A Framework for Multicomponent, Reynolds-Averaged Navier–Stokes Modeling of Hydrodynamic Instability-Induced Turbulent Mixing

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A numerical and theoretical framework is being used to comprehensively evaluate the predictive capabilities and limitations of Reynolds-averaged (RA) mixing models

- Assess merits of lower and higher order closure models for turbulent mixing
  - 2-, 3-, 4-equation
  - 2 dissipation rate/lengthscale
  - Reynolds stress
  - multi-velocity
- Understand implications of using these models for calibration and initialization
  - derive and analyze expressions for self-similar growth parameters: calibration
  - assess complexity of initialization with increasing number of model equations
- Assess predictions of models against a broad range of flows critically and objectively, including self-similar and non-self-similar turbulent flows
  - constant *g* Rayleigh–Taylor, reshocked Richtmyer–Meshkov, shear
  - variable *g* Rayleigh–Taylor, blast waves, shock–turbulence interaction
  - combined instabilities
- Evaluate differences and advantages/disadvantages of ε- and L-based models
  - physics, numerics

To achieve a good balance between predictive capability, model complexity, and robustness, it is important to establish a *point of diminishing returns* where LES should be used instead of RA models

The turbulent kinetic energy and the dissipation rate or lengthscale equation can be expressed in a concise form that unifies the models

- Turbulent kinetic energy and dissipation rate/lengthscale equation ($Z = C_Z K^m \varepsilon^n$ with K–ε and K–L models given by m = 0, n = 1 and m = 3/2, n = -1), where normalized mass flux is $a_j = \overline{\rho' v''_j}/\overline{\rho}$ and Π_K is Sarkar pressure–dilatation model:

$$\begin{aligned}\frac{\partial}{\partial t}(\overline{\rho}\,K) + \frac{\partial}{\partial x_j}(\overline{\rho}\,K\,\widetilde{v}_j) &= a_j\left(\frac{\partial \overline{p}}{\partial x_j} - \boxed{\frac{\partial \overline{\sigma}_{ij}}{\partial x_i}}\right) - \tau_{ij}\,\frac{\partial \widetilde{v}_i}{\partial x_j} + \boxed{\Pi_K} - \left(1 + \boxed{Ma_t^2}\right)\frac{\overline{\rho}\,Z^{1/n}}{C_Z^{1/n}\,K^{m/n}} \\ &+ \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t^Z}{\sigma_K}\right)\frac{\partial K}{\partial x_j}\right]\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\overline{\rho}\,Z) + \frac{\partial}{\partial x_j}(\overline{\rho}\,Z\,\widetilde{v}_j) &= C_{Z0}\,\frac{Z}{K}\,a_j\left(\frac{\partial \overline{p}}{\partial x_j} - \boxed{\frac{\partial \overline{\sigma}_{ij}}{\partial x_i}}\right) - C_{Z1}\,\frac{Z}{K}\,\tau_{ij}^d\,\widetilde{S}_{ij} - \frac{2}{3}\,C_{Z3}\,\overline{\rho}\,Z\,\frac{\partial \widetilde{v}_j}{\partial x_j} \\ &+ \boxed{C_{Z4}\,\frac{Z}{K}\,\Pi_K} - \frac{C_{Z2}}{C_Z^{1/n}}\,\frac{\overline{\rho}\,Z^{1/n+1}}{K^{m/n+1}} + \frac{\partial}{\partial x_j}\left[\left(\boxed{\overline{\mu}} + \frac{\mu_t^Z}{\sigma_Z}\right)\frac{\partial Z}{\partial x_j}\right]\end{aligned}$$

with turbulent viscosity, diffusivity, conductivity $\nu_t^Z = \dfrac{\mu_t^Z}{\overline{\rho}} = C_\mu^Z\,\dfrac{K^{m/n+2}}{Z^{1/n}}\,,\; D_t^Z = \dfrac{\nu_t^Z}{Sc_t}\,,\; \kappa_t^Z = \dfrac{\overline{c}_p\,\mu_t^Z}{Pr_t}$

- Reynolds stress tensor is

$$\tau_{ij} = \frac{2}{3}\,\overline{\rho}\,K\,\delta_{ij} - 2\,\mu_t^Z\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\,\frac{\partial \widetilde{v}_k}{\partial x_k}\right) = \frac{2}{3}\,\overline{\rho}\,K\,\delta_{ij} + \tau_{ij}^d$$

The normalized mass flux a_j can be modeled algebraically (2-equation) or differentially (>2-equation model)

- Algebraic model for *K*–*Z* models:

$$a_j = \frac{\overline{\rho' \, v_j''}}{\overline{\rho}} = \frac{\nu_t^Z}{\sigma_\rho \, \overline{c}_p} \frac{\partial \overline{s}}{\partial x_j} \approx -\frac{\nu_t^Z}{\sigma_\rho \, \overline{\rho}} \left(\frac{\partial \overline{\rho}}{\partial x_j} - \frac{\overline{\rho}}{\overline{\gamma} \, \overline{p}} \frac{\partial \overline{p}}{\partial x_j} \right)$$

- Modeled transport equation for *K*–*Z*–*a*–(*b*) models

$$\frac{\partial}{\partial t}(\overline{\rho} \, a_i) + \frac{\partial}{\partial x_j}(\overline{\rho} \, a_i \, \widetilde{v}_j) = (1 - C_{a0}) \, b \left(\frac{\partial \overline{p}}{\partial x_i} - \boxed{\frac{\partial \overline{\sigma}_{ij}}{\partial x_j}} \right) - \frac{\tau_{ij}}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial x_j} + \overline{\rho} \, a_j \frac{\partial}{\partial x_j} [a_i + (C_{a2} - 1) \, \widetilde{v}_i]$$
$$+ \overline{\rho} \frac{\partial}{\partial x_j}(a_i \, a_j) - \frac{C_{a1}}{C_Z^{1/n}} \frac{\overline{\rho} \, Z^{1/n} \, a_i}{K^{m/n+1}} + \overline{\rho} \frac{\partial}{\partial x_j} \left[\frac{\nu_t^Z}{\sigma_a} \left(\frac{\partial a_i}{\partial x_j} + \frac{\partial a_j}{\partial x_i} \right) \right]$$

