EXPERIENCE WITH TURBULENCE INTERACTION AND TURBULENCE-CHEMISTRY MODELS AT FLUENT INC.

D. Choudhury, S.E. Kim, D.P. Tselepidakis,
and M. Missaghi
Fluent Inc.
Lebanon, New Hampshire

Outline of Talk

- Part I: Turbulence Modeling
  - Challenges in Turbulence Modeling
  - Desirable Attributes of Turbulence Models
  - Turbulence Models in FLUENT
  - Examples using FLUENT
- Part II: Combustion Modeling
  - Turbulence-Chemistry Interaction
  - FLUENT Equilibrium Model
- Concluding Remarks

Part I: Turbulence Modeling and Industrial Flows

- Many industrial flows are turbulent; certainly in the markets that two of our codes, FLUENTand RAMPANT, are focused in.
- Turbulence augments rates of mass, momentum and heat transfer, often by orders of magnitude.
- Most combustion processes involve turbulence and often depend on it.
- Choice of turbulence model dictates the accuracy of CFD predictions.
- There is still a large gap between the state-of-the-art and users' expectations and needs.

Challenges in Turbulence Modeling

- Modeling the correlations: $\overline{\rho u_i' u_j'}$ and $\overline{\rho u_i' \phi}$.
  - Closures based on the "eddy-viscosity" concept (industry's most popular choice)
  - Closures based on transport equations (RSM)
- Modeling an additional transport equation for a scalar quantity to fix the state of turbulence.
  - Most popular choice: the kinetic energy dissipation rate, ε.
  - However, this equation is derived by continuum mechanics-based phenomenological considerations and intuition.
- Modeling of the viscosity-affected, near-wall laminar sublayer.
  - Most popular choice: "Wall-functions" that bridge the turbulent field to the solid wall.
  - However, assumptions involved are not always right.

Desirable Attributes of Turbulence Models in Commercial CFD Codes

- Accuracy and Universality
  - The range of applicability should be as broad as possible.
  - Applicable to complex geometries and unstructured meshes.
- Economy
  - Mathematically simple.
  - Memory and CPU requirements should be moderate and affordable (model formulation and grid distribution requirements).
- Robustness
  - Model should be able to solve a wide range of problems with little or no convergence problems.
  - Computationally efficient (fast execution speed and uses memory sparingly).

Turbulence Models in FLUENT

- k-ε model adequate for simple flows with no significant strain rates.
- RNG k-ε model for separated flows, flows with large streamline curvature, swirling flows, or flows with significant strain rates.
- RSM recommended for swirling flows or highly anisotropic flows.

k-ε Model: Some Comments

- Well-tested, used for over 20 years, limitations well understood.
- It forms a good compromise between universality and economy of use for many engineering problems.
- Subject to the inherent limitations of the Boussinesq's hypothesis, i.e., isotropic eddy-viscosity and Newtonian closure (gradient-diffusion model).
- Many assumptions are introduced in deriving the modeled equations for the turbulent quantities, particularly the ε-equation, making their fidelity limited.
- The constants in the modeled equations are calibrated against simple benchmark experiments.
- As a result, the k-ε model performs poorly in flows with curvature, swirl, rotation, separated flows, low-Reynolds number flows, strongly anisotropic flows, etc.

Renormalization Group (RNG) Based k-ε Model

- Basic theory and derivation are described in Yakhot and Orszag (1986). Further details and applications are in Yakhot, Orszag, Thangam, Speziale, and Gatski (1992), Speziale and Thangam (1992).
- First introduced in a commercial code, FLUENT, in 1992.
- The RNG method is essentially a scale-elimination technique that can be applicable to the Navier-Stokes and other scalar transport equations as well.
- Removal of successively large scales leads to differential transport equation models and associated formula for quantities such as the turbulent Prandtl/Schmidt number.
- The basic form of the RNG-based k-ε equations remains largely the same with the standard k-ε model. But, the constants in the model equations are derived explicitly from theory.
- The ε-equation ends up with an additional source term, a strain-dependent term.
- The RNG model can be integrated directly to a solid wall without using *ad hoc* damping functions or damping terms used in many near-wall models.
- High-Re form of the turbulence kinetic energy and dissipation rate equations derived by RNG procedure are:

$$\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial x_i} = P_k - \varepsilon + \frac{\partial}{\partial x_i}\left(\frac{\nu_T}{\sigma_k}\frac{\partial k}{\partial x_i}\right)$$

$$\frac{\partial \varepsilon}{\partial t} + U_i \frac{\partial \varepsilon}{\partial x_i} = 1.42\frac{\varepsilon}{k}P_k - 1.68\frac{\varepsilon^2}{k} + \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right) - \Re$$

where:

$\sigma_k = \sigma_\varepsilon = 0.7179$

$P_k = 2\nu_T S_{ij} S_{ij}$ is the kinetic energy production

$S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)$ is the mean rate of strain tensor

$\nu_T = C_\mu \frac{k^2}{\varepsilon}$

$\Re = \frac{C_\mu \eta^3 (1-\frac{\eta}{\eta_0})}{1+\beta\eta^3}\frac{\varepsilon^2}{k}$

$\eta = Sk/\varepsilon,\ S = (2\,S_{ij}\,S_{ij})^{\frac{1}{2}}$

$\eta_0 = 4.38,\ \beta = 0.015$

RNG-Based k-ε Model (Cont'd)

- In the low-Re RNG model, a differential relationship exists between $\frac{k}{\sqrt{\varepsilon}}$ and ν_{eff} (Yakhot and Orszag, 1986).
- The turbulent Prandtl/Schmidt number is no longer a constant, and computed from relationships relating the local value of the number to the viscosity ratio (Yakhot and Orszag, 1986).
- In these relations, as $\hat{\nu} \longrightarrow 1, \alpha \longrightarrow \alpha_0$ (the low-Re limit) and as $\hat{\nu} \longrightarrow \infty$, $\sigma = \alpha^{-1} \longrightarrow 0.7179$ (the high-Re limit). Here:

  $\hat{\nu} = \nu_{\text{eff}}/\nu_0$, where $\nu_{\text{eff}} = \nu_0 + \nu_T$

  α = inverse turbulent Prandtl number (σ^{-1})

  α_0 = inverse molecular Prandtl number (σ_0^{-1})

- In the low-Re regions, σ_k and σ_ε are obtained similarly from the Prandtl number relationships, with $\alpha_0 = 1.0$.
- The relationships ensure that in the high-Re number part of the flow where $\hat{\nu} >> 1$:

$$\nu_{\text{eff}} = \nu_T = 0.085 \frac{k^2}{\varepsilon}$$

  and the effective viscosity varies smoothly from the molecular viscosity to the turbulent viscosity.

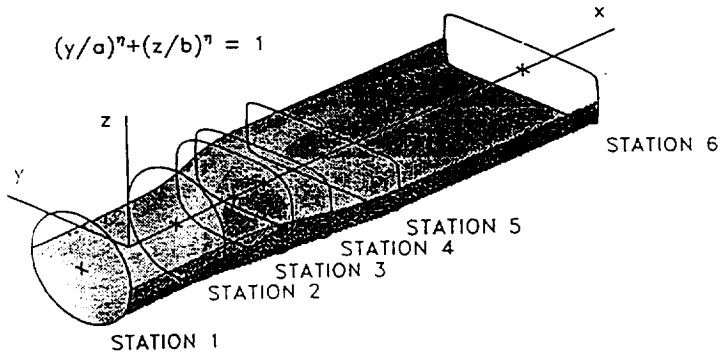
- The low-Re eddy-viscosity formula does not explicitly involve any geometric length scale, i.e., the distance from a solid wall used in the damping functions adopted by most low-Re near-wall models, which is a very convenient feature for calculations for complex three-dimensional geometries.
- In collaboration with the originators of the RNG model, Drs. Yakhot and Orszag, the model has been extended to account for the effects of compressibility, swirl, rotation, and premixed combustion.
- The RNG-based k-ε model also works well with conventional and enhanced (non-equilibrium) wall functions available in Fluent Inc.codes.

