New Developments in Multicomponent Reynolds-Averaged Navier–Stokes Modeling of Reshocked Richtmyer–Meshkov Instability and Turbulent Mixing

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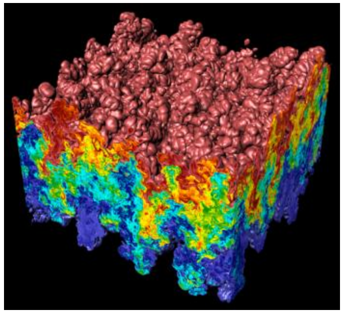
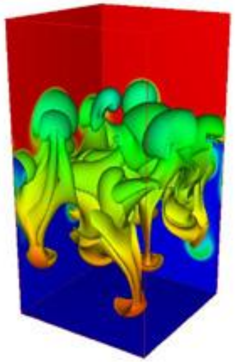
The development of reduced descriptions of turbulent mixing that balance accuracy with cost remains essential

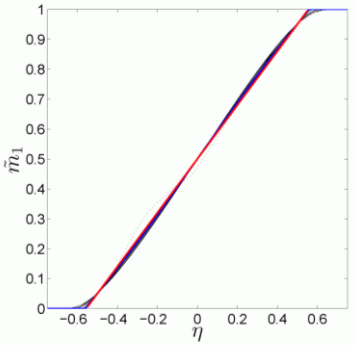
- Simulations and models must account for flow complexities and:
  - broad spectrum of (typically uncertain) initial conditions and range of scales
  - regimes spanning many orders of magnitude (e.g., stellar interiors, ICF): $Re \sim 0\text{–}10^{10}$, $At \sim 10^{-4}\text{–}1$, $Sc \sim 10^{-4}\text{–}10^{3}$



- Direct numerical simulation (DNS): resolve all scales
  - full 3D data available for all fields that can be averaged further
  - ensemble averaging of realizations needed



- Large-eddy simulation (LES)/(M)ILES: resolve "largest" scales
  - "filter" equations and model subgrid terms using resolved-scale fields
  - only resolved fields are available



- Reynolds-averaged (RA) modeling: model all scales
  - ensemble average equations and model unclosed correlations using mean fields
  - turbulent transport equations needed for closures

There are numerous outstanding Reynolds-averaged modeling issues for multifluid turbulent mixing

- Theoretical issues
  - models based on correct and complete unaveraged hydrodynamic equations
  - models better coupled to other physics such as scalar mixing
  - models accounting for transition to large Reynolds number
  - models distinguishing different fluids through their transport properties
  - physics-based initial conditions
  - improved closure submodels and coefficient constraints
- Numerical issues
  - effects of numerically-induced dissipation/diffusion on model physics
  - convergence under spatio-temporal refinement (especially for shocked flows)
  - phasing out model when more flow scales are resolved at higher resolutions

A numerical and theoretical framework has been developed to systematically address these issues

This Reynolds-averaged modeling study advances an improved turbulence model and explores its physical and numerical attributes

- Multicomponent Reynolds-averaged Navier–Stokes (RANS) equations used
  - viscous and thermal effects, and mass and enthalpy diffusion included
  - various dissipation rate and lengthscale-based turbulence models implemented and used for a broad range of cases
  - linear Richtmyer growth rate used to relate initial values of K and ε (or L)
  - a new buoyancy (shock) production closure is used
  - equations solved using a flexible, high-resolution Eulerian method
- RANS simulations are compared with a set of experimental data
  - framework used to develop new modeling approaches and quantify sensitivity of model predictions to coefficients, initial conditions etc.
  - convergence under grid refinement for mixing layer widths, mean fields, and turbulent fields is also considered
  - *numerical dissipation/diffusion effects shown to be important and quantified*

The models are based on the single-velocity, multi-component Reynolds-averaged Navier–Stokes equations

- Mean momentum, total energy, and heavy mass fraction equations are

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{v}_i) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{v}_i\,\widetilde{v}_j) = \overline{\rho}\,g_i - \frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \boxed{\frac{\partial \overline{\sigma}_{ij}}{\partial x_j}}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{e}) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{e}\,\widetilde{v}_j) \quad &= \quad \overline{\rho}\,g_i\,\widetilde{v}_i + \frac{\partial}{\partial x_j}(\overline{p}\,a_j) - \frac{\partial}{\partial x_j}(\overline{p}\,\widetilde{v}_j) - \frac{\partial}{\partial x_j}(\tau_{ij}\,\widetilde{v}_i)\\ &+ \boxed{\frac{\partial}{\partial x_j}(\overline{\sigma}_{ij}\,\widetilde{v}_i)} + \frac{\partial}{\partial x_j}\left(\boxed{\overline{\kappa}\,\frac{\partial \widetilde{T}}{\partial x_j}} + \frac{\mu_t}{\sigma_U}\,\frac{\partial \widetilde{U}}{\partial x_j}\right)\\ &+ \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t}{\sigma_K}\right)\frac{\partial K}{\partial x_j}\right] + \boxed{\frac{\partial \overline{H}_j}{\partial x_j}}\end{aligned}$$

$$\boxed{\widetilde{e} = \frac{\widetilde{v}^2}{2} + \widetilde{U} + K}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,\widetilde{m}_H) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\widetilde{m}_H\,\widetilde{v}_j) = \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\rho}\,\overline{D}} + \frac{\mu_t}{\sigma_m}\right)\frac{\partial \widetilde{m}_H}{\partial x_j}\right]$$

- Boxed molecular transport terms distinguish fluids with *different* mixture viscosities, diffusivities, conductivities etc.