- Requires an algebraic or differential model for *b* in *K*–*Z*–*a*–(*b*) models

$$\frac{\partial}{\partial t}(\overline{\rho} \, b) + \frac{\partial}{\partial x_j}(\overline{\rho} \, b \, \widetilde{v}_j) = -(b+1) \frac{\partial}{\partial x_j}(\overline{\rho} \, a_j) + \overline{\rho} \, a_j \frac{\partial b}{\partial x_j} - \frac{C_{b1}}{C_Z^{1/n}} \frac{\overline{\rho} \, Z^{1/n} \, b}{K^{m/n+1}} + \overline{\rho}^2 \frac{\partial}{\partial x_j} \left(\frac{\nu_t^Z}{\sigma_b \, \overline{\rho}} \frac{\partial b}{\partial x_k} \right)$$

- Rather than solving an equation for *b*, can use an algebraic model in *K*–*Z*–*a* models ($c > 0$ prevents divergence in $At \uparrow 1$ limit)

$$b = \overline{\rho} \, \overline{V} - 1 = [f_1 \, \overline{\rho}_1 + (1 - f_1) \, \overline{\rho}_2] \left[\frac{f_1/(\overline{\rho}_1 + c \, \overline{\rho}) + (1 - f_1)/(\overline{\rho}_2 + c \, \overline{\rho})}{f_1 \, \overline{\rho}_1/(\overline{\rho}_1 + c \, \overline{\rho}) + (1 - f_1) \, \overline{\rho}_2/(\overline{\rho}_2 + c \, \overline{\rho})} \right] - 1$$

Self-similar solutions of 2-, 3-, and 4-equation models for Rayleigh–Taylor flow yield progressively more complex expressions for α*

- *K–L* model

$$\alpha(C_\mu, C_{Ls}, \sigma_\rho, C_{L0}, C_{L2}) = \frac{C_\mu\, C_{Ls}\,(C_{L0} - C_{L2})^2}{8\,\sigma_\rho\,(1 - C_{L0})(1 - C_{L2})}$$

- *K–L–a* model (generalization of Morgan–Wickett expression, but suppressing *At* and *c* dependence for clarity)

$$\alpha(C_{Ls}, C_{L0}, C_{L2}, C_{a1}) = \frac{C_{Ls}\,(C_{L0} - C_{L2})^2}{3\,(1 - C_{L2})[4\,C_{a1}\,(1 - C_{L0}) + C_{Ls}\,(3\,C_{L0} - C_{L2} - 2)]}$$

- *K–L–a–b* model

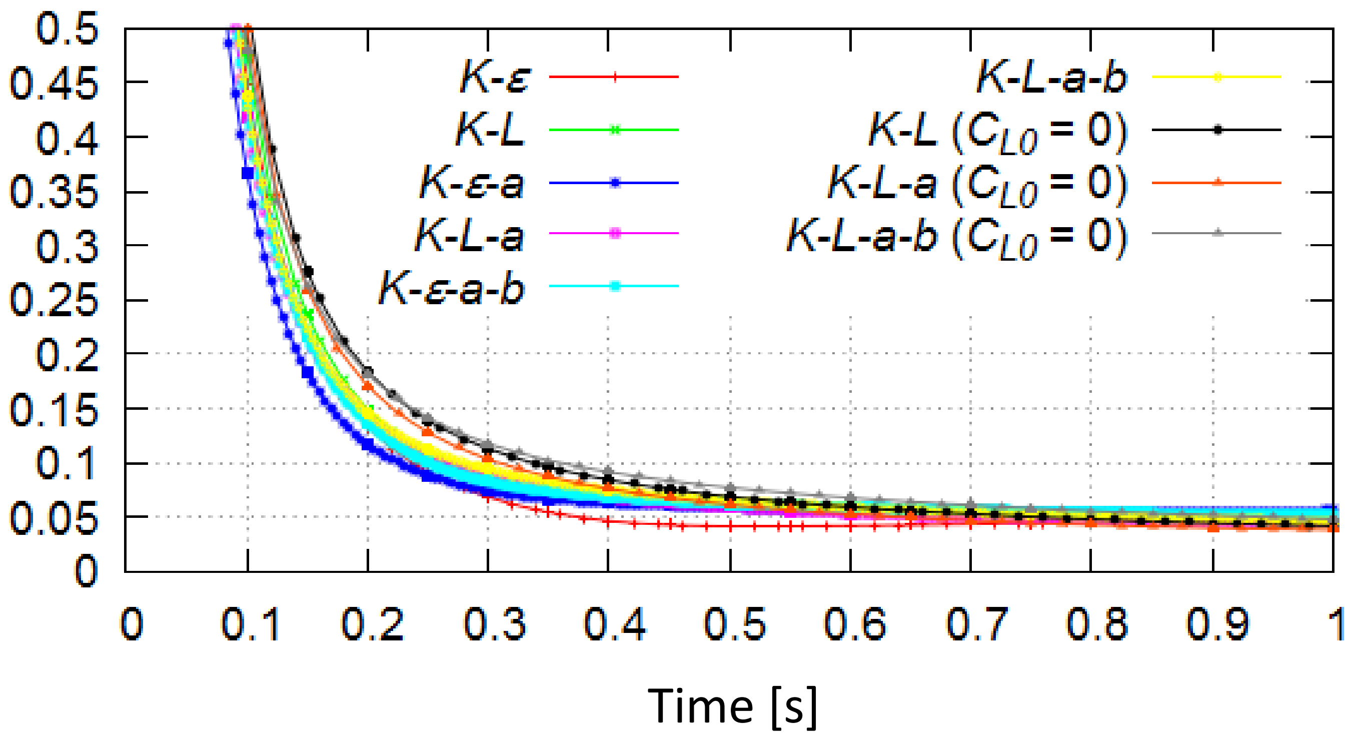
$$\alpha(C_{Ls}, C_{L0}, C_{L2}, C_{a0}, C_{a1}, C_{b2}) = \frac{(C_{L0} - C_{L2})^2}{C_{L2} - 1} \times \frac{2\,C_{b2}\,(C_{L0} - 1)/3 + C_{Ls}\,[2\,C_{a0} - 2 - C_{L0}/3 + (2 - 2\,C_{a0} + 1/3)\,C_{L2}]}{4\,C_{a1}\,(C_{L0} - 1) + 3\,(C_{L2} - C_{L0})\,[2\,C_{b2}\,(C_{L0} - 1) + (C_{L2} - C_{L0})\,C_{Ls}]}$$

