A New Two-Scale Mix Model: Towards a Multi-Component Model of Turbulent Mixing*

Presented to the 8th International Workshop on the Physics of Compressible Turbulent Mixing

Donald E. Eliason, William H. Cabot, and Ye Zhou

AX-Division, Lawrence Livermore National Laboratory

11 December 2001

*This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Abstract

Turbulent mixing of the fluids in a multi-component system is of interest in situations such as inertial confinement fusion (ICF) and core-collapse supernovae[1]. We report results of a project to include a model of turbulent mixing in a multi-component hydrodynamics and physics model called KULL, which is used for ICF. Because KULL is a complex, multi-dimensional model, we have developed a simplified, one-dimensional version called sKULL to speed-up the development of the turbulent mixing model.

Of primary interest in the development of a turbulent mixing model for a multi-component fluid is the question of whether it is necessary to allow each component of the fluid to retain its own velocity. Generally a multi-component, multi-velocity turbulent mixing model should allow separate velocities for each component of the fluid[2]. However, the necessity to carry separate velocities for each component of the fluid greatly increases the memory requirements and complexity of the computer implementation. In contrast, we present a new two-scale formulation of the K-ε turbulent mixing model, with production terms based on a recent scaling analysis[3], which treats all components of the fluid as if they had the same velocity. We also show that our new method for the initial conditions of the uncoupled two-scale K-ε model yields asymptotic growth. Future work will compare the results of using this single velocity model with those from a more complete multi-velocity formulation of turbulent mixing, to decide whether the multi-velocity formulation needs to be used in KULL.

The goal of this work is to develop a turbulent mixing model for the ICF code called KULL

- **Turbulent mixing of the fluids in a multi-component system is of interest in situations such as inertial confinement fusion (ICF) and core-collapse supernovae[1]**
- **We report results of a project to include a model of turbulent mixing in a multi-component hydrodynamics and physics model called KULL, which is used for ICF**
- **Because KULL is a complex, multi-dimensional code, we have developed a simplified, one-dimensional version called sKULL to speed-up the development of the turbulent mixing model**

[1]Remington, B.A., D. Arnett, R.P. Drake, and H. Takabe, Modeling Astrophysical Phenomena in the Laboratory with Intense Lasers, *Science* **284**, 1488 (1999).

Three areas of this research are highlighted

- sKULL reproduces KULL's multi-component hydrodynamics and numerics

- A single velocity, multi-component, two-scale K-$\mathcal{E}$ turbulent mixing model has been developed within sKULL

- A new method for the uncoupled two-scale K-$\mathcal{E}$ initial conditions yields asymptotic growth

We have an appropriate path to develop a turbulent mixing model for KULL

Classic KULL:

ALE Hydrodynamics

Single sKULL:

Duplicates KULL's

ALE Hydrodynamics

Multi-sKULL:

Multi-Component and Multi-Velocity

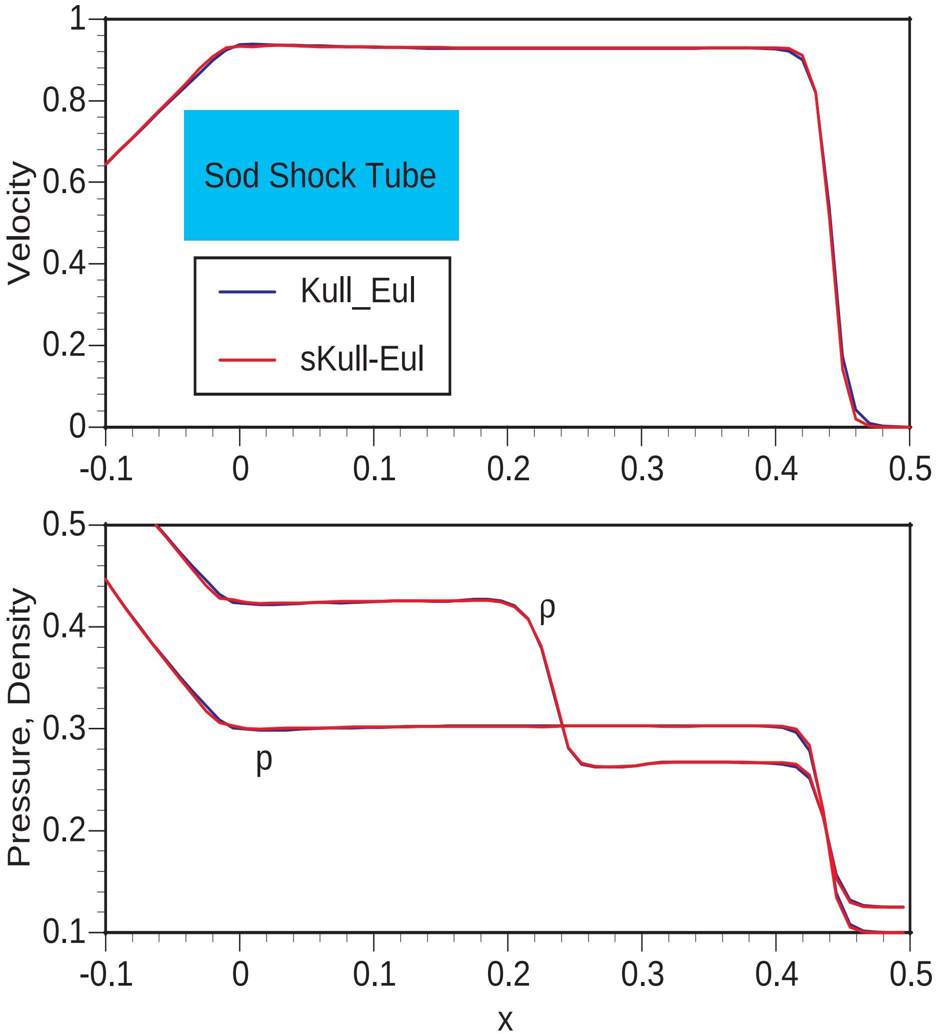
The most general model of turbulent mixing is multi-component and multi-velocity

sKULL is the right platform in which to develop a turbulent mixing model for KULL

- sKULL duplicates KULL's hydrodynamics
  - Side-by-side runs of KULL and sKULL on the Sod shock produce the same results
  - We tested the Lagrangian, Eulerian,and ALE capabilities of sKULL to ensure they matched KULL's

- The simplified nature of sKULL, due both to 1-D and no additional physics, allows it to run more quickly
  - Faster run times lead to shorter turn-around times for testing turbulent mixing models

Side-by-side runs of KULL and sKULL on the Sod shock problem produce the same results

