Single-Velocity, Multi-Component Turbulent Transport Models for Interfacial Instability-Driven Flows

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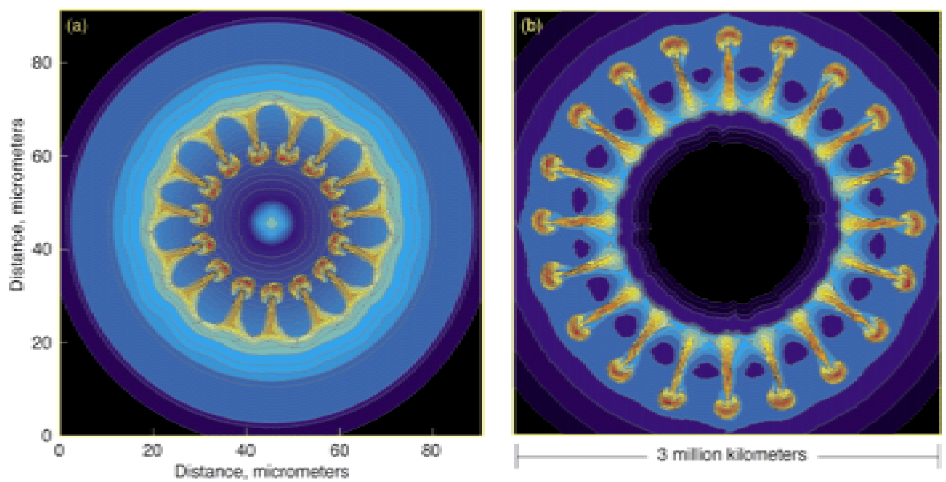
Outline of presentation

- Motivation
  - The need for turbulent transport and mixing models
  - Single- vs. multiple-velocity, multi-component fluid formulations
- Derivation of the Favre-Reynolds averaged single-velocity equations
- Two-equation turbulence models
  - The general K-Z model
  - The K-ε model
  - Derivation of consistent K-l, K-ω, and K-τ models
- Work in progress: *a priori* model tests
  - Determination of model coefficients from experimental data
  - Determination of model coefficients from simulation data
- Conclusions

An *averaged* description of turbulent transport and mixing is needed due to the very wide range of spatio-temporal scales in turbulent mixing layers

- Direct numerical simulation (DNS) cannot attain parameter regimes of interest for astrophysical and inertial confinement fusion (ICF) applications
- Large-eddy simulation (LES) is not yet sufficiently developed
- Interim solution: turbulent transport and mixing models, which have similarities with LES

- Transport models are based on closing terms in the density-weighted averaged equations
  - Reynolds stress tensor
  - Density and energy flux
- These quantities are modeled using an eddy viscosity approximation



Striking similarities exist between hydrodynamic instabilities in (a) inertial confinement fusion capsule implosions and (b) core-collapse supernova explosions. [Image (a) is from Sakagami and Nishihara, *Physics of Fluids B* **2**, 2715 (1990); image (b) is from Hachisu et al., *Astrophysical Journal* **368**, L27 (1991).]

ICF **supernova**

Single-velocity formulations of multi-component flow are significantly less complex than multiple-velocity formulations

- Single-velocity, multi-component fluid formulations:
  - Equations systematically derived from reacting flow theory
  - Equations have nearly the same form as the *single-fluid*, compressible fluid dynamics equations
  - Additional fluxes involving a diffusion velocity are present
  - The diffusion velocity is obtained, and these fluxes are expressed in terms of a mass diffusion flux
- Multiple-velocity, multi-component fluid formulations:
  - Require multiple advection terms equal to number of fluids
  - Require fluid dynamic fields for every fluid, so the number of equations to model and solve is large
  - Require phenomenological modeling of interfacial source terms arising from interfacial averaging: drag, added mass terms, etc.

The derivation of the single-velocity equations begins with the full, *N*-fluid equations expressing mass, momentum, and energy conservation

- In compact form, these equations are (r labels each fluid):

$$\frac{\partial}{\partial t}(\rho^r \phi^r_\alpha) + \frac{\partial J^r_{\alpha\beta}[\phi^r]}{\partial x_\beta} = F^r_\alpha + S^r_\alpha$$