- Observations
  - additional equations add (and subtract) coefficients, and there may be insufficient physical constraints to completely determine all coefficients
  - a_i and *b* equations do not apparently add new physics, but are required for closure (e.g., 2- and 4-equation models can both be calibrated to predict a particular, constant α)
  - models are all based on an isotropic eddy viscosity, with Boussinesq model for Reynolds stress

*Joint work with summer student Tucker A. Hartland

The evolution of the mixing layer parameters indicates that all of the models can be calibrated to achieve self-similarity with a specified $\alpha \approx 0.05$

Mixing layer parameter $\alpha(t) = h(t) / (At\ g\ t^2)$

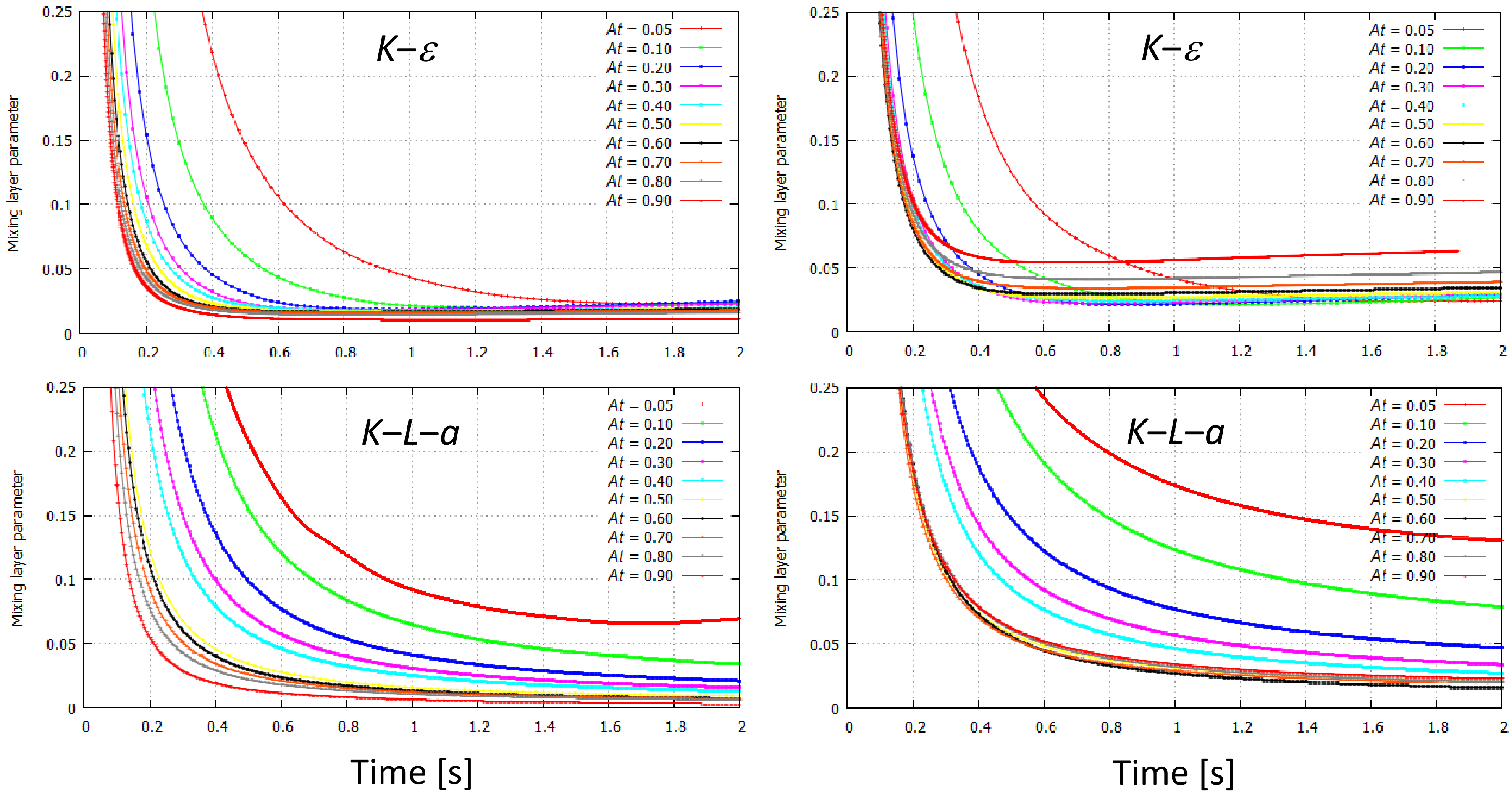


Models approach self-similarity at different rates

- Self-similar growth parameters α can be derived analytically for constant g for each model
- Allows models to be calibrated to same late-time growth (at least for small At)
- No longer true for complex accelera-tions such as g off, g reversed, or g accel/decel/accel

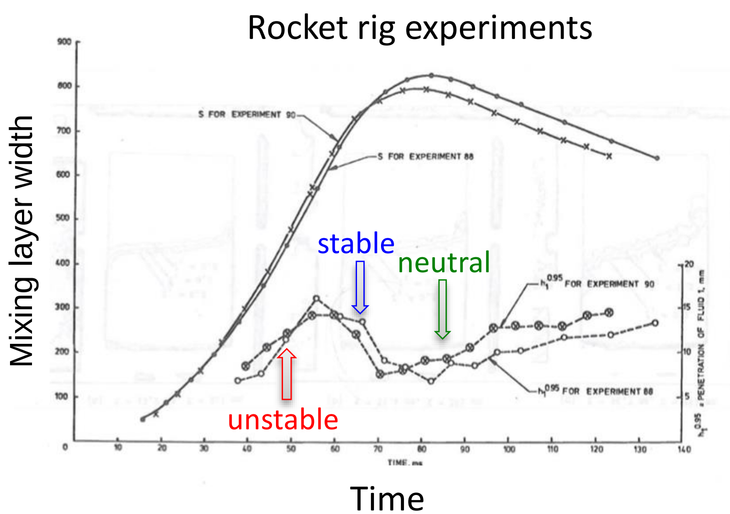
The *K–ε* model is consistent with *miscible* Rayleigh–Taylor mixing, while the *K–L–a* model is consistent with *immiscible* mixing