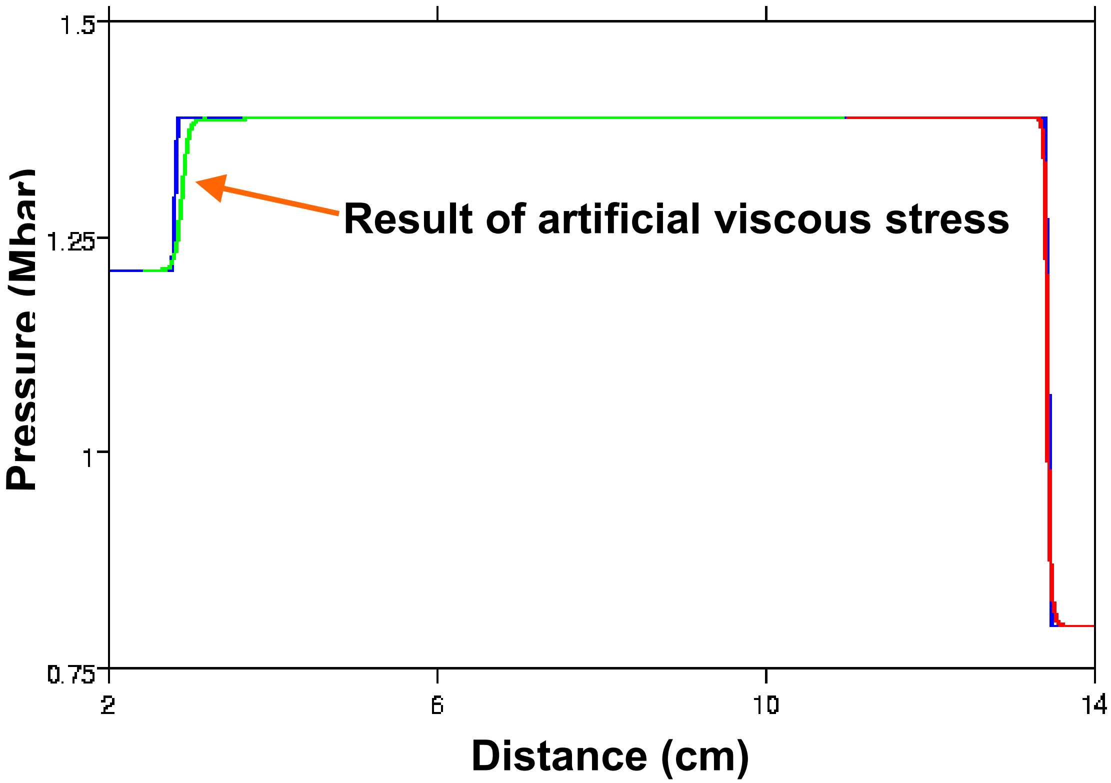


- Duplication of KULL results on selected problems w/ sKULL verifies that we've duplicated KULL's numerics
- Sod (1978) shock tube problem:

$\rho = 1$	$\rho = 0.125$
$p = 1$	$p = 0.1$
$u = 0$	$u = 0$

- Standard test problem
- Compared Lagrangian, Eulerian, and ALE results to ensure that the results from the two codes agreed

sKULL MC-1V's simulation of the Benjamin air-SF_6 shock tube agrees well with the exact solution



- Benjamin *et al.* (1993) air-SF_6 shock tube:

Air*	SF_6
$\rho = 1.27\times10^{-3}$	$\rho = 4.85\times10^{-3}$
$u = 1.05\times10^{4}$	$u = 0$
$p = 1.21\times10^{6}$	$p = 8.00\times10^{5}$

Shock (Ma=1.2) →

- Pressure results from the MC-1V Lagrangian simulation versus exact solution at time 232 μs show good agreement

A multi-component, multi-velocity (MC-MV) approach needs to be considered for the turbulent mixing model

- In RTI/RMI, zones may contain more than one component, each with its own velocity
  - Component interactions (e.g., drag) can lead to mixing
  - From the rocket rig experiments, this led David Youngs (AWE) to create his MC-MV mixing model[2]

- The MC-MV equations add a great deal of complexity
  - Carrying separate velocities increases the memory requirement
  - The drag term may require an implicit treatment

[2]Youngs, D.L., *Laser & Particle Beams* **12**, 725 (1994).

sKULL will be used to test multi-velocity versus single velocity-based turbulent mixing models

Because of sKULL's simplified nature it is faster and cheaper than KULL

- **The extra memory requirement of MC-MV will be manageable**
- **Additional computation for interactions will be do-able**
- **Different numerical treatments of the drag term can be tested (explicit vs. implicit vs. iterated)**

Faster and cheaper makes sKULL the ideal platform to test whether MC-MV might be needed in KULL

The MC-MV equations (Youngs[2]) add a great deal of complexity

ALE: "Grid Velocity" u = $\begin{cases} u_r\text{, Lagrangian} \\ 0\text{, Eulerian} \end{cases}$