Molecular transport coefficients and ratio of specific heats are expressed in binary mixture form

- Molecular transport coefficients $\phi = \mu$, D, and κ (dynamic viscosity, mass diffusivity, and thermal conductivity) are

$$\overline{\phi} = \frac{\phi_H \,\widetilde{m}_H / \sqrt{MW_H} + \phi_L \,(1 - \widetilde{m}_H) / \sqrt{MW_L}}{\widetilde{m}_H / \sqrt{MW_H} + (1 - \widetilde{m}_H) / \sqrt{MW_L}}$$

(H and L denote heavy and light; $MW_{H,L}$ is molecular weight)

- Mixture ratio of specific heats is

$$\overline{\gamma} = \frac{c_{pH} \,\widetilde{m}_H + c_{pL} \,(1 - \widetilde{m}_H)}{c_{vH} \,\widetilde{m}_H + c_{vL} \,(1 - \widetilde{m}_H)}$$

($c_{pH,L}$, $c_{vH,L}$ are specific heats at constant pressure, volume)

- Arbitrary gas pairs available

The mechanical turbulence equation includes all of the terms that should be present

- Turbulent kinetic energy equation is (Π_K is pressure–dilatation and a_j is mass flux)

$$\frac{\partial}{\partial t}(\overline{\rho}\,K) + \frac{\partial}{\partial x_j}(\overline{\rho}\,K\,\widetilde{v}_j) = a_j\,\frac{\partial \overline{p}}{\partial x_j} - \tau_{ij}\,\frac{\partial \widetilde{v}_i}{\partial x_j} - \overline{\rho}\,\epsilon + \boxed{\Pi_K} + \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t}{\sigma_K}\right)\frac{\partial K}{\partial x_j}\right]$$

with turbulent viscosity

$$\nu_t = \frac{\mu_t}{\overline{\rho}} = C_\mu\,\frac{K^2}{\epsilon} \quad \text{or} \quad \nu_t = \frac{\mu_t}{\overline{\rho}} = C_\mu\,\sqrt{K}\,L$$

requiring a transport equation for turbulent kinetic energy dissipation rate ε or lengthscale L (several models available for Π_K)

- Reynolds stress tensor is (buoyancy generalization also available)

$$\tau_{ij} = \frac{2}{3}\,\overline{\rho}\,K\,\delta_{ij} - 2\,\mu_t\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\,\frac{\partial \widetilde{v}_k}{\partial x_k}\right) \quad , \quad \widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right)$$

The second mechanical equation is for the turbulent kinetic energy dissipation rate or lengthscale

- Turbulent kinetic energy dissipation rate and lengthscale equations are

$$\frac{\partial}{\partial t}(\overline{\rho}\,\epsilon) + \frac{\partial}{\partial x_j}(\overline{\rho}\,\epsilon\,\widetilde{v}_j) = C_{\epsilon 0}\,\frac{\epsilon}{K}\,a_j\,\frac{\partial \overline{p}}{\partial x_j} - C_{\epsilon 1}\,\frac{\epsilon}{K}\tau^d_{ij}\,\frac{\partial \widetilde{v}_i}{\partial x_j} - \frac{2}{3}\,C_{\epsilon 3}\,\overline{\rho}\,\epsilon\,\frac{\partial \widetilde{v}_j}{\partial x_j} - C_{\epsilon 2}\,\frac{\overline{\rho}\,\epsilon^2}{K} + \boxed{C_{\epsilon 4}\,\frac{\epsilon}{K}\Pi_K} + \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right]$$

$$\epsilon \propto \frac{K^{3/2}}{L}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\,L) + \frac{\partial}{\partial x_j}(\overline{\rho}\,L\,\widetilde{v}_j) = C_{L0}\,\frac{L}{K}\,a_j\,\frac{\partial \overline{p}}{\partial x_j} - C_{L1}\,\frac{L}{K}\tau^d_{ij}\,\frac{\partial \widetilde{v}_i}{\partial x_j} - \frac{2}{3}\,C_{L3}\,\overline{\rho}\,L\,\frac{\partial \widetilde{v}_j}{\partial x_j} - C_{L2}\,\overline{\rho}\,\sqrt{K} + \boxed{C_{L4}\,\frac{L}{K}\Pi_K} + \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t}{\sigma_L}\right)\frac{\partial L}{\partial x_j}\right]$$

- A modeled transport equation can be used for a_j or an algebraic closure

$$a_j = -\frac{\nu_t}{\sigma_\rho\,\overline{\rho}}\left(\frac{\partial \overline{\rho}}{\partial x_j} - \boxed{\frac{\overline{\rho}}{\overline{\gamma}\,\overline{p}}\,\frac{\partial \overline{p}}{\partial x_j}}\right)$$