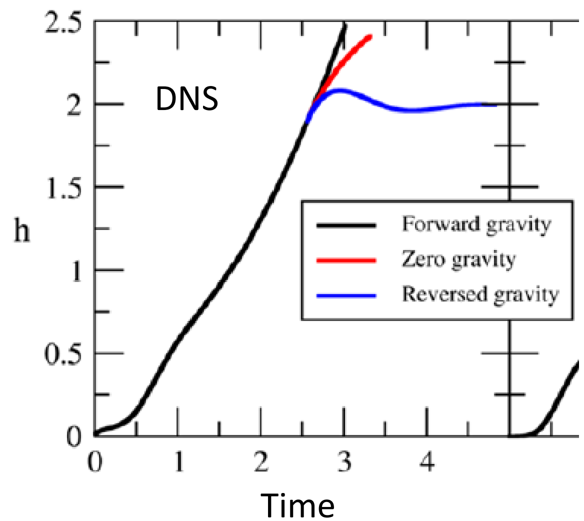
Bubble (left) and spike (right) mixing layer parameters $\alpha_{b,s}(t) = h_{b,s}(t) \,/\, (At\, g\, t^2)$



Rayleigh–Taylor mixing cases with several complex accelerations were compared to determine if the models could reproduce experimental and DNS data

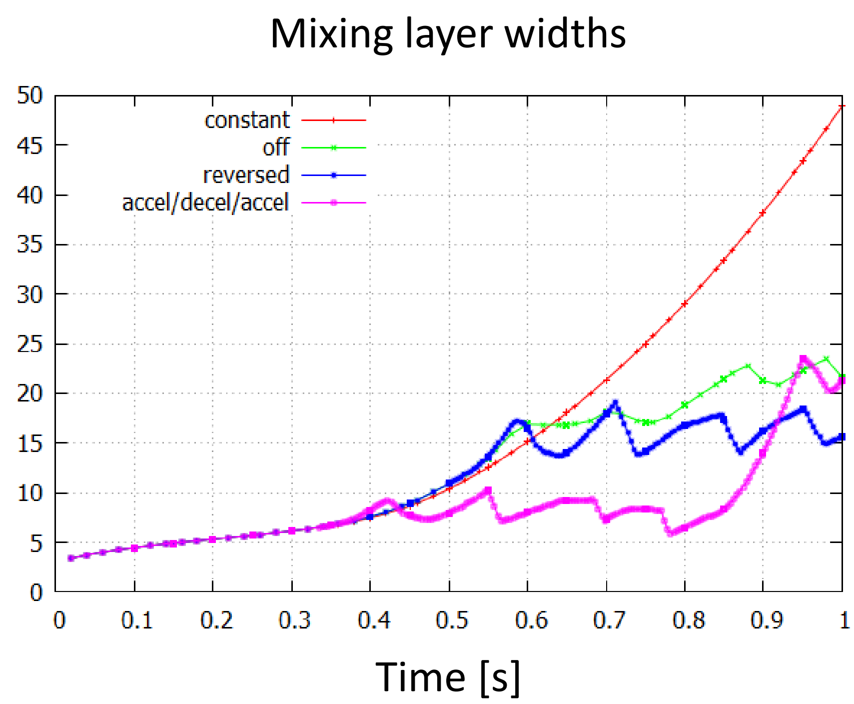
- Models applied to At = 0.5 Rayleigh–Taylor flows with (g_0 = 2000 cm/s^2)
  - constant: $g = -g_0$ (unstable)
  - off: $g = -g_0$ for $t < t_{end}/2$ (unstable) $g = 0$ for $t > t_{end}/2$ (neutral)
  - reversed: $g = -g_0$ for $t < t_{end}/2$ (unstable) $g = g_0$ for $t > t_{end}/2$ (stable)
  - accel/decel/accel: $g = -g_0$ for $t < t_{end}/3$ (unstable) $g = g_0$ for $t_{end}/3 \leq t \leq 2t_{end}/3$ (stable) $g = -g_0$ for $t > 2t_{end}/3$ (unstable)





complex g cases have lower widths than constant g case

Turning off, reversing, or alternating the sign of the acceleration is reflected in the mixing widths: the K–ε model results are consistent with expectations