  – where the fields, fluxes, forces, and sources are

$$\rho^r \phi^r_\alpha = \begin{pmatrix} \rho^r \\ \rho^r v^r_\alpha \\ \rho^r e^r \\ \rho^r \phi^r \end{pmatrix}, \quad J^r_{\alpha\beta} = \begin{pmatrix} \rho^r v^r_\beta \\ \rho^r v^r_\alpha v^r_\beta + p^r \delta_{\alpha\beta} - \sigma^r_{\alpha\beta} \\ (\rho^r e^r + p^r) v^r_\beta - v^r_\alpha \sigma^r_{\alpha\beta} + \Phi^{\mathrm{rad},r}_\beta \\ \rho^r \phi^r v^r_\beta + \Phi^{\phi,r}_\beta \end{pmatrix}$$

$$F^r_\alpha = \begin{pmatrix} 0 \\ \rho^r g_\alpha \\ 0 \\ 0 \end{pmatrix}, \quad S^r_\alpha = \begin{pmatrix} R^r \\ v^r_\alpha R^r \\ H^r R^r + \rho^r g_\alpha v^r_\alpha \\ \phi^r R^r \end{pmatrix}$$

These fields are defined so that summing appropriate expressions over each fluids recovers the non-reacting, single-fluid equations

- The quantities ρ^r, v_α^r, U^r, φ^r, $\Phi_\alpha^{rad,r}$, Φ^r, g_α, R^r, and H^r are the density, velocity, internal energy, scalar, radiative flux, scalar flux, acceleration, reaction rate, and heat of formation
- The pressure, viscous stress tensor, and total energy are

$$p^r = p^r(\rho^r, U^r)$$

$$\sigma^r_{\alpha\beta} \equiv \mu^r\left(\frac{\partial v^r_\alpha}{\partial x^\beta} + \frac{\partial v^r_\beta}{\partial x^\alpha}\right) + \left(\xi^r - \frac{2\,\mu^r}{d}\right)\delta_{\alpha\beta}\,\frac{\partial v^r_\gamma}{\partial x_\gamma}$$

$$e^r = \frac{v_r^2}{2} + U^r + \rho\, m^r H^r - \mathbf{g} \bullet \mathbf{x}$$

- Consistency with the single-fluid equations is obtained with the constraints

$$\sum_{r=1}^N \rho^r \phi^r_\alpha = \rho\,\phi_\alpha \quad , \quad \sum_{r=1}^N J^r_{\alpha\beta} = J_{\alpha\beta}$$

$$\sum_{r=1}^N F^r_\alpha = F_\alpha \quad , \quad \sum_{r=1}^N S^r_\alpha = S_\alpha$$

$$\sum_{r=1}^N R^r = 0 \quad , \quad \sum_{r=1}^N \phi^r_\alpha R^r = 0$$

The single-velocity equations are obtained by decomposing the velocity into a mean velocity plus a diffusion velocity

- Introduce the local mass fraction of fluid *r*

$$m^r(\mathbf{x},t) \equiv \frac{\rho^r}{\rho} \quad , \quad \sum_{r=1}^{N} m^r(\mathbf{x},t) = 1$$

- Write the velocity of fluid *r* as

$$\mathbf{v}^r = \mathbf{v} + \mathbf{V}^r \quad , \quad \mathbf{v} \equiv \sum_{r=1}^{N} m^r \mathbf{v}^r$$

where V^r is the diffusion velocity, which expresses the molecular transport caused by the concentration gradient in fluid *r*

- The identity

$$\sum_{r=1}^{N} m^r \mathbf{V}^r = 0$$

is central to the derivation of the single-velocity equations

The single-velocity equations are a consequence of the previous identities

- Substituting the velocity decomposition into the multi-component equations, summing, and using the previous identities gives the single-velocity equations

$$\frac{\partial}{\partial t}(\rho\,\phi_\alpha) + \frac{\partial J_{\alpha\beta}}{\partial x_\beta} = F_\alpha + S_\alpha$$

- The fields and fluxes are

$$\rho\,\phi_\alpha = \begin{pmatrix} \rho \\ \rho\, v_\alpha \\ \rho\, e \\ \rho\,\phi \end{pmatrix} \qquad J_{\alpha\beta} = \begin{pmatrix} \rho\, v_\beta \\ \rho\, v_\alpha\, v_\beta + p\,\delta_{\alpha\beta} - \sigma_{\alpha\beta} \\ (\rho\, e + p) v_\beta - v_\alpha\,\sigma_{\alpha\beta} + \Phi_\beta^{\mathrm{rad}} \\ \rho\,\phi\, v_\beta + \Phi_\beta^\phi \end{pmatrix} + \begin{pmatrix} 0 \\ -\sigma_{\alpha\beta}^D \\ J_\beta^e \\ J_\beta^\phi \end{pmatrix}$$

where the last term in $J_{\alpha\beta}$ depends on the diffusion velocity and must be modeled

The forces, sources, and other quantities are defined as follows

- The forces and sources are

$$F_\alpha = \begin{pmatrix} 0 \\ \rho g_\alpha \\ 0 \\ 0 \end{pmatrix} \qquad S_\alpha = \begin{pmatrix} 0 \\ 0 \\ \rho g_\alpha v_\alpha \\ 0 \end{pmatrix} + \sum_{r=1}^{N} \begin{pmatrix} 0 \\ 0 \\ H^r R^r \\ 0 \end{pmatrix}$$