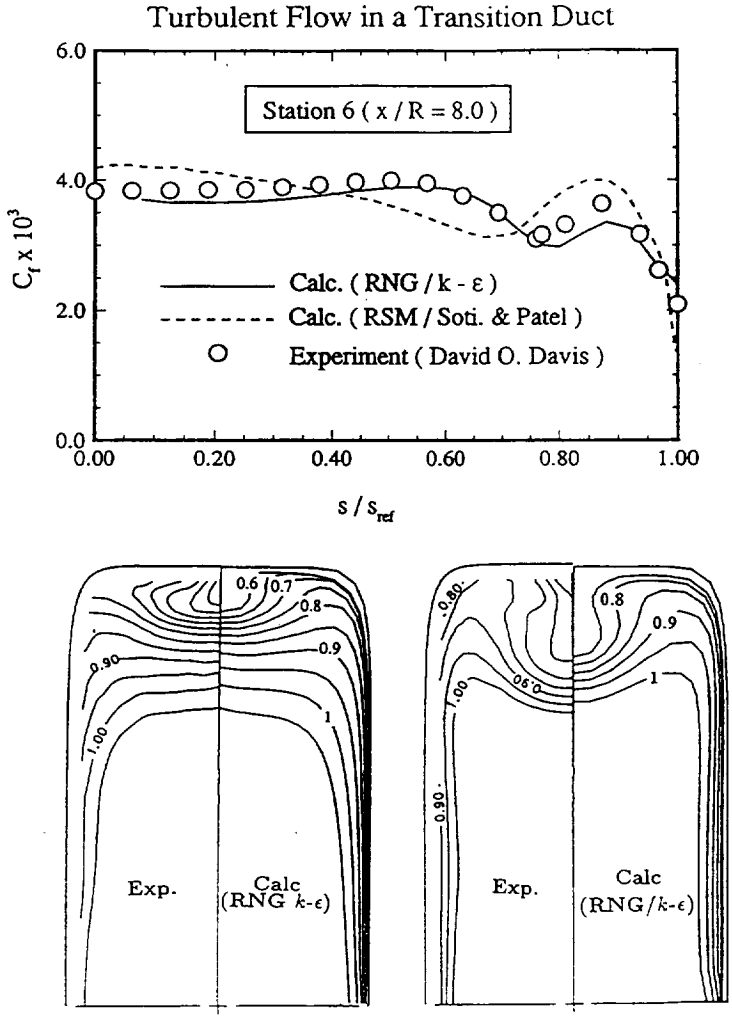
The Reynolds-Stress Model in FLUENT

- RSM solves transport equations for the Reynolds stresses: $\overline{u_i' u_j'}$ (4 equations in 2D problems, 6 equations in 3D problems).
- RSM is the level of modeling that has a well established track record of out-performing eddy-viscosity models in complex flows.
- It is computationally more expensive and more inclined to divergence and stability problems.
- The simple and most widely tested form of the Launder, Reece and Rodi (1975) form is used.
- The interpolation technique for co-located grids of Rhie and Chow (1983) is used.
- It offers the best choice for highly anisotropic flows.

Example 1: Circle-to-Rectangle Transition Duct

- Measured by Davis (1991).
- $Re_D = 3.9 \times 10^5$.
- Solution Domain.
  - Upstream Inlet Boundary: $x/D = -1.0$
  - Downstream Exit Boundary: $x/D = 8.0$
  - A Quadrant of the duct modeled.