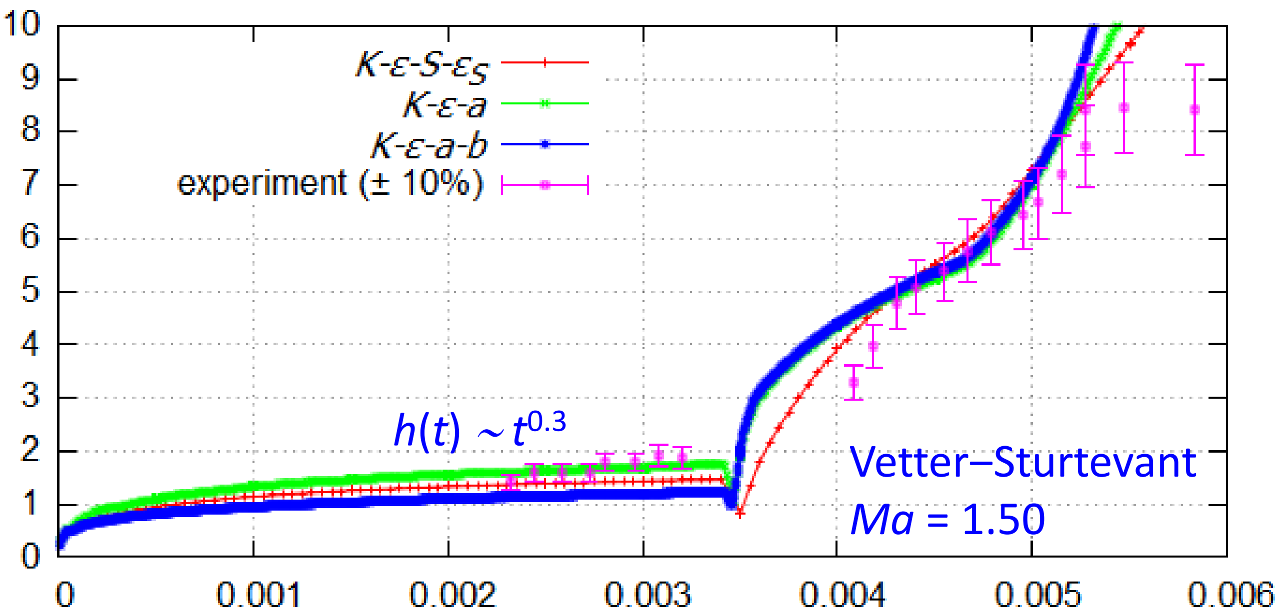


all complex g cases have inhibited mixing layer widths

- Results are not shown for K–L, K–L–a, and K–L–a–b models
  - some versions of K–L and K–L–a–b model are able to predict g off case
  - other cases fail or continue to grow similarly to constant g case
  - $C_{L0} = 0$ cases tend to fail more than $C_{L0} \neq 0$ cases
- *L* equation does not allow sufficient stabilizing mechanisms to inhibit growth of *L*
  - in a model with $C_{L0} = 0$, L equation does not directly respond to changes in g

The ε-based models generally predict qualitatively and quantitatively similar mixing widths for reshocked Richtmyer–Meshkov unstable flow

Mixing layer width based on 2–98% cutoff in X_H



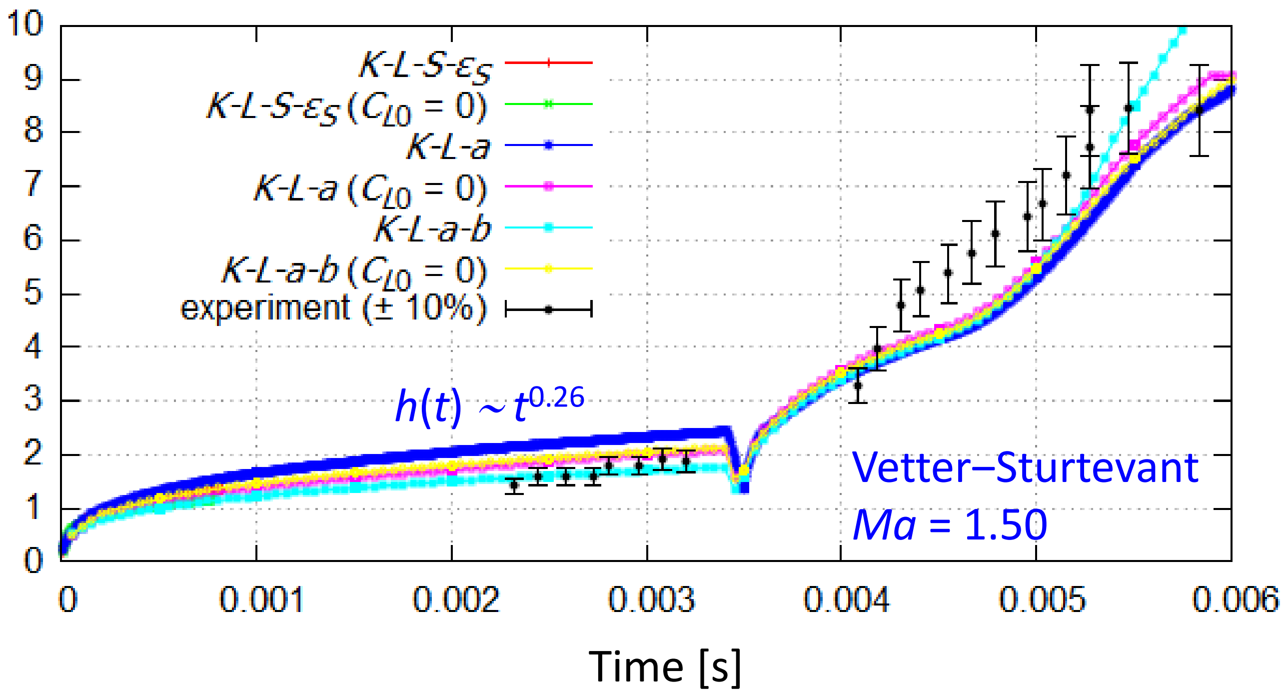
Time [s]

ε is slaved to K, leading to similar ν_t, and therefore to similar widths

- Models reasonably well capture pre- and post-reshock growth
- a-based models have steeper post-reshock growth rates and tend to overpredict growth
- Adjustments can bring predictions into closer agreement
- $\theta \approx 0.30$ determined by value of C_{Z2} (i.e., $C_{\varepsilon 2} = 1.92$)

The *L*-based models also generally predict qualitatively and quantitatively similar mixing widths