- The total density, pressure, radiative flux, viscous stress tensor, dynamic viscosity, and bulk viscosity are

$$\rho \equiv \sum_{r=1}^{N} \rho^r \qquad p \equiv \sum_{r=1}^{N} p^r(\rho^r, U^r) \qquad \Phi_\alpha^{\mathrm{rad}} \equiv \sum_{r=1}^{N} \Phi_\alpha^{\mathrm{rad},r}$$

$$\sigma_{\alpha\beta} \equiv \mu\left(\frac{\partial v_\alpha}{\partial x^\beta} + \frac{\partial v_\beta}{\partial x^\alpha}\right) + \left(\xi - \frac{2\mu}{d}\right)\delta_{\alpha\beta}\frac{\partial v_\gamma}{\partial x_\gamma}$$
$$+\sum_{r=1}^{N} \mu^r\left(\frac{\partial V_\alpha^r}{\partial x^\beta} + \frac{\partial V_\beta^r}{\partial x^\alpha}\right) + \left(\xi^r - \frac{2\mu^r}{d}\right)\delta_{\alpha\beta}\frac{\partial V_\gamma^r}{\partial x_\gamma}$$

$$\mu \equiv \sum_{r=1}^{N} \mu^r \quad , \quad \xi \equiv \sum_{r=1}^{N} \xi^r$$

The diffusive fluxes are defined as follows

- The multi-component viscous diffusion stress tensor is

$$\sigma^{D}_{\alpha\beta} \equiv -\rho \sum_{r=1}^{N} m^{r} V^{r}_{\alpha} V$$

- The diffusive energy flux is

$$J^{e}_{\alpha} \equiv \rho \sum_{r=1}^{N} m^{r} e^{r} V^{r}_{\alpha}$$

- The diffusive scalar flux is

$$J^{\phi}_{\alpha} \equiv \rho \sum_{r=1}^{N} m^{r} \phi^{r} V^{r}_{\alpha}$$

The averaged equations are obtained by introducing the Favre-Reynolds decompositions and averaging

- The Favre-Reynolds decompositions are

$$\phi_\alpha^r(\mathbf{x},t) = \tilde{\phi}_\alpha^r(\mathbf{x},t) + \phi_\alpha^r(\mathbf{x},t)''$$

$$\rho^r(\mathbf{x},t) = \overline{\rho}^r(\mathbf{x},t) + \rho^r(\mathbf{x},t)' \qquad p^r(\mathbf{x},t) = \overline{p}^r(\mathbf{x},t) + p^r(\mathbf{x},t)'$$

- The Favre average is

$$\tilde{\phi}_\alpha \equiv \frac{\overline{\rho\phi_\alpha}}{\overline{\rho}}$$

- The Favre-averaged multi-component fluid dynamics equations are

$$\frac{\partial}{\partial t}(\overline{\rho}\,\tilde{\phi}_\alpha) + \frac{\partial \overline{J}_{\alpha\beta}}{\partial x_\beta} = \overline{F}_\alpha + \overline{S}_\alpha$$

The Favre-averaged fields and fluxes are defined as follows

- The fields and fluxes are

$$\overline{\rho}\,\widetilde{\phi}_{\alpha} = \begin{pmatrix} \overline{\rho} \\ \overline{\rho}\,\widetilde{v}_{\alpha} \\ \overline{\rho}\,\widetilde{e} \\ \overline{\rho}\,\widetilde{\phi} \end{pmatrix}$$

$$\overline{J}_{\alpha\beta} = \begin{pmatrix} \overline{\rho}\,\widetilde{v}_{\beta} \\ \overline{\rho}\,\widetilde{v}_{\alpha}\,\widetilde{v}_{\beta} + \overline{p}\,\delta_{\alpha\beta} - \widetilde{\sigma}_{\alpha\beta} - \widetilde{\sigma}^{D}_{\alpha\beta} \\ (\overline{\rho}\,\widetilde{e} + \overline{p})\widetilde{v}_{\beta} - \widetilde{v}_{\alpha}\,\widetilde{\sigma}_{\alpha\beta} + \overline{\Phi}^{\mathrm{rad}}_{\beta} + \widetilde{J}^{e}_{\beta} \\ \overline{\rho}\,\widetilde{\phi}\,\widetilde{v}_{\beta} + \overline{\Phi}^{\phi}_{\beta} + \widetilde{J}^{\phi}_{\beta} \end{pmatrix} + \begin{pmatrix} 0 \\ -\overline{\sigma''_{\alpha\beta}} - \overline{\sigma^{D''}_{\alpha\beta}} + \overline{\rho}\,\widetilde{v''_{\alpha}\,v''_{\beta}} \\ \overline{p'\,v''_{\beta}} - \overline{v''_{\alpha}\,\sigma''_{\alpha\beta}} + \overline{\Phi^{\mathrm{rad}''}_{\beta}} + \overline{J^{e''}_{\beta}} + \overline{\rho}\,\widetilde{e''\,v''_{\beta}} \\ \overline{\Phi^{\phi''}_{\beta}} + \overline{J^{\phi''}_{\beta}} + \overline{\rho}\,\widetilde{\phi''\,v''_{\beta}} \end{pmatrix}$$

