Numerical Modeling of Mixing Processes - What Can LES Offer?

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**Objective**

- To evaluate whether LES can be used effectively to model fluid behavior in engineering applications

**Outline**

- Brief Summary of Turbulence Models
- Introduction to Large Eddy Simulation (LES)
- Examples
  - Bluff Body Jet
  - HEV Static Mixer
Modeling Turbulence

- Turbulence is a 3D transient phenomenon
  - Fluctuations cover a wide range of time and length scales
- Turbulence models range from approximate to highly rigorous:
  - steady-state isotropic models
  - transient 3D models of entire spectrum
- Models are incorporated into the Navier-Stokes equations using a variety of methods

The Turbulence Spectrum

- Many scales of turbulent eddies exist:
  - Large eddies contain most of the turbulent kinetic energy
    - Scale sizes are on the order of the flow passages
  - Energy cascades from large to small eddies
  - Small eddies dissipate the energy they receive from larger eddies in the spectrum
- Difficulty in turbulence modeling is trying to accurately capture the contributions of all scales in the spectrum
Direct Numerical Simulation (DNS)

- Navier-Stokes equations are solved on a fine grid using a small time-step
- Goal is to capture the smallest turbulence scales
  - Large scales are captured as well
- Result is accurate, 3D, transient behavior
- Great for simple flows, but computationally intensive
  - Not suited to industrial applications with cpu resources available today

The Cost of DNS

- The number of grid points per dimension needed to resolve the small scales is
  \[ N_{1D} \sim \text{Re}_t^{3/4}, \quad \text{Re}_t = \frac{\rho \sqrt{k \ell}}{\mu} \]
- The number of grid points needed for a 3D DNS simulation is
  \[ N_{3D} \sim \text{Re}_t^{9/4} \]
- The overall cost, including time step, of the computational effort\(^1\) is \( \sim \text{Re}_t^3 \)

\(^1\)Reynolds, W.C. Turbulence at the Crossroads, pp. 313-342 (1990)
RANS Turbulence Models 1

- Velocities are described by an equilibrium ($v_o$) and fluctuating ($v'$) contribution:

$$v_i = v_{oi} + v'_i$$

- Momentum equations are rewritten, then time-averaged (Reynolds Averaged Navier-Stokes equations)
  - Averaging eliminates terms with $v'$ as a factor
  - Terms with $v_i v_j'$ remain
  - These Reynolds stresses are computed with a turbulence model
  - Impact on transport equations is through the effective viscosity: $\mu_{eff} = \mu + \mu_o$ (1 and 2 equation models)

RANS Turbulence Models 2

- Many flavors exist, such as:
  - $k-\epsilon$: Robust, popular 2-equation model using constants taken from simple, high Re flows
    - isotropic turbulence effects
    - $\mu_{eff}$ is a scalar
  - RSM: 5-equation (2D) or 7-equation (3D) model
    - non-isotropic turbulence effects makes this suitable for highly swirling flows
Large Eddy Simulation (LES)

- LES is midway between DNS and RANS in terms of:
  - rigor
  - computational requirement
- Spectrum of turbulent eddies in the Navier-Stokes equations is “filtered”
  - The filter is a function of the grid size
  - small eddies are removed, and modeled using a subgrid-scale (SGS) model
  - large eddies are retained, and solved for directly using a transient calculation

Filtered Variables

- A variable, \( \phi(x') \), is filtered using a filter function, \( G \)
  \[
  \tilde{\phi}(x) = \int_G \phi(x')G(x, x')dx'
  \]
- \( G \) is a function of the cell volume
  \[
  G(x, x') = \begin{cases} 
  1/V & \text{for } x' \in V \\
  0 & \text{otherwise}
  \end{cases}
  \]
  Thus
  \[
  \tilde{\phi}(x) = \frac{1}{V} \int_{V} \phi(x')dx', \quad x' \in V
  \]
Filtered Transport Equations

- The filtered continuity and momentum equations use filtered variables:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \tilde{u}_j}{\partial x_j} = 0
\]

and

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_j}
\]

\(\tau_{ij}\) is the filtered stress tensor
\(\sigma_{ij}\) are the subgrid-scale Reynolds stresses