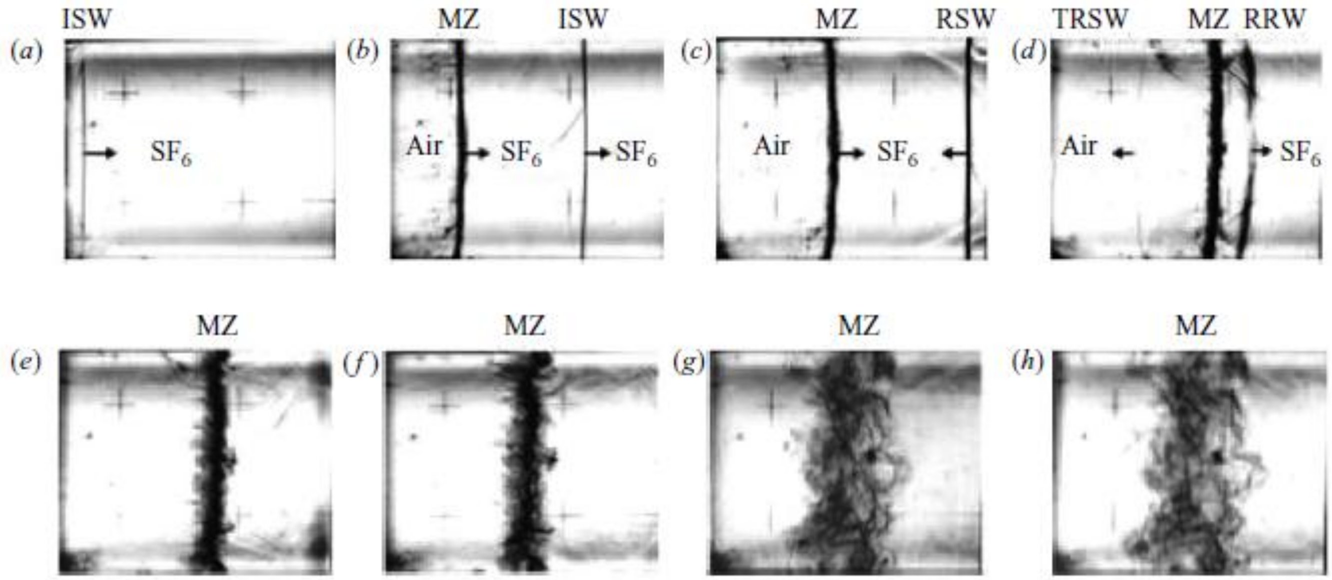
no limiting, shock detection, or ν_t modifications needed

The equations are solved using a conservative, Eulerian WENO finite-difference method with many options

- Weighted essentially nonoscillatory (WENO) reconstruction for advective fluxes (could be another scheme, e.g., PPMLR/DE, MUSCL, TVD, HLLE/C, compact etc.)
  - 1^{st}-, 3^{rd}-, 5^{th}- or 9^{th}-order with various options for weights
  - local Lax–Friedrichs flux splitting
  - Roe averaging using left/right state variables generalized to include turbulent fields and mixture γ
  - transformation to/from characteristic space using left/right eigenvector matrices of $(n + 4) \times (n + 4)$ flux Jacobian (n-equation turbulence model)
  - option for reconstruction in physical space, *avoiding eigensystem operations*
- Spatial derivatives in viscous/diffusive and other source terms computed using central differencing
  - standard central or centered WENO 2^{nd}-, 4^{th}-, 6^{th}- or 10^{th}-order derivatives
- 3^{rd}-order TVD Runge–Kutta time-evolution scheme
  - Courant condition includes molecular and turbulent transport coefficients

Reshocked Richtmyer–Meshkov instability is a shock-driven instability generating turbulent mixing

- Impulsive acceleration of perturbed interface initially separating different density fluids results in growth of perturbations
- Interpenetration and mixing of light and heavy fluid occurs
- Reshock occurs when mixing layer is compressed by a reflected shock (see Leinov et al. [J. Fluid Mech. 626 (2009), 449])
- Experiments and simulations show that reshock significantly *increases mixing layer growth rates* and *generates turbulent mixing*



A new physics-based prescription for initializing the turbulent fields has been applied to many cases

- Initial mean fields left and right of shock set by:
  - ambient conditions, Mach number, and Rankine–Hugoniot relations
  - sharp initial interface (mass fractions)
- Initial turbulent fields set by assuming that initial turbulent kinetic:
  - energy $K(x,0)$ is a small fraction of mean (post-shock) kinetic energy (At^* is post-shock Atwood number)

$$K(x,0) = K_0 \, \frac{At^* \, \widetilde{v}(x,0)^2}{2} \quad , \quad K_0 \approx 10^{-2}$$

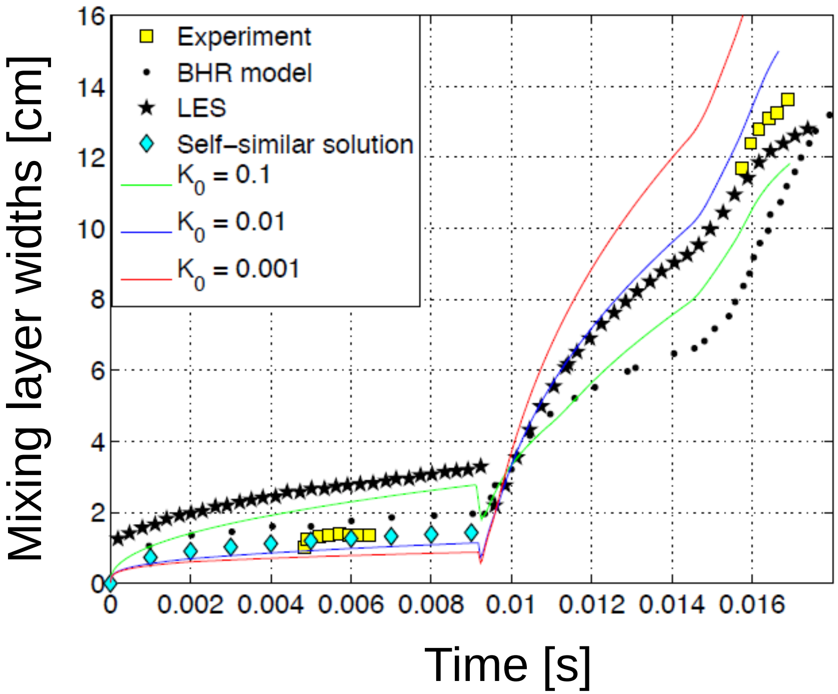
  - energy dissipation rate $\epsilon(x,0)$ or lengthscale $L(x,0)$ related to $K(x,0)$ by linear Richtmyer growth rate $\omega = At^* \, k_{rms} \, |\Delta v|$

$$\epsilon(x,0) = K(x,0)\,\omega \ \text{ or } \ L(x,0) = \frac{\sqrt{K(x,0)}}{\omega}$$