The Favre-averaged forces and sources are defined as follows

- The forces and sources are

$$\overline{F}_\alpha = \begin{pmatrix} 0 \\ \overline{\rho}\, g_\alpha \\ 0 \\ 0 \end{pmatrix}$$

$$\overline{S}_\alpha = \begin{pmatrix} 0 \\ 0 \\ \overline{\rho}\, g_\alpha \widetilde{v}_\alpha \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \overline{\rho' v''_\alpha}\, g_\alpha + \sum_r \left(\overline{H^r}\,\overline{R^r} + \overline{H^{r\prime\prime} R^{r\prime\prime}} \right) \\ 0 \end{pmatrix}$$

- At large Reynolds numbers, the viscous stress terms and diffusive fluxes are assumed to be negligible compared to the Reynolds stress tensor and turbulent fluxes

A gradient diffusion approximation is usually used to model the turbulent stresses and fluxes

- The gradient diffusion approximation is

$$\overline{\rho \phi''_\alpha v''_j} = \overline{\rho}\, \widetilde{\phi''_\alpha v''_\beta} = -\frac{\partial}{\partial x^j}\left(\frac{\nu_t}{\sigma_{\phi\alpha}} \overline{\rho}\, \tilde{\phi}_\alpha \right)$$

$$\tau_{ij} \equiv \overline{\rho v''_i v''_j} = \overline{\rho}\, \widetilde{v''_i v''_j}$$

$$= 2\, \overline{\rho}\, \widetilde{E''} \frac{\delta_{ij}}{3} - 2\, \overline{\rho}\, \nu_t \left(\widetilde{S}_{kj} - \frac{\delta_{kj}}{3} \frac{\partial \tilde{v}_l}{\partial x_l} \right)$$

$$\overline{\rho' v''_j} = -\frac{\partial}{\partial x_j}\left(\frac{\nu_t}{\sigma_\rho} \overline{\rho} \right)$$

- The eddy viscosity

$$\nu_t = C_\mu \left(\widetilde{E''} \right)^{\frac{m+2n}{n}} \left(\widetilde{Z''} \right)^{-\frac{1}{n}}$$

is determined by the solution of transport equations for two turbulence variables *K* (= *E*'') and

$$\widetilde{Z''} \equiv C_Z \left(\widetilde{E''} \right)^m \left(\widetilde{\epsilon''} \right)^n$$

The turbulent kinetic energy equation is closed as follows

- The unclosed turbulent kinetic energy equation is

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{E''}\right)+\frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{E''}\,\widetilde{v}_j\right)$$

$$=\underbrace{\left(\overline{\rho}\,\overline{v''_i}+\overline{\rho'\,v''_i}\right)g_i}_{\text{force production}}-\underbrace{\frac{\partial}{\partial x_j}\left(\frac{\overline{\rho\,v''^2\,v''_j}}{2}+\overline{p'\,v''_j}-\overline{v''_i\,\sigma''_{ij}}-\overline{v''_i\,\sigma^{D''}_{ij}}\right)}_{\text{turbulent diffusion}}$$

$$+\underbrace{\widetilde{v}_i\,\frac{\partial}{\partial x_j}\left(\overline{\rho\,v''_i\,v''_j}\right)}_{\text{mean velocity production}}-\underbrace{\overline{v''_i}\,\frac{\partial\overline{p}}{\partial x_i}}_{\text{pressure work}}+\underbrace{\overline{p'\,\frac{\partial v''_j}{\partial x_j}}}_{\text{pressure-dilatation}}-\underbrace{\overline{\sigma''_{ij}\,\frac{\partial v''_i}{\partial x_j}}-\overline{\sigma^{D''}_{ij}\,\frac{\partial v''_i}{\partial x_j}}}_{\text{kinetic energy dissipation rate}}$$

- Use the gradient diffusion approximation to close the diffusion term and density flux, and (Ma_t is the turbulent Mach number)

$$\overline{p'\,\frac{\partial v''_i}{\partial x_j}}=\overline{\rho}\left(\alpha_2\,\tau_{ij}\,\frac{\partial\widetilde{v}_i}{\partial x_j}+\alpha_3\,Ma_t\,\widetilde{\epsilon''}\right)Ma_t^2$$

$$\overline{v''_i}=-\frac{\overline{\rho'\,v''_i}}{\overline{\rho}}=\frac{\nu_t}{\overline{\rho}\,\sigma_\rho}\,\frac{\partial\overline{\rho}}{\partial x^i}$$