"ALE"-like,

g = 0 if shock tube,

Interactions,

Turbulence Transport

$$\frac{\partial x}{\partial t} = u$$

$$\frac{\partial (f_r \rho_r)}{\partial t} = -\frac{\partial}{\partial x}\left[f_r \rho_r (u_r - u)\right] - f_r \rho_r \frac{\partial u}{\partial x}$$

$$\frac{\partial (f_r \rho_r u_r)}{\partial t} = -\frac{\partial}{\partial x}\left[f_r \rho_r u_r (u_r - u)\right] - f_r \rho_r u_r \frac{\partial u}{\partial x} - f_r \frac{\partial P}{\partial x} + f_r \rho_r g$$

$$+ \sum_s (D_{rs} + M_{rs}) - m_r \frac{\partial \tau}{\partial x}$$

$$\frac{\partial (f_r \rho_r e_r)}{\partial t} = -\frac{\partial}{\partial x}\left[f_r \rho_r e_r (u_r - u)\right] - f_r \rho_r e_r \frac{\partial u}{\partial x} - h_r P_r \frac{\partial \bar{u}}{\partial x}$$

$$+ \frac{\partial}{\partial x}\left(f_r \rho_r \nu_r \frac{\partial e_r}{\partial x} \right) + f_r \varepsilon$$

Because of the MC-MV equations' complexity, we've first developed a single velocity version, MC-1V

sKULL MC-1V Lagrangian equations with a new two-scale K-ε mixing model

$$\frac{dx}{dt} = u$$

$$\frac{dV_r}{dt} \approx h_r \frac{dV}{dt}, V = \sum_r V_r$$

$$\rho \frac{Du}{Dt} = -\frac{\partial P}{\partial x} - \frac{\partial \tau}{\partial x}$$

Reynolds stress

Turbulent dissipation

$$f_r \rho_r \frac{De_r}{Dt} = -h_r P_r \frac{\partial u}{\partial x} + f_r \rho_r \varepsilon_t + \frac{\partial}{\partial x}\left(f_r \rho_r \frac{\nu_r}{\sigma_e} \frac{\partial e_r}{\partial x} \right)$$

Kinematic viscosity/Schmidt number

The use of the compressibility in the effective pressure allows the simplification to single velocity

$$P = \frac{\sum_r P_r f_r K_r}{\sum_r f_r K_r}, \quad P_r = p_r + q_r$$

Effective pressure (includes artificial viscosity)

$$K_r^{-1} = \rho_r \left.\frac{\partial P_r}{\partial \rho_r}\right|_{e_r} + \frac{P_r}{\rho_r} \left.\frac{\partial P_r}{\partial e_r}\right|_{\rho_r}, \quad h_r = \frac{f_r K_r}{\sum_s f_s K_s}$$

Inverse effective compression;

Relative com-pression

For an ideal gas and $q_r = 0$, $K_r^{-1} = \gamma_r p_r$ (adiabatic compres-sibility), and $h_r = [f_r/(\rho_r\ c_r^2)]/[\sum_s f_s/(\rho_s\ c_s^2)]$ (Youngs[2])

The viscosity for energy diffusion and Reynolds stress comes from the two-scale K-ε model

$$\tau = \tfrac{2}{3}\rho K_p - \tfrac{4}{3}\rho \nu_p \frac{\partial u}{\partial x}$$ **Reynolds stress**

$$\nu_\alpha = \nu_0 + \nu_{T\alpha}$$ **Kinematic visc.**

Molecular (ν_0) **Turbulent** ($\nu_{T\alpha}$)

$$\nu_{T\alpha} = C_\mu \frac{K_\alpha^2}{\varepsilon_\alpha}$$

Equations for K_α and ε_α are needed for closure

The two-scale K-ε equations describe evolution of the production and turbulence scales

$$\frac{DK_p}{Dt} = P_{R*} - \varepsilon_p + \frac{\partial}{\partial x}\frac{\nu_p}{\sigma_K}\frac{\partial K_p}{\partial x} - \frac{\tau}{\rho}\frac{\partial u}{\partial x}$$

Production scale

Production

$$\frac{DK_t}{Dt} = \varepsilon_p - \varepsilon_t + \frac{\partial}{\partial x}\frac{\nu_t}{\sigma_K}\frac{\partial K_t}{\partial x}$$