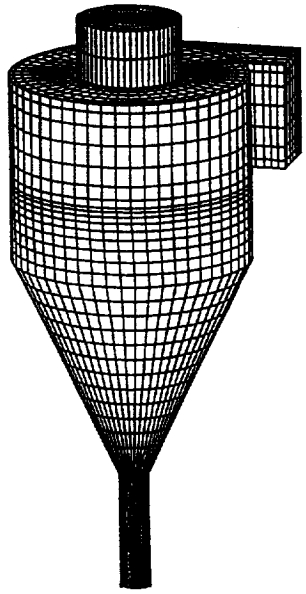


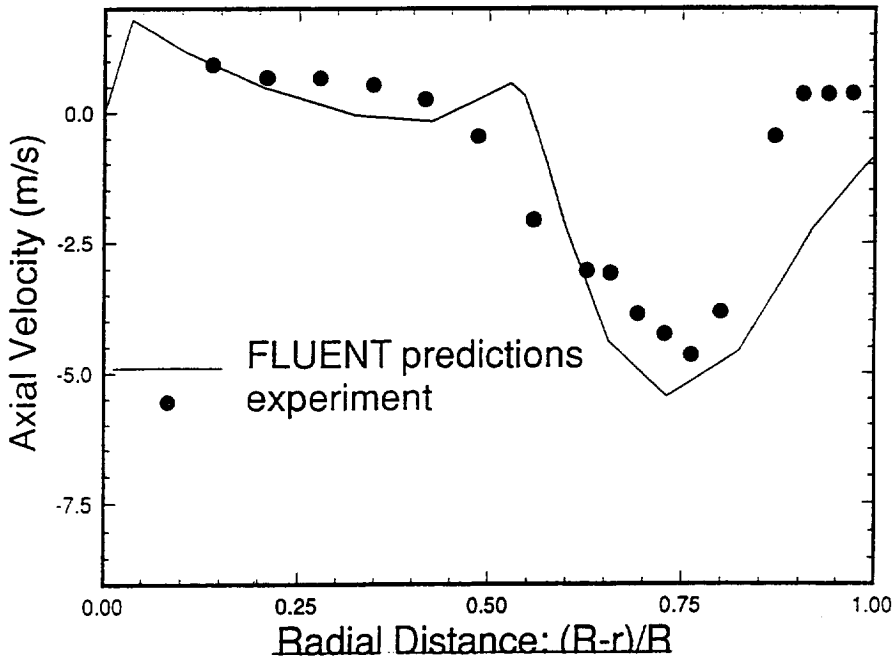


Contours of computed streamwise velocity
(RNG-based k-ϵ model)

Example 2:
Cyclone Sparator

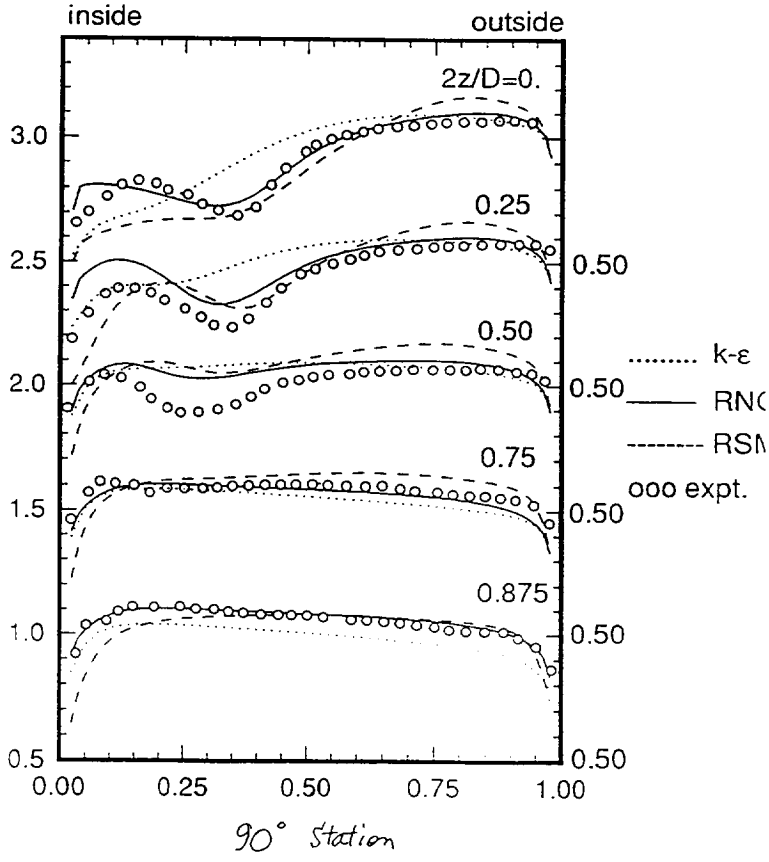
- Measured by Qing (1983).
- RSM is used.
- Cylindrical 55 × 23 × 41 grid.