The modeled turbulent kinetic energy dissipation rate transport equation is obtained as follows

- The turbulent kinetic energy dissipation rate equation is obtained by multiplying the turbulent kinetic energy equation by ε/K and a dimensionless constant for each term:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{\epsilon''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{\epsilon''}\,\widetilde{v}_j\right)$$

$$= \underbrace{C_{\epsilon 0}\,\frac{\widetilde{\epsilon''}}{\widetilde{E''}}\left(\overline{\rho}\,\overline{v_i''} + \overline{\rho' v_i''}\right) g_i}_{\text{force production}} + \underbrace{C_{\epsilon 1}\,\frac{\widetilde{\epsilon''}}{\widetilde{E''}}\,\widetilde{v}_i\,\frac{\partial}{\partial x_j}\left(\overline{\rho\, v_i'' v_j''}\right)}_{\text{mean velocity production}}$$

$$- \underbrace{C_{\epsilon 2}\,\overline{\rho}\,\frac{\left(\widetilde{\epsilon''}\right)^2}{\widetilde{E''}}}_{\text{kinetic energy dissipation rate}} - \underbrace{\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\epsilon}\,\frac{\partial \widetilde{\epsilon''}}{\partial x^j}\right)}_{\text{turbulent diffusion}}$$

$$- \underbrace{C_{\epsilon 3}\,\frac{\widetilde{\epsilon''}}{\widetilde{E''}}\,\overline{v_i''}\,\frac{\partial \overline{p}}{\partial x_i}}_{\text{pressure work}} + \underbrace{C_{\epsilon 4}\,\frac{\widetilde{\epsilon''}}{\widetilde{E''}}\,\overline{p'\,\frac{\partial v_i''}{\partial x_i}}}_{\text{pressure-dilatation}}$$

The modeled *Z* transport equation is obtained from the *K* and ε equations as follows

- Using the *K* and ε equations,

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{Z''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{Z''}\,\widetilde{v}_j\right) = \overline{\rho}\left(\frac{\partial}{\partial t} + \widetilde{v}_j\,\frac{\partial}{\partial x_j}\right)\widetilde{Z''}$$

$$= \overline{\rho}\,\widetilde{Z''}\left[\frac{m}{\widetilde{E''}}\left(\frac{\partial}{\partial t} + \widetilde{v}_j\,\frac{\partial}{\partial x_j}\right)\widetilde{E''} + \frac{n}{\widetilde{\epsilon''}}\left(\frac{\partial}{\partial t} + \widetilde{v}_j\,\frac{\partial}{\partial x_j}\right)\widetilde{\epsilon''}\right]$$

$$= m\,\frac{\widetilde{Z''}}{\widetilde{E''}}\left[\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{E''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{E''}\,\widetilde{v}_j\right)\right]$$

$$+ n\,\frac{\widetilde{Z''}}{\widetilde{\epsilon''}}\left[\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{\epsilon''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{\epsilon''}\,\widetilde{v}_j\right)\right]$$

$$= \frac{\widetilde{Z''}}{\widetilde{E''}}\left(m + n\,C_{\epsilon_K}\right)\left[\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{E''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{E''}\,\widetilde{v}_j\right)\right]$$

The turbulent diffusion term is transformed as follows

- Substituting

$$\widetilde{\epsilon''} = \left[\frac{\widetilde{Z''}}{C_Z \left(\widetilde{E''}\right)^m} \right]^{1/n}$$

it follows that

$$\widetilde{Z''} \left[\frac{m}{\widetilde{E''}} \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial \widetilde{E''}}{\partial x^j} \right) + \frac{n}{\widetilde{\epsilon''}} \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \widetilde{\epsilon''}}{\partial x^j} \right) \right]$$

$$= \frac{m \widetilde{Z''}}{\widetilde{E''}} \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial \widetilde{E''}}{\partial x^j} \right) + \frac{\partial}{\partial x_j} \left[\frac{\mu_t}{\sigma_\epsilon} \left(\frac{\partial \widetilde{Z''}}{\partial x^j} - \frac{m \widetilde{Z''}}{\widetilde{E''}} \frac{\partial \widetilde{E''}}{\partial x^j} \right) \right]$$

$$+ \frac{\mu_t}{n \sigma_\epsilon} \left(\frac{\partial \widetilde{Z''}}{\partial x^j} - \frac{m \widetilde{Z''}}{\widetilde{E''}} \frac{\partial \widetilde{E''}}{\partial x^j} \right) \left(\frac{1-n}{\widetilde{Z''}} \frac{\partial \widetilde{Z''}}{\partial x_j} - \frac{m}{\widetilde{E''}} \frac{\partial \widetilde{E''}}{\partial x_j} \right)$$