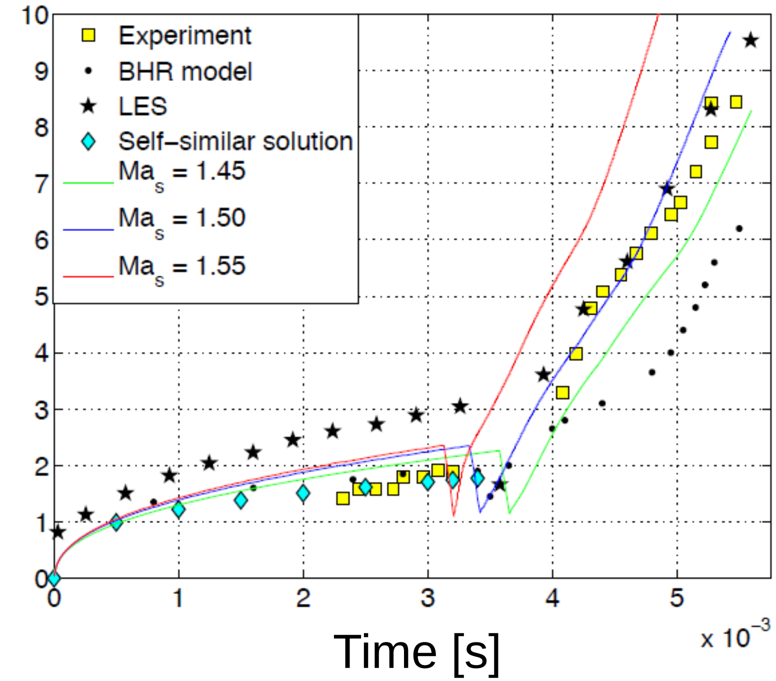
  - *avoids using Kolmogorov scaling* $\epsilon(x,0) \propto K(x,0)^{3/2}/L(x,0)$ (only valid for fully-developed, equilibrium turbulence) with arbitrary $L(x,0)$
  - relates $\epsilon(x,0)$ to physical parameters: dominant <u>perturbation wavenumber</u> $k_{rms} = 2\pi/\lambda_{rms}$, <u>shock strength</u> (Δv) and <u>gas pair</u> (At^*)

Very good agreement with Vetter–Sturtevant Ma_s = 1.24 and 1.50 data was obtained using the K–ε model*

Vetter–Sturtevant Ma_s = 1.24



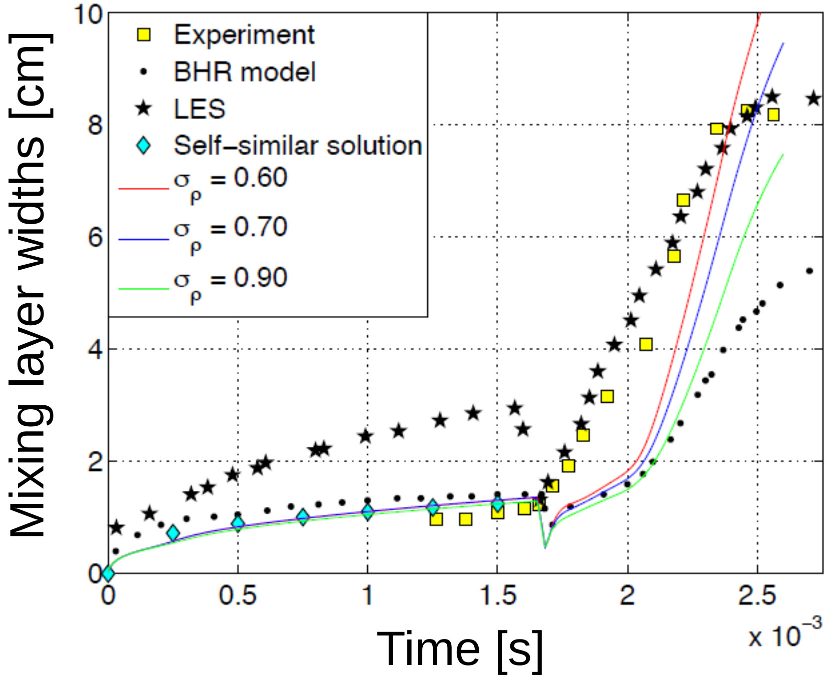
Vetter–Sturtevant Ma_s = 1.50

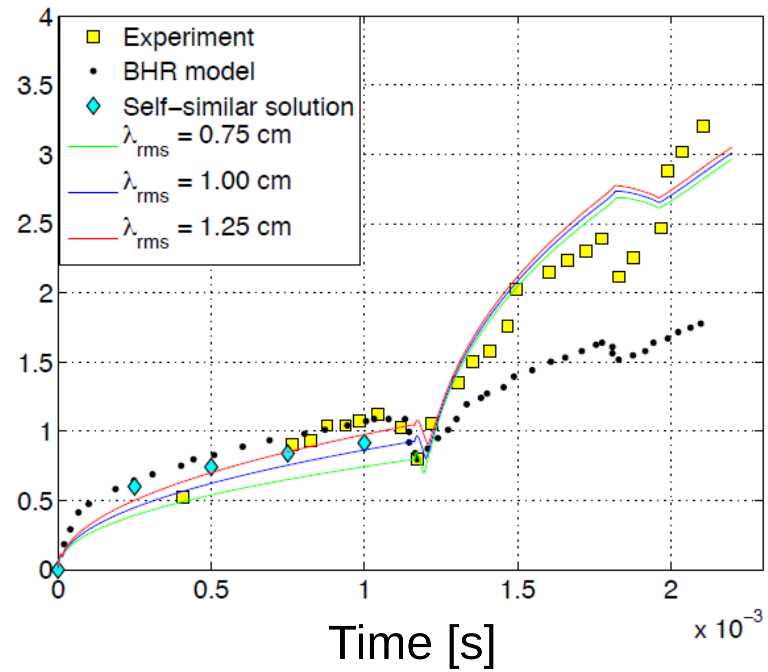


- Grid-converged widths for $C_{\varepsilon 0}$ = 0.90 and σ_ρ = 0.90, $\sigma_m = \sigma_U = \sigma_K = \sigma_\varepsilon$ = 0.5 ($C_{\varepsilon 1}$ = 1.44, $C_{\varepsilon 2}$ = 1.92 , $C_{\varepsilon 3}$ = 2.00)
- Effects of initial conditions and Mach number variation examined for Ma_s = 1.24 and 1.50, respectively