Mixing layer width based on 2–98% cutoff in X_H

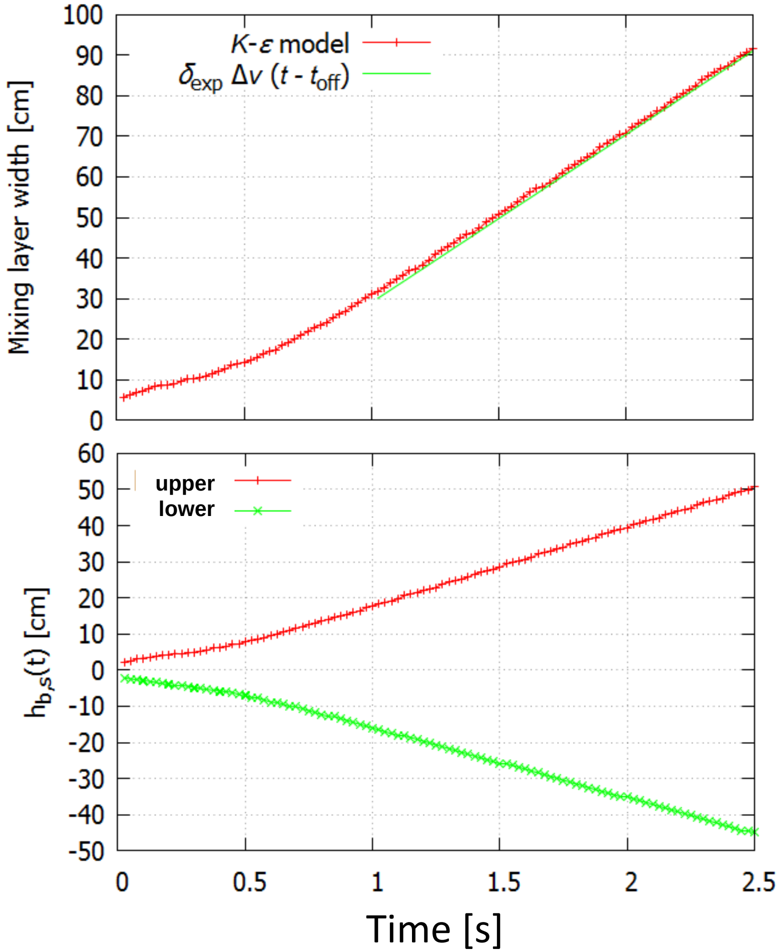


L is slaved to *K*, leading to similar ν_t, and therefore to similar mixing widths

- When run consistently with ε-based models, *L*-based models
  - overpredict pre-reshock widths
  - underpredict post-reshock widths
- ε- and *L*-based models may respond differently to interaction of reflected rarefaction with layer
- Adjustments can bring predictions into closer agreement with data
- $\theta \approx 0.26$ determined by value of C_{L2} = -0.42

The K–ε model using the standard values $C_{\varepsilon 1}$ = 1.44 and $C_{\varepsilon 2}$ = 1.92 predicts the linear growth rate of the v_1/v_2 = 0.6 Bell–Mehta (1990) air/air shear layer very well

Shear layer width based on 5–95% cutoff in v_y



- Mean shear momentum equation is

$$\bar{\rho}\left(\frac{\partial}{\partial t}+\tilde{v}_x\,\frac{\partial}{\partial x}\right)\tilde{v}_y=\frac{\partial\bar{\sigma}_{yx}}{\partial x}-\frac{\partial\tau_{yx}}{\partial x}=\frac{\partial}{\partial x}\left[(\bar{\mu}+\mu_t)\,\frac{\partial\tilde{v}_y}{\partial x}\right]$$

- Initial mean shear velocity is

$$\tilde{v}_y(x,0)=\frac{v_1+v_2}{2}-\frac{v_1-v_2}{2}\,\mathrm{erf}\left[\frac{2\,(x-x_c)}{\delta_*}\right]$$

  - lower, upper velocities v_1 = 900, v_2 = 1500 cm/s
  - δ_* = 5 cm is profile width, x_c = 125 cm is centerline

- $K(x,0) = 0.01(\Delta v)^2/2$, $\varepsilon(x,0) = K(x,0)^{3/2}/L(x,0)$ with $L(x,0)$ = 0.44 cm (boundary layer thickness)

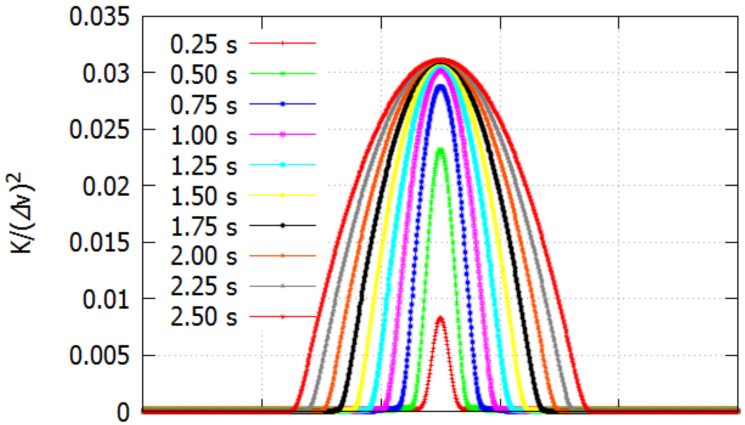
- Self-similar width of air/air shear layer is

$$h(t)=\delta_{\exp}\,|\Delta v|\,t\quad,\quad\delta_{\exp}=0.069$$

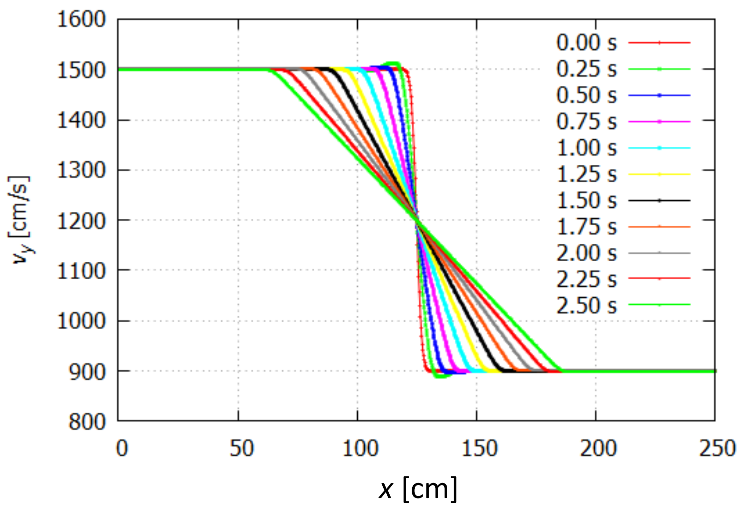
- Following early transient, upper and lower stream widths are nearly symmetric

The K–ε model using the standard values $C_{\varepsilon 1} = 1.44$ and $C_{\varepsilon 2} = 1.92$ predicts a $K(x_{int})/(\Delta v)^2$ in reasonably good agreement with the Bell–Mehta data