Finally, the modeled form of the Z transport equation is as follows

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\widetilde{Z''}\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\,\widetilde{Z''}\,\widetilde{v}_j\right) = \overline{\rho}\left(\frac{\partial}{\partial t} + \widetilde{v}_j \frac{\partial}{\partial x_j}\right)\widetilde{Z''}$$

$$= \underbrace{C_{Z0}\,\frac{\widetilde{Z''}}{\widetilde{E''}}\left(\overline{\rho}\,\overline{v_i''} + \overline{\rho' v_i''}\right) g_i}_{\text{force production}} + \underbrace{C_{Z1}\,\frac{\widetilde{Z''}}{\widetilde{E''}}\,\widetilde{v}_i\,\frac{\partial}{\partial x_j}\left(\overline{\rho\, v_i'' v_j''}\right)}_{\text{mean velocity production}} - \underbrace{C_{Z2}\,\overline{\rho}\,\frac{\widetilde{Z''}\,\widetilde{\epsilon''}}{\widetilde{E''}}}_{\text{kinetic energy dissipation rate}}$$

$$\underbrace{- \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial \widetilde{Z''}}{\partial x^j}\right] - \frac{m\,\widetilde{Z''}}{\widetilde{E''}}\,\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\,\frac{\partial \widetilde{E''}}{\partial x^j}\right)}_{\text{turbulent diffusion}}$$

$$\underbrace{+ m\,\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\epsilon}\,\frac{\widetilde{Z''}}{\widetilde{E''}}\,\frac{\partial \widetilde{E''}}{\partial x^j}\right) - \frac{\mu_t}{n\,\sigma_\epsilon}\left(\frac{\partial \widetilde{Z''}}{\partial x^j} - \frac{m\,\widetilde{Z''}}{\widetilde{E''}}\,\frac{\partial \widetilde{E''}}{\partial x^j}\right)\left(\frac{1-n}{\widetilde{Z''}}\,\frac{\partial \widetilde{Z''}}{\partial x_j} - \frac{m}{\widetilde{E''}}\,\frac{\partial \widetilde{E''_k}}{\partial x_j}\right)}_{\text{turbulent diffusion}}$$

$$- \underbrace{C_{Z3}\,\frac{\widetilde{Z''}}{\widetilde{E''}}\,\overline{v_i''}\,\frac{\partial \overline{p}}{\partial x_i}}_{\text{pressure work}} + \underbrace{C_{Z4}\,\frac{\widetilde{Z''}}{\widetilde{E''}}\,\overline{p'\,\frac{\partial v_i''}{\partial x_i}}}_{\text{pressure-dilatation}}$$

The coefficients in the modeled Z transport equation are obtained from those in the ε equation

- The coefficients in the standard K-ε model are

$$\sigma_k = 1.0 \quad , \quad \sigma_\epsilon = 1.3 \quad , \quad C_{\epsilon 1} = 1.44 \quad , \quad C_{\epsilon 2} = 1.92$$

$$C_{\epsilon 0} = C_{\epsilon 4} = 1.0$$

- The coefficients in the Z equation are

$$C_{Z0} \equiv m + n\, C_{\epsilon 0} \quad , \quad C_{Z1} \equiv m + n\, C_{\epsilon 1} \quad , \quad C_{Z2} \equiv m + n\, C_{\epsilon 2}$$

$$C_{Z3} \equiv m + n\, C_{\epsilon 3} \quad , \quad C_{Z4} \equiv m + n\, C_{\epsilon 4}$$

- Different choices of m and n yield different 2-equation models:
  - $\widetilde{E''}$-$\widetilde{\epsilon''}$ with m = 0 and n = 1 (turbulent energy dissipation)
  - $\widetilde{E''}$-$\widetilde{\ell''}$ with m = 3/2 and n = -1 (turbulent lengthscale)
  - $\widetilde{E''}$-$\widetilde{\omega''}$ with m = -1 and n = 1 (turbulent frequency)
  - $\widetilde{E''}$-$\widetilde{\tau''}$ with m = 1 and n = -1 (turbulent timescale)

The *K*-*Z* model simplifies for several special types of turbulent flows, which can be used to tune the model coefficients

- Isotropic turbulence: power-law decaying solutions
  - Production terms proportional to τ_{ij}, the turbulent diffusion terms, and the mean velocity vanish

- Free shear flows (plane wake; mixing layer; plane, round, and radial jet): far-field, self-similar, statistically-stationary solutions
  - Solutions depend on the similarity variable $\eta = y/x$