*see Morán-López, J. T. & Schilling, O. 2013 Multicomponent Reynolds-averaged Navier–Stokes simulations of reshocked Richtmyer–Meshkov instability-induced mixing. *High Energy Density Physics* 9, 112–121

Good agreement with Vetter–Sturtevant Ma_s = 1.98 and Poggi et al. Ma_s = 1.45 data was also obtained using the K–ε model*

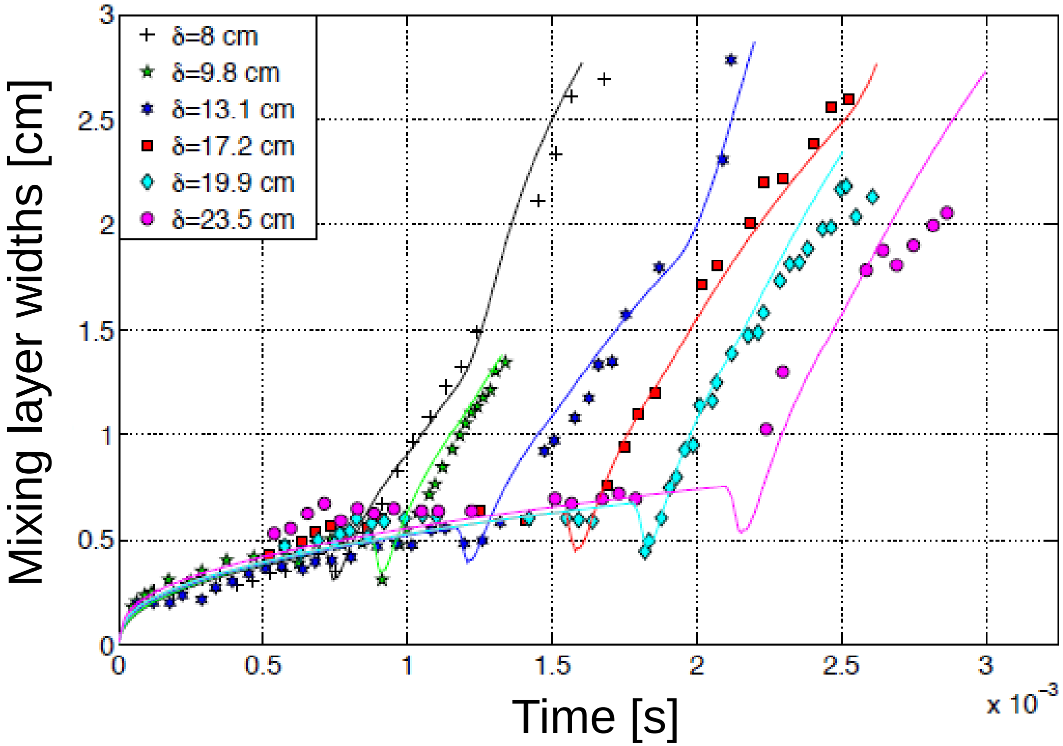




- Grid-converged widths for $C_{\varepsilon 0}$ = 0.90 and σ_ρ = 0.90, $\sigma_m = \sigma_U = \sigma_K = \sigma_\varepsilon = 0.5$ ($C_{\varepsilon 1}$ = 1.44, $C_{\varepsilon 2}$ = 1.92 , $C_{\varepsilon 3}$ = 2.00)
- Effects of changing σ_ρ and initial perturbation wavelength λ_{rms} examined for Ma_s = 1.98 and 1.45, respectively

*see Morán-López, J. T. & Schilling, O. 2013 Multicomponent Reynolds-averaged Navier–Stokes simulations of reshocked Richtmyer–Meshkov instability-induced mixing. *High Energy Density Physics* 9, 112–121