Turbulence scale

$$\frac{D\varepsilon_p}{Dt} = C_{p1}\frac{\varepsilon_p}{K_p}P_{R*} - C_{p2}\frac{\varepsilon_p^2}{K_p} + \frac{\partial}{\partial x}\frac{\nu_p}{\sigma_\varepsilon}\frac{\partial \varepsilon_p}{\partial x}$$

$$\frac{D\varepsilon_t}{Dt} = C_{t1}\frac{\varepsilon_p\varepsilon_t}{K_t} - C_{t2}\frac{\varepsilon_t^2}{K_t} + \frac{\partial}{\partial x}\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon_t}{\partial x}$$

The production terms P_{R*} for the two-scale K-ε equations parameterize mixing caused by RTI or RMI

Based on a recent scaling analysis[3] of RT and RM instabilities, the production term may be written as

Rayleigh-Taylor

$$P_{RT} = 4C_{RT}\varepsilon_p^{1/2}(gA)^{3/4}(k_0^{-1/4} - k_1^{-1/4})$$

Richtmyer-Meshkov

$$P_{RM} = 2C_{RM}\varepsilon_p^{1/2}(A\Delta u)^{3/2}(k_1^{1/2} - k_0^{1/2})$$

[3]Zhou, Y., A scaling analysis of turbulent flows driven by Rayleigh-Taylor and Richtmyer-Meshkov instabilities, *Phys. Fluids* **13**, 538–543 (2001).

Wave numbers k_0 and k_1 for the production terms evolve with the flow

Initially k_0 and k_1 are set by the initial perturbation scales, but thereafter evolve according to the computed production and turbulence scales

Production scale

Rayleigh-Taylor

$$k_0 = \left[\frac{\frac{4}{7} C_{RT} \varepsilon_p^{1/2} (gA)^{1/4}}{\frac{4}{7} C_{RT} \varepsilon_p^{1/2} (gA)^{1/4} k_1^{-3/4} + K_p} \right]^{4/3}$$

Richtmyer-Meshkov

$$k_0 = \frac{4 C_{RM}^2 \varepsilon_p A \Delta u}{\left[2 C_{RM} \left(\varepsilon_p A \Delta u \right)^{1/2} k_1^{-1/2} + K_p \right]^2}$$

Turbulence scale

$$k_1 = \varepsilon_t \left(\tfrac{3}{2} C_K / K_t \right)^{3/2}$$

RT or RM

The change in total energy is due to production minus dissipation and surface fluxes

$$\underbrace{\frac{D}{Dt}\int \rho\left(\tilde{u}^2/2+e+K\right)dV}_{\text{Total Energy Change}} = \underbrace{\int \rho\left(P_{R^*}-\varepsilon_t\right)dV}_{\text{Production - Dissipation}} - \underbrace{\left[u\left(P+\tau\right)+F_e+F_K\right]_S}_{\text{Surface Fluxes}}$$

Total Energy Change

Production - Dissipation

Surface Fluxes

$$F_e = -\frac{\nu}{\sigma_K}\frac{\partial e}{\partial x}, F_{K_\alpha} = -\frac{\nu_\alpha}{\sigma_K}\frac{\partial K_\alpha}{\partial x}$$

$$F_K = F_{K_p} + F_{K_t}$$

Diffusive fluxes of internal and turbulent kinetic energies

Results from Orszag and Speziale will be used to provide ICs for the two-scale turbulent mixing model

- **Steve Orszag's work for the ASCI Turbulence Group:**

$$K_p < \tilde{P}_{R0}\sqrt{\nu_0 / C_\mu}, \quad \tilde{P}_{R0} = \boxed{P_{R0}} / \varepsilon_{p0}^{1/2}$$

Initial RT or RM Production

$$\frac{C_\mu K_{p0}^2}{\nu_0} < \varepsilon_{p0} < \tilde{P}_{R0}^2$$

If violated: too much turbulence initially, interface dies out

If violated: no turbulent viscosity develops, Orszag's high Re run blew up

- **Is this result consistent w/ Speziale's fixed point analysis?**

The result using Orszag's approach is consistent with Speziale's fixed point analysis