– Turbulent boundary layers: power-law solutions in the logarithmic layer
  - Sufficiently far from the boundary, the eddy viscosity dominates the molecular viscosity and the advection terms are negligible

The *K-Z* model equations have power-law solutions for isotropic turbulence

- The model equations reduce to coupled ordinary differential equations

$$\frac{dK}{dt} = -\epsilon \qquad \frac{dZ}{dt} = -C_{Z2}\,\frac{Z}{K}\,\epsilon$$

- The initial conditions are $K(0) = K_0$ and $Z(0) = Z_0 = C_Z K_0^m \epsilon_0^n$
- The corresponding solutions are

$$\frac{K(t)}{K_0} = \left[1 + \left(\frac{C_{Z2}-m-n}{n}\right)\frac{\epsilon_0}{K_0}\,t\right]^{-n/(C_{Z2}-m-n)}$$

$$= \left[1 + (C_{\epsilon 2} - 1)\frac{\epsilon_0}{K_0}\,t\right]^{-1/(C_{\epsilon 2}-1)}$$

$$\frac{Z(t)}{Z_0} = \left[\frac{K(t)}{K_0}\right]^{C_{Z2}} = \left[\frac{K(t)}{K_0}\right]^{m+nC_{\epsilon 2}}$$

- Experimentally, $K(t) \propto t^{1.34}$, which determines $C_{\varepsilon 2}$ (or C_{Z2})

The *K*-*Z* model equations have similarity solutions for free shear flows

- The model equations reduce to (and are solved by transforming to the similarity variable)

$$\left(\overline{v}_x \frac{\partial}{\partial x} + \overline{v}_y \frac{\partial}{\partial y}\right)K = \tau_{xy} \frac{\partial \overline{v}_x}{\partial y} - \epsilon + \frac{1}{y^r} \frac{\partial}{\partial y}\left(y^r \frac{\nu_t}{\sigma_k} \frac{\partial K}{\partial y}\right)$$

$$\left(\overline{v}_x \frac{\partial}{\partial x} + \overline{v}_y \frac{\partial}{\partial y}\right)Z = C_{Z1} \frac{Z}{K} \nu_t \left(\frac{\partial \overline{v}_i}{\partial x_j}\right)^2 - C_{Z2} \frac{Z}{K} \epsilon$$

$$+\frac{1}{y^r} \frac{\partial}{\partial y}\left(y^r \frac{\nu_t}{\sigma_\epsilon} \frac{\partial Z}{\partial y}\right) + \frac{mZ}{Ky^r} \frac{\partial}{\partial y}\left(y^r \frac{\nu_t}{\sigma_k} \frac{\partial K}{\partial y}\right) - \frac{m}{y^r} \frac{\partial}{\partial y}\left(y^r \frac{\nu_t}{\sigma_\epsilon} \frac{Z}{K} \frac{\partial K}{\partial y}\right)$$

$$+\frac{\nu_t}{n\sigma_\epsilon}\left(\frac{\partial Z}{\partial y} - \frac{mZ}{K} \frac{\partial K}{\partial y}\right)\left(\frac{1-n}{Z} \frac{\partial Z}{\partial y} - \frac{m}{K} \frac{\partial K}{\partial y}\right)$$

where $r = 1$ corresponds to a round jet and $r = 0$ otherwise, and the shear stress is

$$\tau_{xy} = \nu_t \frac{\partial \overline{v}_x}{\partial y}$$

The *K-Z* model equations have similarity solutions for the mixing layer

- The solutions have the form

$$\overline{v}_x(x,y) = \Delta v\, \overline{v}_x(\eta)$$

$$K(x,y) = (\Delta v)^2 K(\eta)$$

$$Z(x,y) = C_Z\, (\Delta v)^{2m}\, K(\eta)^m \left[\frac{(\Delta v)^3}{x} \right]^n \epsilon(\eta)^n$$

where $v = v_1 - v_2$ is the velocity difference between the two streams

The *K-Z* model equations have solutions consistent with the law-of-the-wall in bounded flows

- The Reynolds-averaged and *K-Z* equations reduce to

$$\frac{\partial}{\partial y}\left(\mu_t \frac{\partial \overline{v}_x}{\partial y}\right) = 0$$

$$\mu_t \left(\frac{\partial \overline{v}_x}{\partial y}\right)^2 + \frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_K}\frac{\partial K}{\partial y}\right) - \rho\epsilon = 0$$

$$C_{Z1}\frac{Z}{K}\mu_t\left(\frac{\partial \overline{v}_x}{\partial y}\right)^2 - C_{Z2}\,\rho\,\frac{Z}{K}\epsilon + \frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_\epsilon}\frac{\partial Z}{\partial y}\right)$$

$$+\frac{mZ}{K}\,\frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_k}\frac{\partial K}{\partial y}\right) - m\frac{\partial}{\partial y}\left(\frac{\mu_t}{\sigma_\epsilon}\frac{Z}{K}\frac{\partial K}{\partial y}\right)$$

$$+\frac{\mu_t}{n\,\sigma_\epsilon}\left(\frac{\partial Z}{\partial y} - \frac{mZ}{K}\frac{\partial K}{\partial y}\right)\left(\frac{1-n}{Z}\frac{\partial Z}{\partial y} - \frac{m}{K}\frac{\partial K}{\partial y}\right) = 0$$