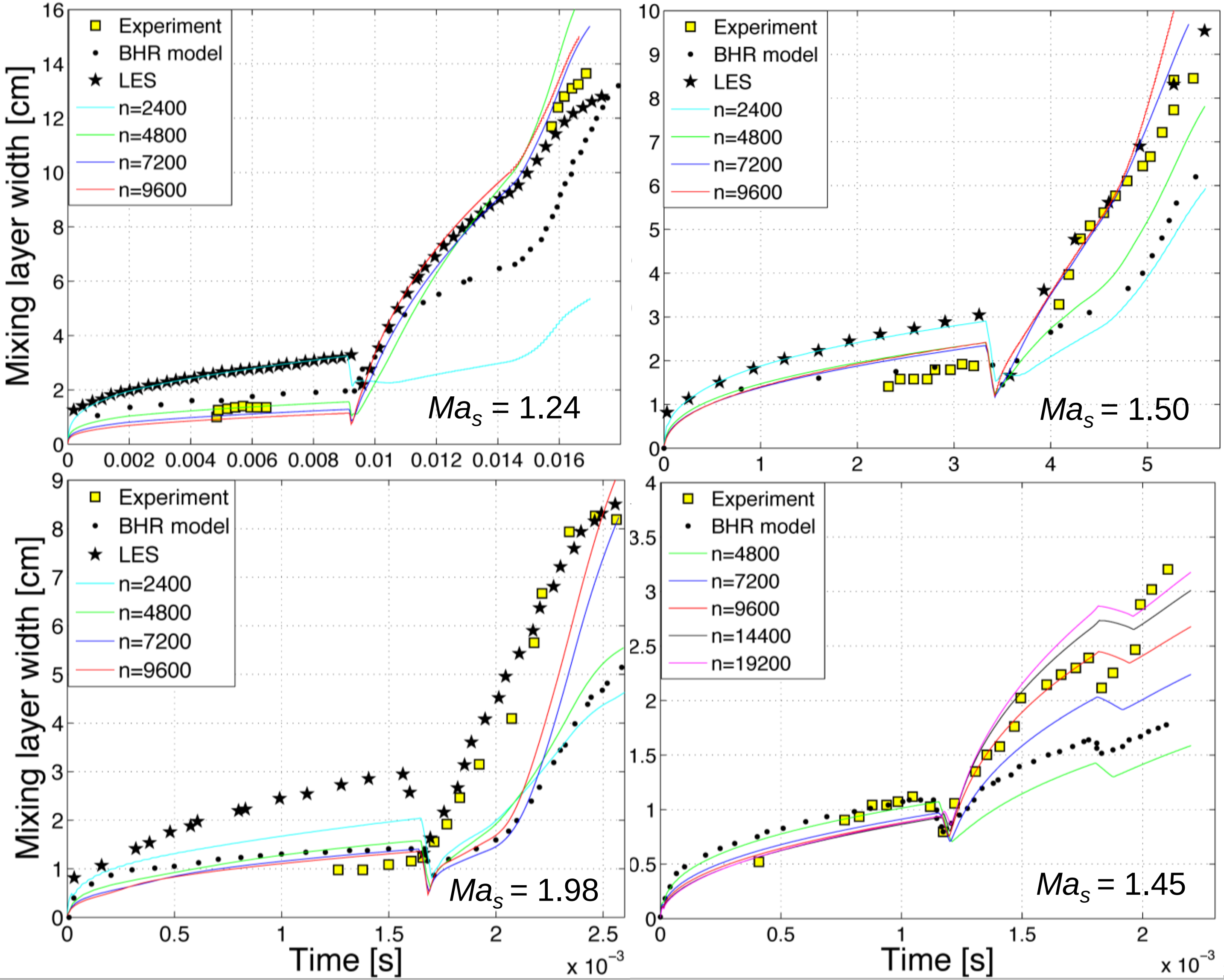
Very good agreement with the Leinov et al. Ma_s = 1.20 data for different test section lengths (reshock times) was also obtained*



- Predicted, grid-converged widths also agree very well with 3D ALE simulations by Leinov et al. for three test section lengths
- RANS predictions consistent with experiments: as δ is increased (reshock of increasingly nonlinear mixing layers), post-reshock growth rates increase

*see Morán-López, J. T. & Schilling, O. 2013 Multicomponent Reynolds-averaged Navier–Stokes simulations of Richtmyer–Meshkov instability and mixing induced by reshock at different times. *Shock Waves* (in press)

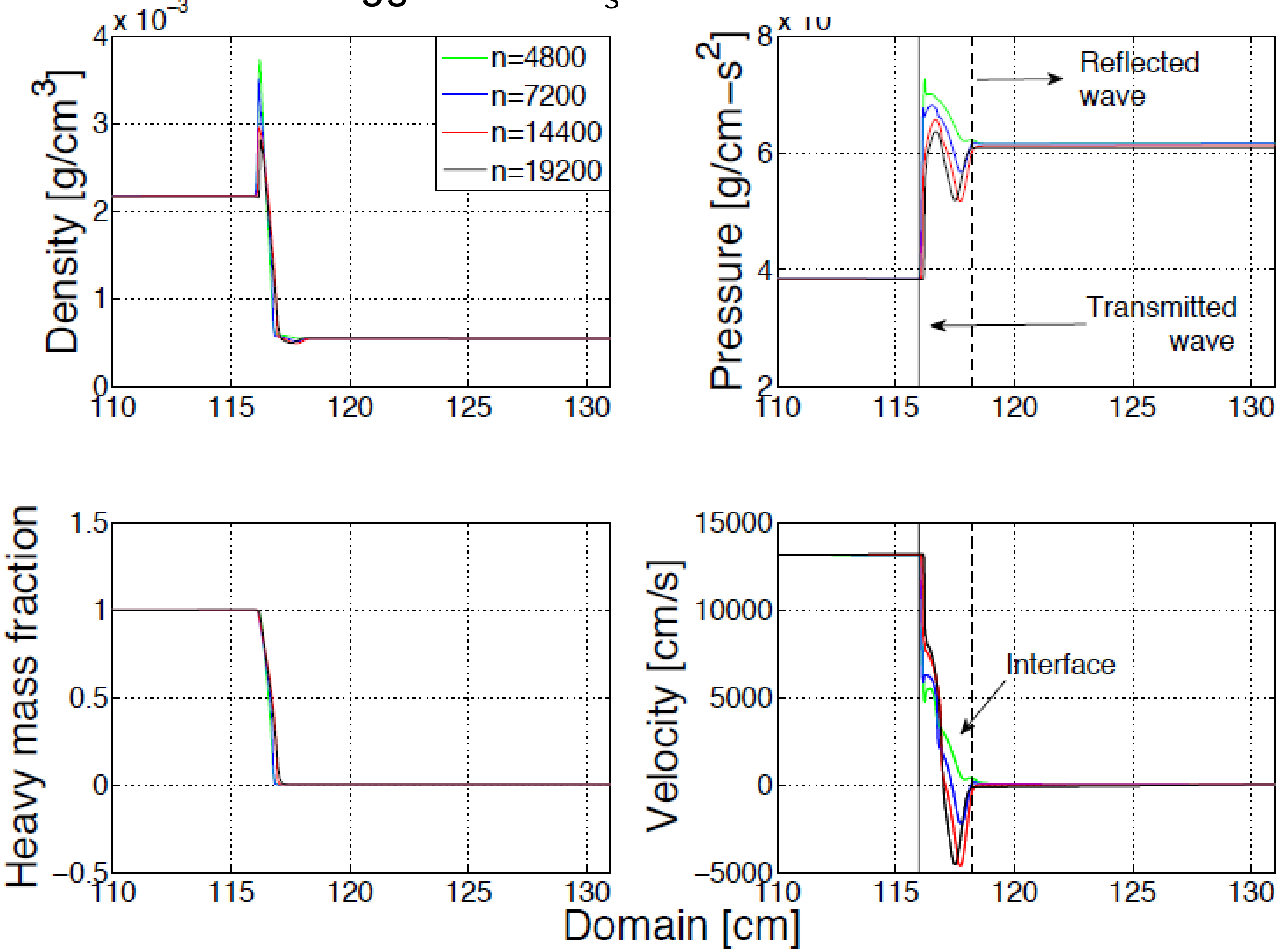
The turbulent mixing layer widths converge under spatial grid refinement