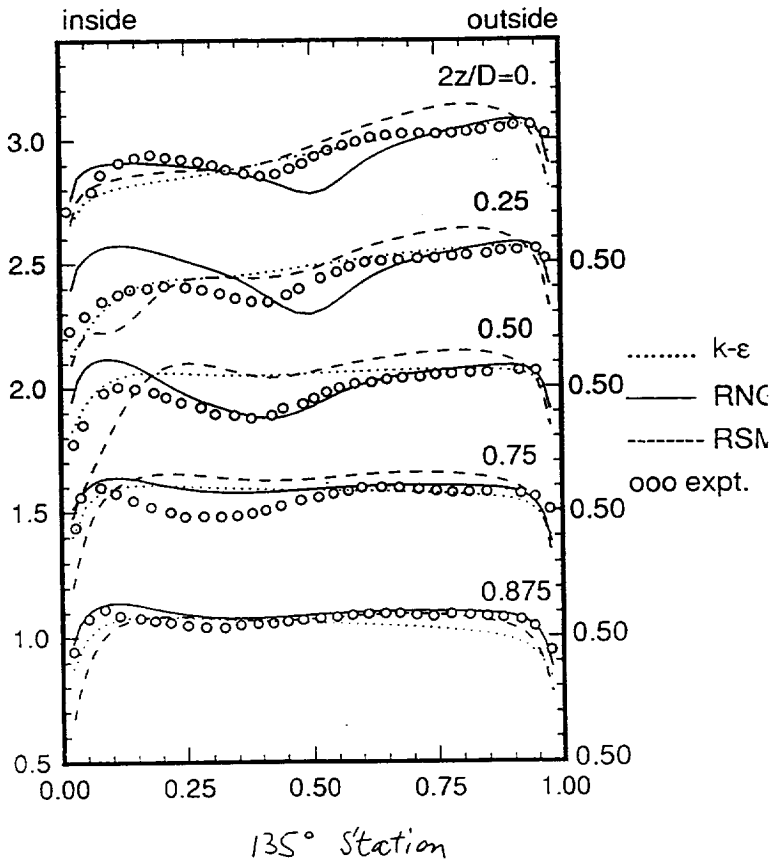




Example 3:
180° Bend of Square-Cross Section

- Solution Domain
  - Upstream Boundary: $5.0D_H$ from the start of the bend
  - Downstream Boundary: $5.0D_H$ from the end of the bend
  - A symmetric half of the duct modeled.
- Mesh
  - Orthogonal $101 \times 47 \times 27$
  - Distance from the wall $\approx 0.01D_H$





Part II:
Combustion Modeling

- With environmental awareness, legislations on combustion-generated pollutants such as NO_x, SO_x carbon monoxide, soot, unburnt hydrocarbons, etc. have become increasingly tougher.
- Combustion simulation in industrial applications can help us to design combustors with higher efficiencies and lower pollutant emissions.
- The combustion process involves some of the most complex phenomena such as chemistry, multiphase flow, turbulence, heat transfer and the interaction between these phenomena.
- Here we focus on gaseous combustion in which the reactants may be mixed or non-mixed prior to flowing into the combustor.