- The solutions have the form (where v_τ is the friction velocity, κ is the von Kármán constant, and C, D, C_Z are constants)

$$\overline{v}_x = \frac{v_\tau}{\kappa}\log y + C \quad , \quad K = D\,v_\tau^2 \quad , \quad Z = C_Z D^m\, v_\tau^{2m+3n}\left(\frac{1}{\kappa\,y}\right)^n$$

Application to asymptotically self-similar Rayleigh-Taylor mixing

- The turbulence production term is of the form

$$P_Z = C_{Z1} \frac{\widetilde{Z''}}{\widetilde{E''}} \tau_{ij} \frac{\partial \tilde{v}_i}{\partial x_j}$$

- Assume that at sufficiently late times, the scaling of the mixing layer width is

$$h(t) = \alpha \, At \, g \, t^2$$

and that turbulence variables are proportional to this lengthscale and the corresponding velocity scale

- Then, *K*, ε, and *Z* are

$$\widetilde{E''} = \frac{\widetilde{v''^2}}{2} \propto \left(\frac{dh}{dt} \right)^2 \propto 4(\alpha \, At \, g)^2 t^2 \qquad \widetilde{\epsilon''} = \frac{\partial \widetilde{E''_k}}{\partial t} \propto 8(\alpha \, At \, g)^2 \, t$$

$$\widetilde{Z''} = C_Z \left(\widetilde{E''} \right)^m \left(\widetilde{\epsilon''} \right)^n \propto (\alpha \, At \, g)^{2m+2n} \, t^{2m+n}$$

In Rayleigh-Taylor mixing the eddy viscosity and Reynolds stress tensor scale as follows

- The eddy viscosity scales as

$$\nu_t = \left(\widetilde{E''}\right)^{\frac{m+2n}{n}} \left(\widetilde{Z''}\right)^{-\frac{1}{n}} \propto (\alpha A t g)^2 t^3$$

- The Reynolds stress scales as

$$\tau_{ij} = 2\overline{\rho}\,\widetilde{E''}\,\frac{\delta_{ij}}{d} - 2\overline{\rho}\,\nu_t \left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{d}\frac{\partial \widetilde{v}_k}{\partial x_k}\right)$$

$$\propto 2\overline{\rho}(\alpha A t g)^2 t^2 \left[\frac{4}{d}\delta_{ij} - \left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{d}\frac{\partial \widetilde{v}_k}{\partial x_k}\right) t\right]$$

- Therefore, if the Favre-averaged strain-rate tensor dimensionally scales as (q_{ij} is dimensionless)

$$\widetilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial \widetilde{v}_i}{\partial x_j} + \frac{\partial \widetilde{v}_j}{\partial x_i}\right) \propto q_{ij}\,\frac{1}{h(t)}\,\frac{dh(t)}{dt} \propto \frac{1}{t}$$

then $\tau_{ij} \propto 2\overline{\rho}(\alpha A t g)^2 t^2 \left(\frac{5}{d}\delta_{ij} - q_{ij}\right)$ and

$$P_Z \propto (\alpha A t g)^{2(m+n)}\, t^{2m+n-1}\, \overline{\rho}\left(\frac{5}{d}\delta_{ij} - q_{ij}\right) q_{ij}$$

Conclusions

- The methodology presented here provides a systematic and self-consistent approach to the derivation of 2-equation turbulent transport models
  - This provides an improved *l* transport equation
  - Also provides a consistent expression for the diffusion and cross diffusion terms, which are important in many flow (e.g., near a boundary)
- Several canonical turbulent flows can be used to reduce the model equations and specify model parameters before application to interfacial-instability induced turbulence
- The general *Z* equation is consistent with the t^2 scaling of the mixing layer width
- Both an ω and a τ equation were derived as alternatives to the ε and *l* equation
  - τ may be a better physical variable than ε and *l*

Work in progress

- Completion of solutions for canonical turbulent flows
- Completion of solutions for Rayleigh-Taylor instability-induced turbulence
- Commencement of examination of model parameters and forms of modeled terms using high-resolution DNS data
- Eventually, application to Richtmyer-Meshkov instability-induced turbulence