- Ma_s = 1.24, 1.50, 1.98: 161 cm domain
  - Δx = 0.07, 0.03, 0.02, 0.01 cm
  - 86, 260, 485, 1000 points in layer
  - LES had Δx = 0.21 cm
- Ma_s = 1.45: 131 cm domain
  - Δx = 0.03, 0.02, 0.01, 0.009, 0.007 cm
  - 53, 113, 270, 333, 457 points in layer

The mean fields, which are the principal quantities predicted by the model, converge

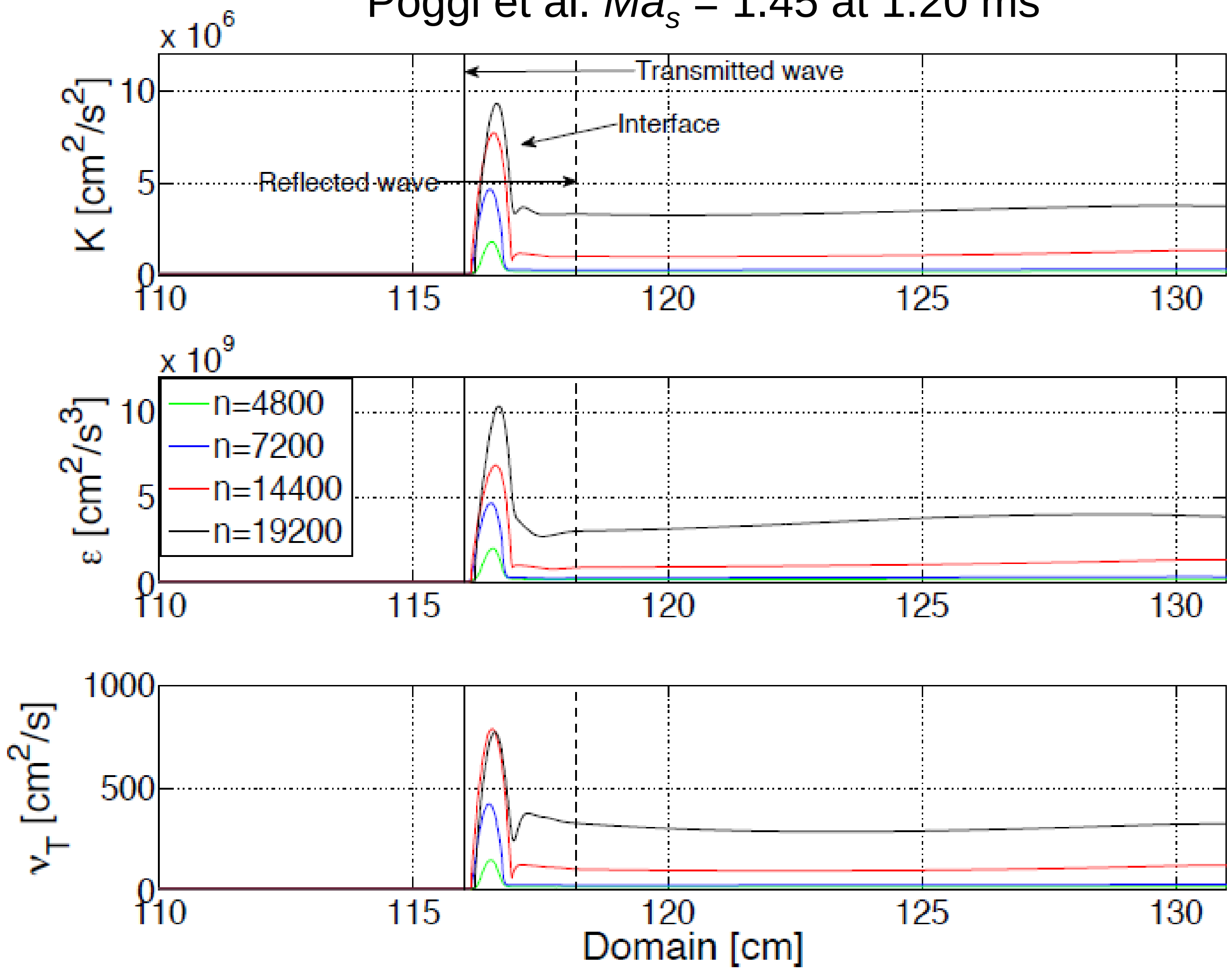
Poggi et al. Ma_s = 1.45 at 1.20 ms



- peak density and pressure overpredicted on coarse grids
- velocity poorly resolved on coarse grids
- similar results for Ma_s = 1.24, 1.50 and 1.98 cases
- heavy-to-light transition requires more points than light-to-heavy