Turbulence-Chemistry Interaction

- Accurate simulation of turbulent combustion requires a thorough assessment of the way turbulence and chemistry interact. The reaction rate and flame structure primarily depend on this interaction.
- In turbulent flames, chemical rates can be significantly different than those in laminar flames (sometimes several orders of magnitude), and the mean chemical rate is not the same as the rate calculated based on mean values of the various scalars:

$$\bar{r}(\theta_1, \theta_2, ...) \neq r(\bar{\theta}_1, \bar{\theta}_2, ...)$$

- Turbulent-chemistry interaction is best characterized by the Damkohler number which is the ratio of characteristic flow time to chemical reaction time:

$$Da = \frac{\tau_E}{\tau_r} = \frac{\ell}{\ell_f} \frac{U_\ell}{U'}$$

- When $Da << 1$ chemical reactions are orders of magnitude slower than turbulent mixing and the influence of turbulence on reaction can be neglected.
- When $Da >> 1$ chemical reactions are very fast and hence combustion is controlled by turbulent mixing.

- At high Da we can exploit the laminar flame concept: turbulent flame is comprised of an array of laminar flames (flamelets). Hence chemical rate expressions can be those obtained in laminar flames and the effect of turbulence can be characterized through the probability density function (pdf).
- For turbulent diffusion flame, the pdf is usually expressed in terms of a scalar which can best characterize mixing, e.g., the mixture fraction. Since the rate of reaction is much higher than the mixing rate, we can assume that the reaction system is at equilibrium. The effect of turbulence is simply felt by the fluctuations in the mixture fraction. The mean value of any scalar in the flame is simply:

$$\bar{\theta} = \int_0^1 \theta(\xi) P(\xi) d\xi$$

- For turbulent premixed flames the pdf is usually expressed in terms of a scalar which can best characterize the reaction progress, e.g., normalized temperature:

$$\bar{r} = \int_0^1 r(c) p(c) dc$$

FLUENT Equilibrium Model

- For turbulent diffusion flames we use a two-moment beta pdf and equilibrium data to calculate various thermo-chemical scalars in the flame.
- To obtain equilibrium data we use the popular CHEMKIN library of SANDIA, fully interfaced with our codes. CHEMKIN contains data on all important gaseous fuels, combustion intermediates and products as well as their properties.
- We obtain the mean mixture fraction and its variance from their respective conservation equations:

$$\frac{\partial}{\partial x_i}(\rho u_i \bar{\xi}) = \frac{\partial}{\partial x_i}(\frac{\mu_t}{\sigma_t}\frac{\partial \bar{\xi}}{\partial x_i})$$

$$\frac{\partial}{\partial x_i}(\rho u_i \overline{\xi'^2}) = \frac{\partial}{\partial x_i}(\frac{\mu_t}{\sigma_t}\frac{\partial \overline{\xi'^2}}{\partial x_i}) + \frac{2\mu_t}{\sigma_t}(\frac{\partial \bar{\xi}}{\partial x_i})^2 - C_d \rho \frac{\epsilon}{k}\overline{\xi'^2}$$

- To save computational time we calculate the integrals before the CFD calculations.

Concluding Remarks

- As of now, we provide our users with three turbulence models:
  - the "conventional" k-ϵ model,
  - the ReNormalization Group model,
  - the Reynolds-Stress Model.
- The Renormalization group k-ϵ model has broadened the range of applicability of two-equation turbulence models.
- The Reynolds-stress model has proved useful for strongly anisotropic flows such as those encountered in cyclones, swirlers and combustors.
- Issues remain, such as near-wall closure, with all classes of models.
- Collaborative research with ICOMP will not only serve to further quantify applicability of turbulence models but may bring to market new ideas in the field of turbulence modeling for industrial flows.