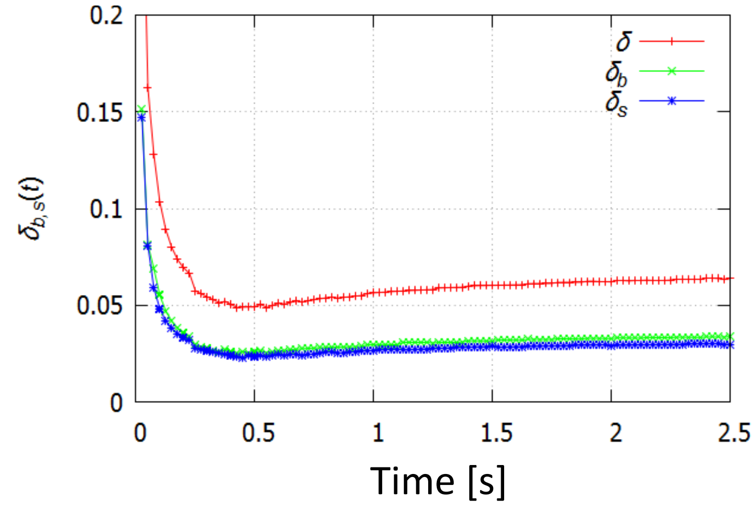
Normalized turbulent kinetic energy



Mean shear velocity

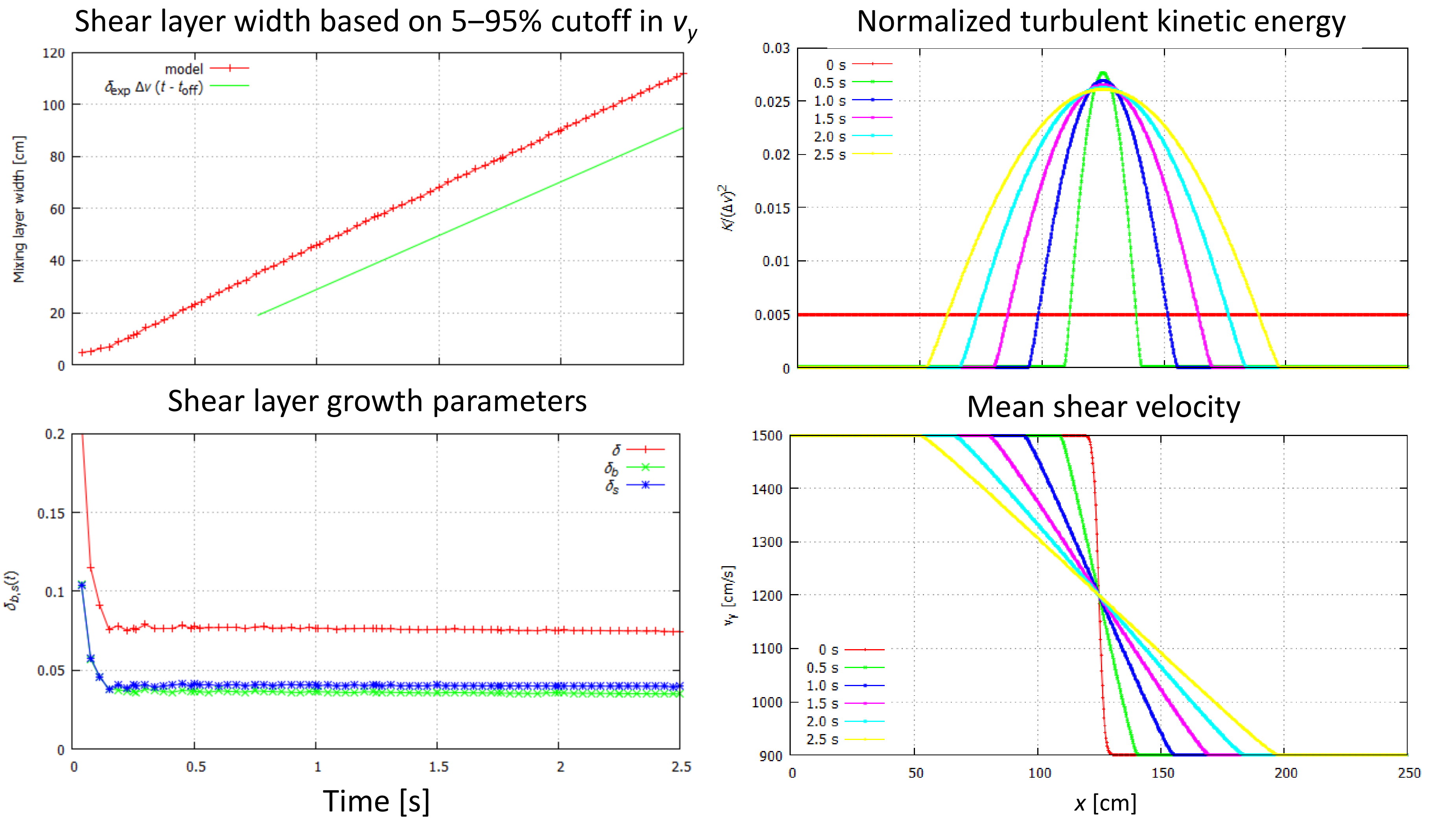


Shear layer growth parameters



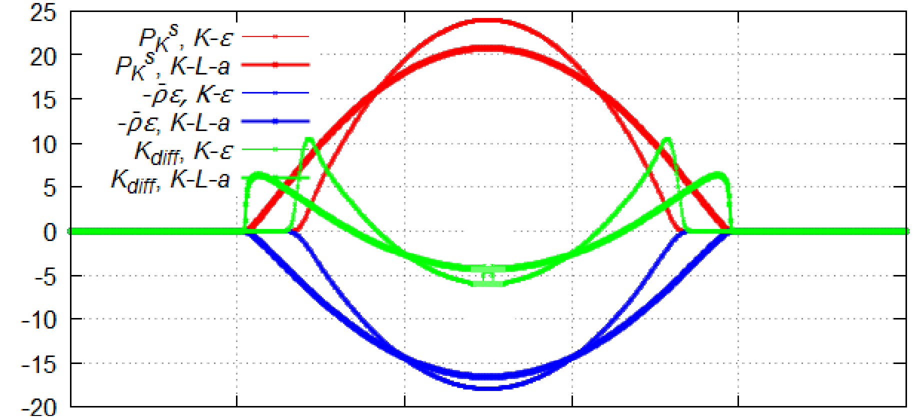
- $K(x_{int})/(\Delta v)^2$ reaches steady value ≈0.032, underpredicting data (≈0.035) ~9%
- Layer width grows linearly in time, with $\delta \sim 0.065$, underpredicting data ~6%
- Shear velocity diffuses due to turbulence, and becomes linear across layer