The turbulent fields K and ε do not converge, but the turbulent viscosity does converge

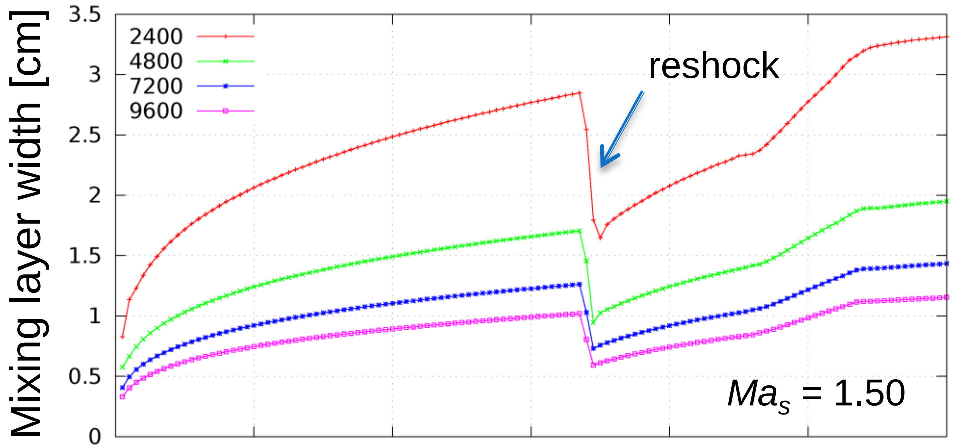
Poggi et al. Ma_s = 1.45 at 1.20 ms



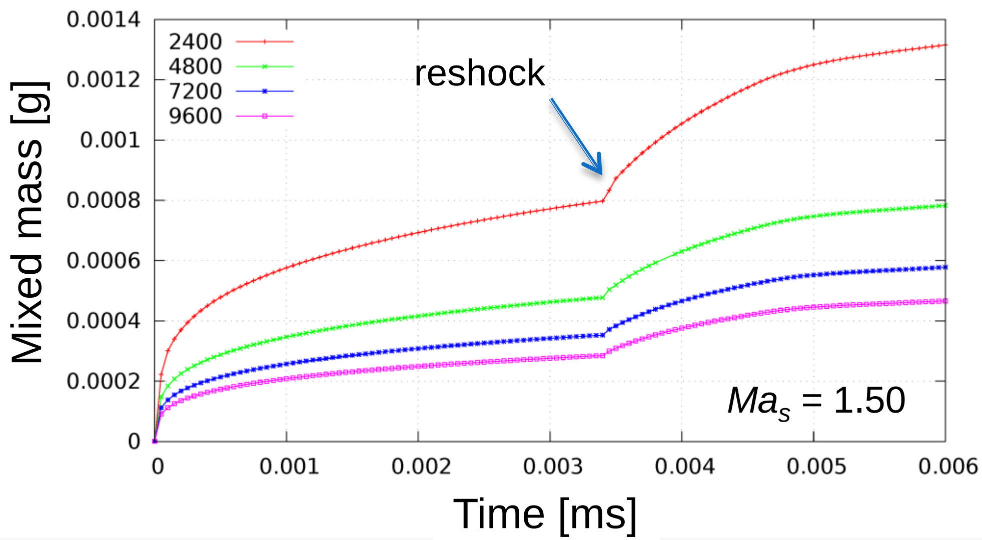
- $K \propto 1/\Delta x$ and $\varepsilon \propto 1/(\Delta x)^2$ still growing: very sensitive to model details, shocks, waves, grid
- $\nu_t \propto K^2/\varepsilon$ converges within layer
- mass fraction diffusion (i.e., layer width) $\propto \nu_t$
- similar results for Ma_s = 1.24, 1.50 and 1.98 cases

Eulerian methods require many grid points to minimize *mixing from numerical dissipation/diffusion*

Mixing layer width *with turbulence model off*



Mixed mass *with turbulence model off*



- Lagrangian methods give zero width without a turbulence model
- Eulerian methods give nonzero width due to:
  - dissipative upwinding
  - diffusive errors from remaps
  - truncation errors
- Advection of fields (including mass fraction) induces numerical diffusion
- Turbulence vs. numerical model contribution small on coarse grids
- *Mixed mass* quantifies mass of light (air) and heavy (SF_6) gas mixed by purely numerical effects

$$mm(t) = L_x^2 \int_0^{L_x} \overline{\rho}(x,t)\, \widetilde{m}_H(x,t)\, \widetilde{m}_L(x,t)\, \mathrm{d}x$$

- Width and mixed mass grow with shallower power-laws as grid refined

A general numerical framework is being used for development and assessment of turbulence models

- Implemented many multicomponent Reynolds-averaged turbulence models in a flexible high-resolution Eulerian numerical framework
  - K–ε and K–L based, and extensions of models to include scalar turbulence
  - molecular transport based on full Navier–Stokes equations
- Applied an advanced K–ε model to ten Ma_s = 1.20–1.98 reshocked Richtmyer–Meshkov experiments (a validation suite for $At = \pm 0.67$)
  - new production term closure with no limiters, shock detection or modified ν_t
  - introduced new initialization of turbulent fields based on physical parameters
  - converged mixing layer widths are in good agreement with data
  - post-reshock widths are most sensitive to variations in $C_{\varepsilon 0}$ and σ_ρ
- Explored convergence of widths, mean fields, and turbulent fields
  - K and ε do not converge, but ν_t, mean fields and widths do converge
  - quantified numerical diffusion effects on layer width using mixed mass