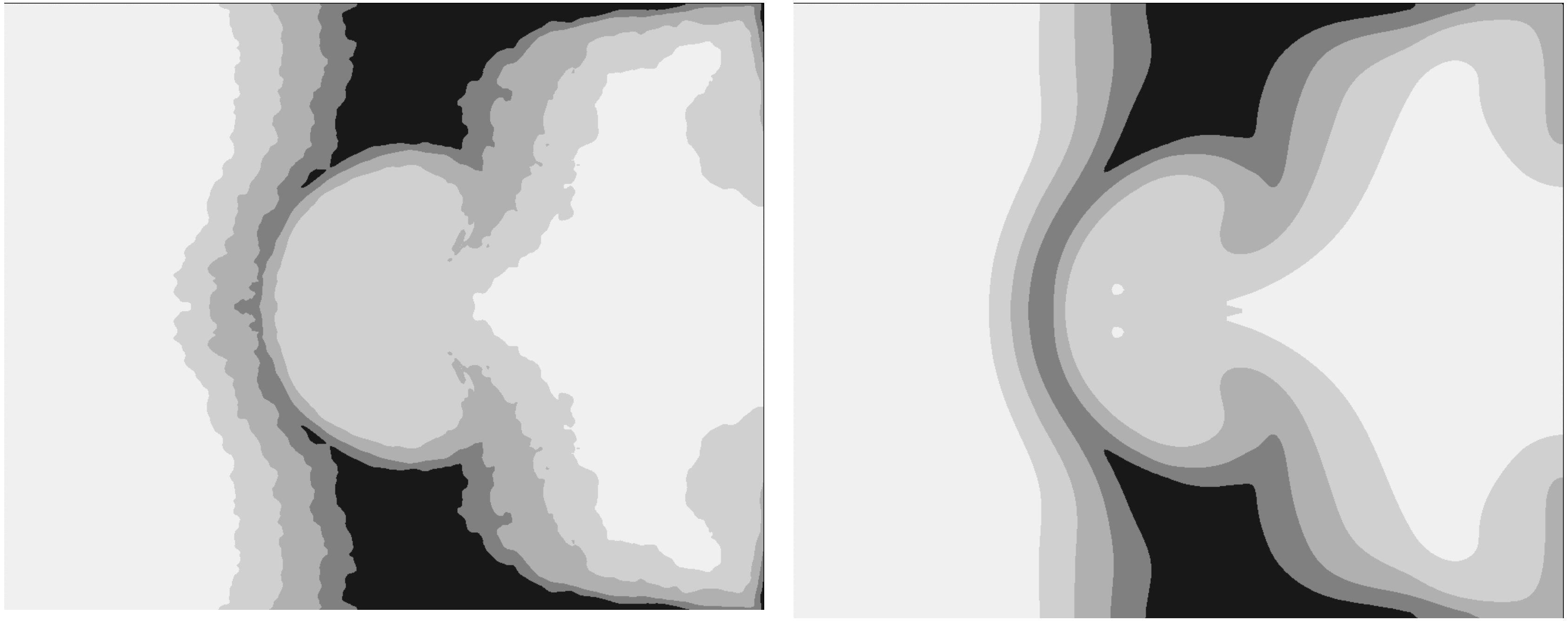
Contours of SF_6 volume fraction averaged in z-direction