Using the coefficients derived from the K–ε model for the K–L model gives the correct growth rate but a $K(x_{int})/(\Delta v)^2$ that is too low and a much larger width

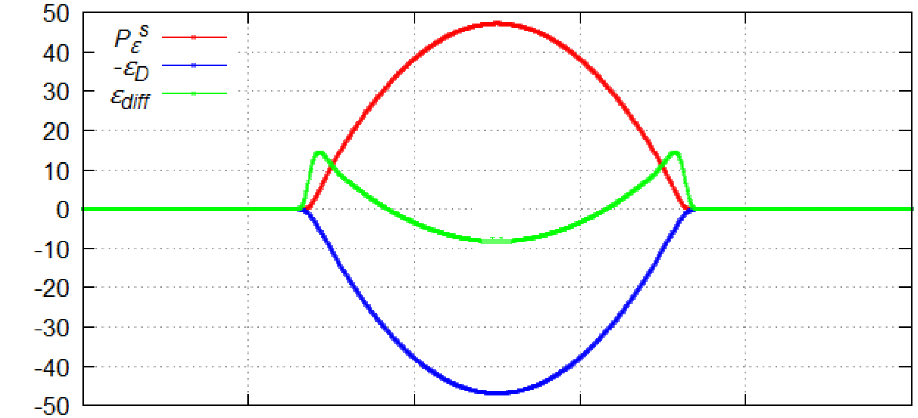


The turbulent budgets from the K–ε and K–L model indicate significant differences in the roles of the production, destruction, and turbulent diffusion terms

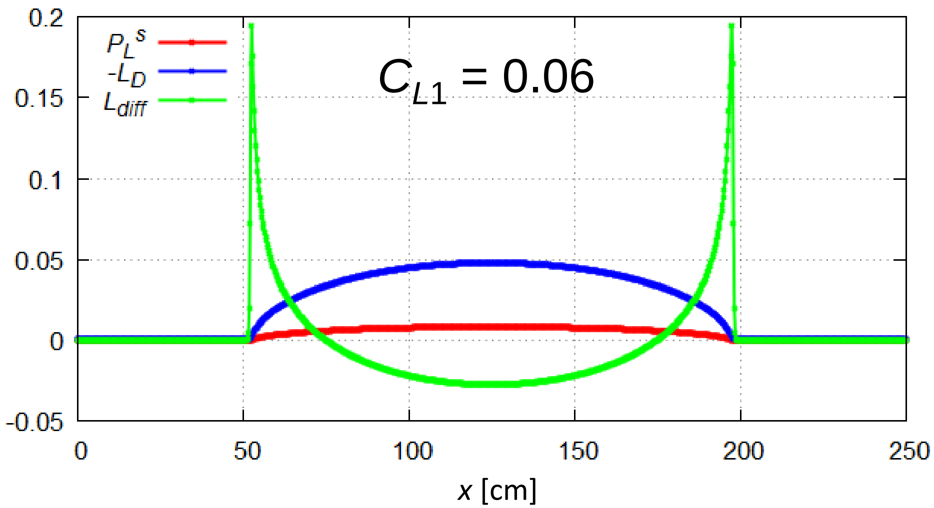
Comparison of K equation budgets



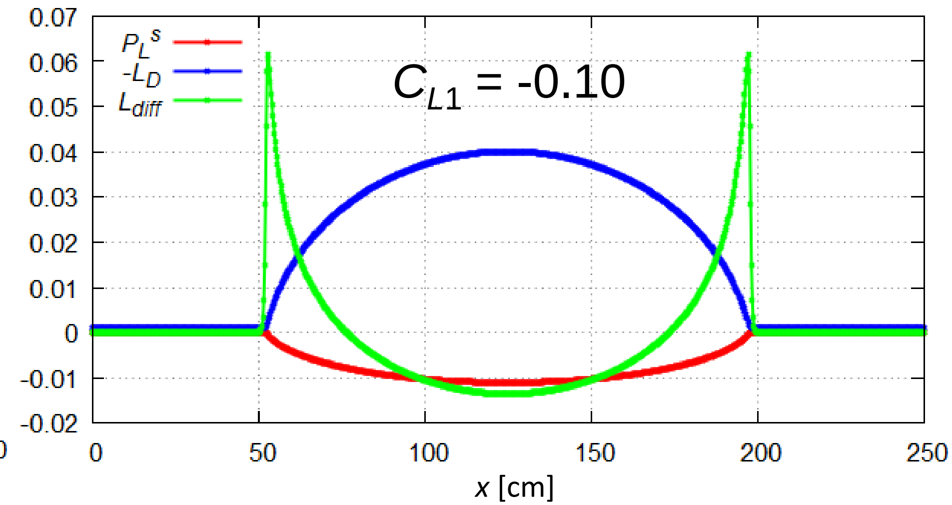
ε equation budget



L equation budget



L equation budget



A multicomponent RANS modeling framework is being used to investigate the detailed predictions of many ε- and L-based models applied to turbulent mixing

- Predictions were compared for Rayleigh−Taylor mixing
  - similarity analysis predicts a constant α for 2- and 4-equation models, and an *At*-dependent α for 3-equation models (from *b* closure model)
  - similarity can calibrate each model to a given α
  - models attain self-similar growth at slightly different rates
  - 2- (but not 3- or 4-) equation models predict reduced widths for stabilizing accelerations
- Predictions were compared for reshocked Richtmyer−Meshkov mixing
  - models predict similar trends before and after reshock
  - ε- or L-based models with algebraic or differential closures for a_j predict similar widths
- Predictions were compared for shear flow
  - $K-\varepsilon$ model predicts growth rate and $K(x_{int})/(\Delta v)^2$ in good agreement with experiment
  - $K-L$ model does not predict *both* of these quantities well *simultaneously*

- Applications to:
  - canonical flows do not provide evidence that higher order closures are more predictive
  - $K-\varepsilon$ model provides best predictions for complex acceleration and shear flows
  - assumption $\varepsilon = C_{Ls}\, K^{3/2}/L$ in L-based models, and L equation itself (having mostly >0 terms on right side) lead to poor predictions for flows with stabilizing mechanisms or shear