- **The "fixed points" from Speziale's analysis[4] act as attractors**
- **Initialize with fixed points that are consistent with desired long-term behavior**
  - ↓ **Leads more quickly to the desired long-term state**
- **Speziale's analysis yields the following fixed points:**

$$\varepsilon_{pf} = f_p P_{R0}, \varepsilon_{tf} = f_t \varepsilon_{pf}$$

$$f_p = (C_{p1} - 1)/(C_{p2} - 1), f_t = (C_{t1} - 1)/(C_{t2} - 1)$$

suggesting

$$\varepsilon_{p0} = f_p^2 \tilde{P}_{R0}^2$$

↓ **consistent with Orszag's approach if $f_p < 1$**

[4]Speziale, C.G., and N. Mac Giolla Mhuiris, On the prediction of equilibrium states in homogeneous turbulence, *J. Fluid Mech.*, **209**, 591-615 (1989).

The Orszag-Speziale ICs yield asymptotically growing solutions for the two-scale turbulent mixing model

• Current recommended values C_{p1} = 1.5, C_{p2} = 2 give f_p = 1/2

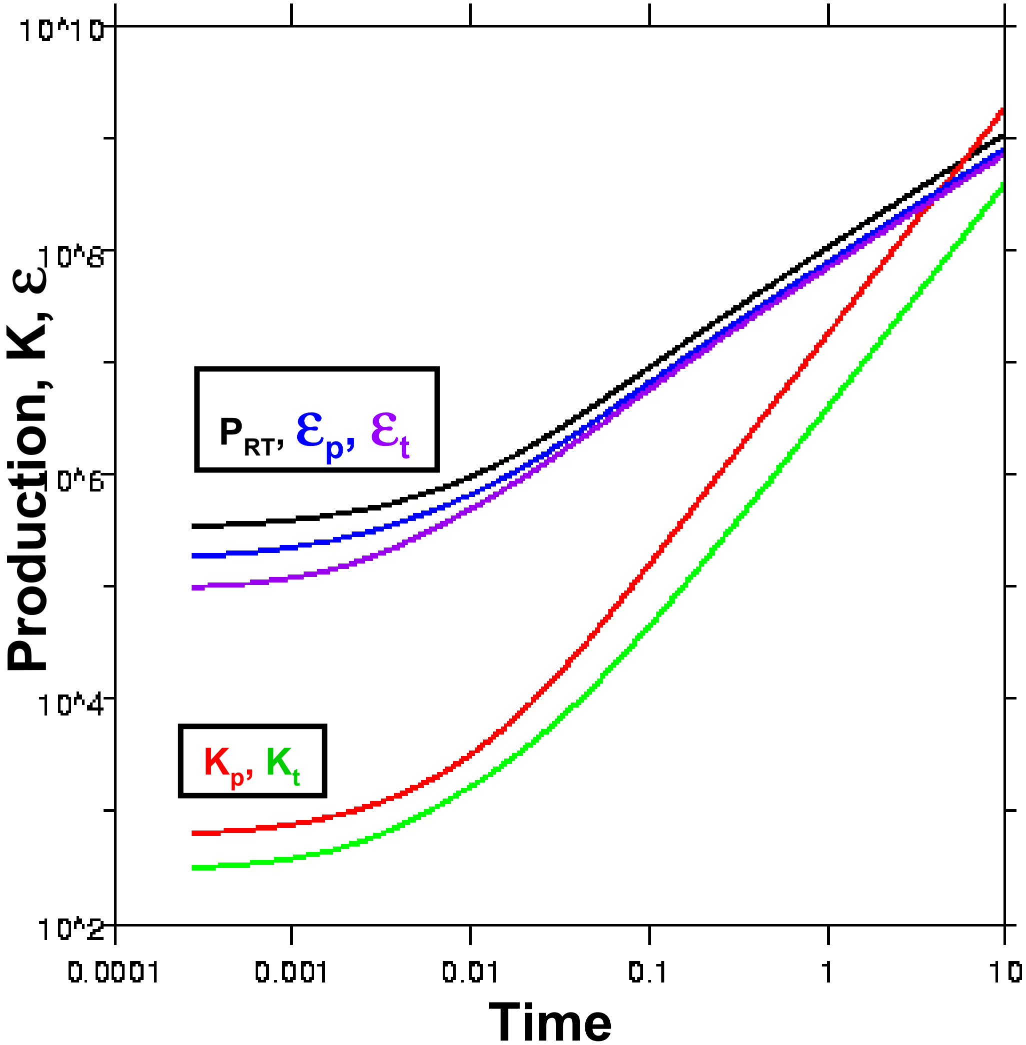
↓ The result using Orszag's approach is consistent with Speziale's fixed point analysis