contour values: 0.05, 0.3, 0.7, 0.95



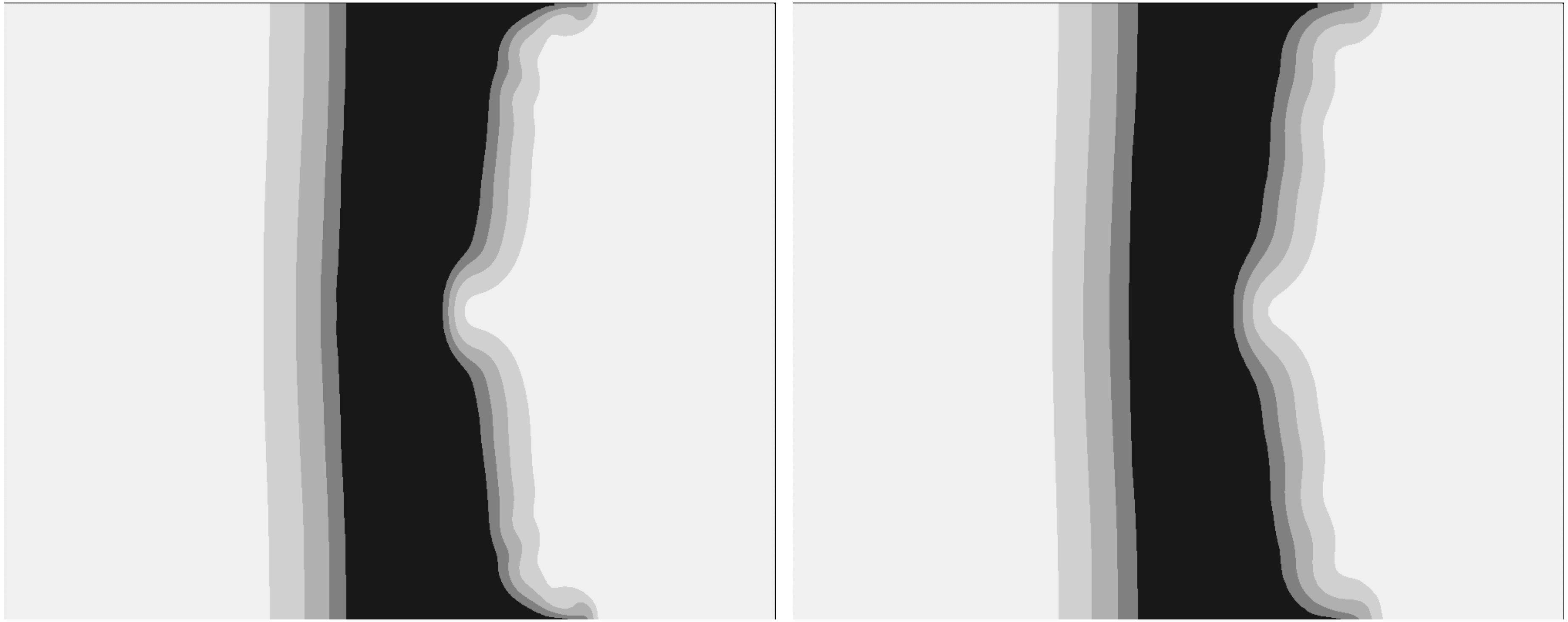
T=3.0ms

TURMOIL3D:400x320x160 2D model:160 zones vertical



T=4.0

TURMOIL3D: 400x320x160   2D model: 160 zones vertical



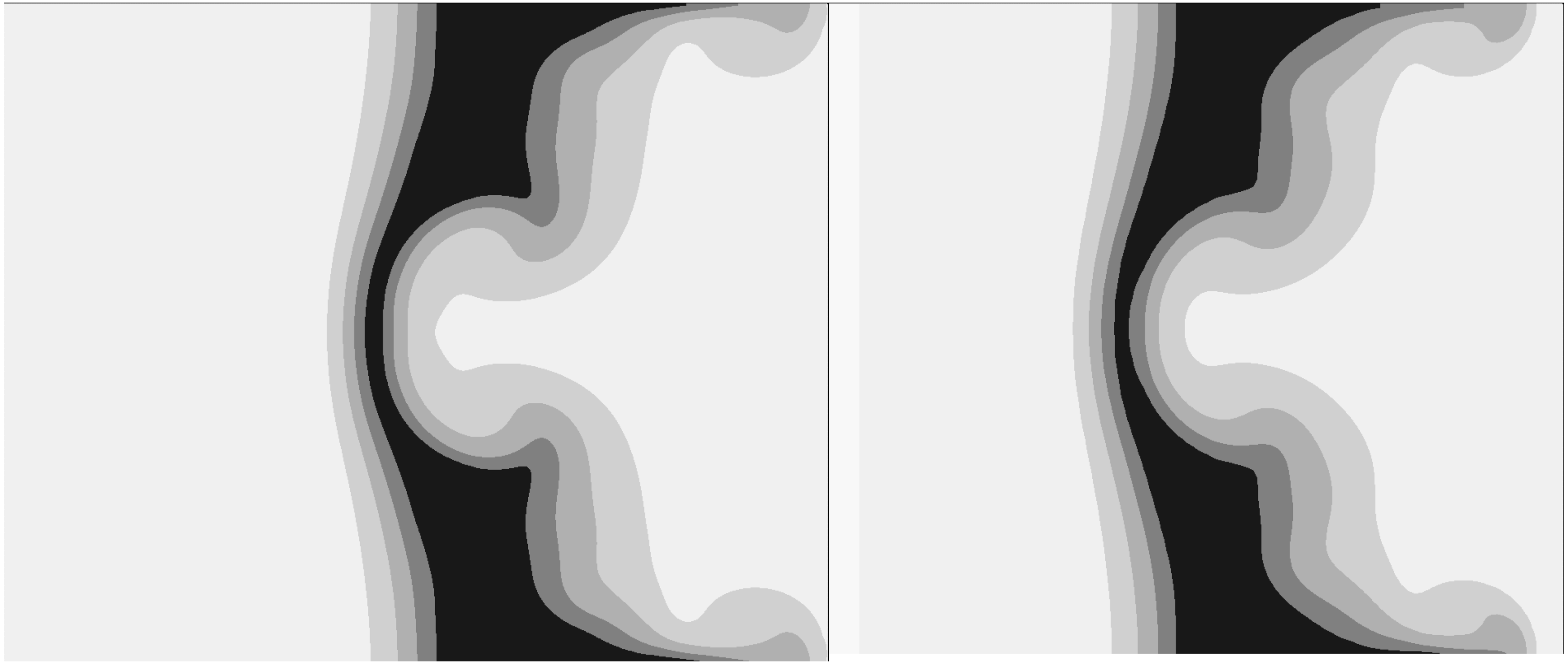
T=2.0ms

2D model

160 zones vertical

2D model

80 zones vertical



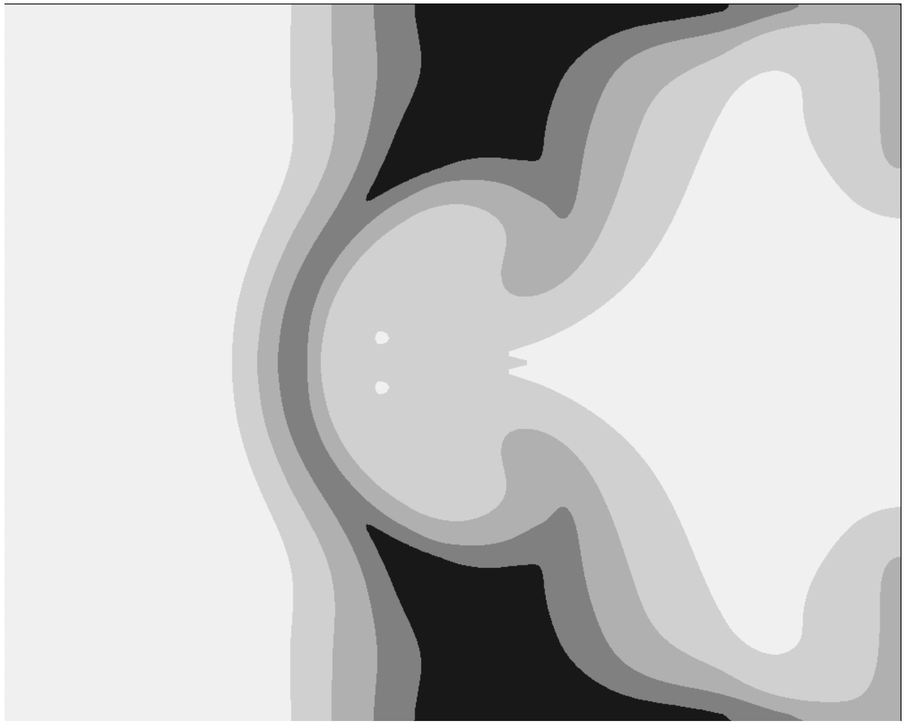
T=3.0 ms

2D model

160 zones vertical

2D model

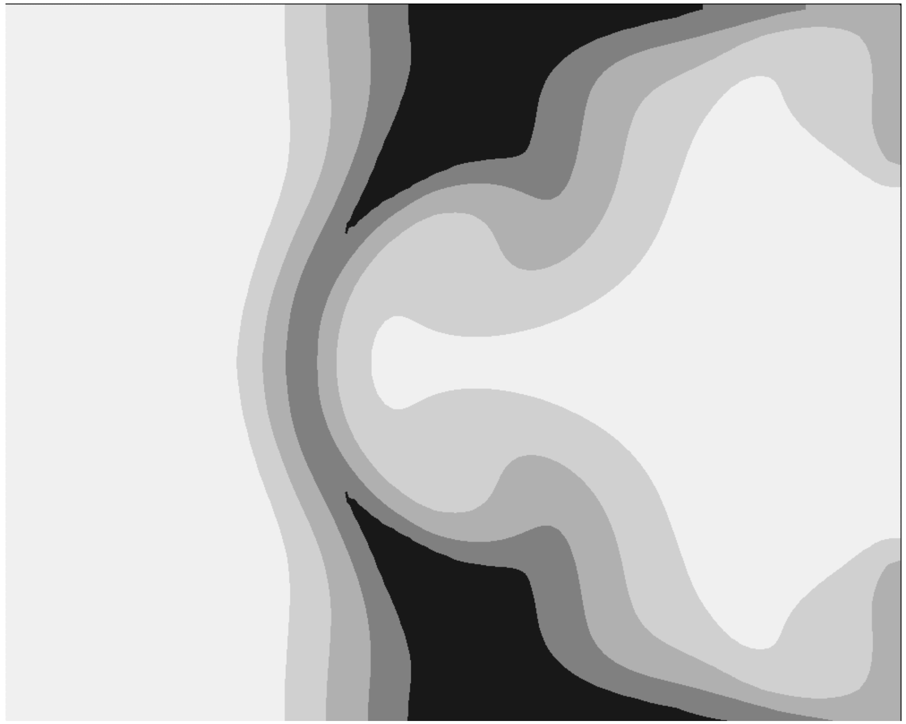
80 zones vertical



T=4.0

2D model

160 zones vertical



2D model

80 zones vertical

CONCLUDING REMARKS

- Robust numerical method devised. Sensitivity to mesh size reduced by the use of van Leer advection and initial conditions model.

- Successful comparison of turbulent mixing model with 3D LES.

- 3D LES for simplified problems will play a very useful role in the validation of the 2D turbulence model for application to real problems.

- Plan to implement the mixing model in 2D ALE hydrocode, using a simple extension of the numerical technique.