↓ Also consistent with constraints $C_{*2} > 1$ and $C_{*2} > C_{*1} > 1/2$ needed to get asymptotically growing solutions

• Solution of the two-scale turbulent mixing model equations as ODEs using the Orszag-Speziale ICs produced the expected asymptotically growing results

↓ The Orszag-Speziale ICs will be used in the two-scale turbulent mixing model for sKULL MC-1V

A test of the Orszag-Speziale ICs w/ the uncoupled two-scale K-ε model yields asymptotic growth



Rayleigh-Taylor Test

- gA = 4000
- $k_1(0) = 10k_0(0) = 20\pi$
- $C_K = C_{RT} = 1.5$
- $C_{p1} = 1.5$, $C_{p2} = 2.0$
- $C_{t1} = 1.08$, $C_{t2} = 1.15$

• Constraints for asymptotic growth are satisfied, and asymptotic growth achieved

Consistency with a stand-alone ODE solution demonstrates that the uncoupled two-scale K-ε equations have been correctly implemented in sKULL

Summary and Future Work

● A simplified version of the ICF code KULL has been developed which reproduces KULL’s multi-component hydrodynamics

- ■ The purpose of simplified KULL, sKULL, is to serve as a test-bed for implementation of multi-component turbulent mixing models
- ■ Tests show that sKULL faithfully duplicates KULL’s numerics

● A single velocity, multi-component, two-scale K-ε turbulent mixing model has been developed within sKULL

- ■ A new method for the uncoupled two-scale K-ε initial conditions yields asymptotic growth

● Future work will compare these single velocity results with those from a more complete multi-velocity formulation of turbulent mixing, to decide whether the multi-velocity formulation needs to be used in KULL

Table of Symbols #1

Quantity	Description
D_{rs}	Drag force on fluid r due to fluid s
e_r	Specific internal energy of fluid r
ε_p	Dissipation at production scale
ε_t	Dissipation at turbulence scale
f_r	Volume fraction of fluid r
g	Acceleration (e.g., gravitational)
h_r	Relative compressibility of fluid r
K_p	Turbulence kinetic energy at production scale
K_t	Turbulence kinetic energy at turbulence scale
m_r	Mass fraction of fluid r

Table of Symbols #2

Quantity	Description
M_{rs}	Added mass effect for fluid r due to fluid s
ν_{0r}	Molecular viscosity of fluid r
$\nu_T = \nu_p + \nu_t$	Total turbulent viscosity
ν_p	Turbulent viscosity, production scale
ν_t	Turbulent viscosity, turbulence scale
$\nu_r = \nu_{0r} + \nu_T$	Total viscosity of fluid r
$P_r = p_r + q_r$	Effective pressure of fluid r
$P = p + q$	Effective mean pressure
$p = \sum_r h_r p_r$	Mean pressure
$p_r = p_r(\rho_r, e_r)$	Pressure of fluid r from EOS

Table of Symbols #3

Quantity	Description
$q = \sum_r f_r q_r$	Mean artificial viscous stress
q_r	Artificial viscous stress of fluid r
$\rho = \sum_r f_r \rho_r$	Mean density
ρ_r	Density of fluid r
t	Time
u	Mean velocity
$\bar{u} = \sum_r f_r \bar{u}_r$	Volume-weighted mean velocity
$\bar{u}_r = u_r + \frac{\nu_r}{\rho_r} \frac{\partial \rho_r}{\partial x}$	Volume-weighted velocity of fluid r
u_r	Velocity of fluid r
x	Position at time t