Subgrid-Scale (SGS) Modeling

- SGS Reynolds stresses are modeled by

\[
\sigma_{ij} - \frac{1}{3} \delta_{ij} \sigma_{kk} = -2 \mu_s S_{ij}
\]

where \(\mu_s\) is the subgrid-scale eddy viscosity and \(S_{ij}\) is the rate of strain tensor

- Two models in FLUENT 5 are:

<table>
<thead>
<tr>
<th>Smagorinsky SGS model</th>
<th>RNG SGS model</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mu_s = \rho L^2 \sqrt{2S_y S_y})</td>
<td>(\mu_s = \mu \left[ 1 + C \left( \frac{\mu_s^2 \mu_{\text{min}}}{\mu^2} - C \right) \right]^{1/3})</td>
</tr>
</tbody>
</table>
| \(L = \min\left( \kappa d, C_s V^2 \right) \) | \(\mu_s = \left( 0.157 V^3 / \sqrt{2S_y S_y} \right) \)
**Bluff-Body Jet**

- Cold flow in a bluff-body coaxial burner
- A range of length and time scales exists

![Bluff Body Jet Flow Pattern](image)

**Bluff Body Jet Flow Pattern**

Time averaged flow pattern from LES simulations.
**Bluff-Body Jet Axial Velocities**

- Transient, 3D solution done with LES*
- Steady-state, 2D axisymmetric solutions done with $k$-$\varepsilon$ and RSM**
- Comparison with experiment

<table>
<thead>
<tr>
<th></th>
<th>$v_{\text{axial}}(x/D=0.8)$</th>
<th>$v_{\text{axial}}(x/D=1.3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>33.5 m/s</td>
<td>12.7 m/s</td>
</tr>
<tr>
<td>LES \textit{(t-averaged)}</td>
<td>35.2</td>
<td>13.2</td>
</tr>
<tr>
<td>RSM</td>
<td>26.4</td>
<td>7.5</td>
</tr>
<tr>
<td>$k$-$\varepsilon$</td>
<td>25.5</td>
<td>7.7</td>
</tr>
</tbody>
</table>

*420,000 cells  ** 30,000 cells

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**HEV Static Mixer**

- Circular or square cross-section pipe with sets of tabs mounted on the walls
- Flow around tabs is unsteady, with counter-rotating longitudinal vortices, and hairpin vortices

Source: “Kenics Static Mixers” brochure, 1996.
Previous Models

- Assumptions:
  - Eight-fold symmetry.
  - Steady state flow with RANS model

- Results:
  - Longitudinal vortices observed

- Disadvantages:
  - Hairpin vortices not observed
  - Under-prediction of mixing near center
  - No material exchange between areas surrounding tabs

Geometries Studied

- Two models studied
  - Square duct
    - $0.1 \times 0.1 \times 1$ m$^3$
    - Air at 30 m/s
    - Re $\sim 200k$
  - Cylindrical pipe
    - $D = 0.05$ m
    - Water at 0.12 m/s
    - Re $\sim 5000$

- Both models:
  - 500k cells
  - Unstructured grid
**Square Duct Results: RNG k-ε**

Longitudinal vortices are symmetric and stable.

Between 3rd and 4th tabs

2-D downstream of last tabs

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**Square Duct Results: LES**

**Longitudinal Vortices - 1**

Between third and fourth sets of tabs

T = 0.1429 s

T = 0.1486 s
**Square Duct Results: LES**

*Longitudinal Vortices - 2*

2-D downstream of last set of tabs

- T = 0.1429 s
- T = 0.1486 s

**Cylindrical Pipe Results: LES**

*Hairpin Vortices - 1*

- T = 6.40 s
- T = 6.43 s
Cylindrical Pipe Results: LES
Hairpin Vortices - 2

T = 6.46 s

T = 6.53 s

Hairpin Vortex Animation
Cylindrical Pipe Results: LES
Longitudinal Vortices - 1

Cylindrical - At Tip of Last Set of Tabs

Cylindrical Pipe Results: LES
Longitudinal Vortices - 2

Cylindrical - At Tip of Last Set of Tabs
Longitudinal Vortices Animation

Effective Viscosity Comparison

Ratio between effective viscosity and molecular viscosity

Re = 5000  Re = 2E5

Subgrid LES  k-E RNG  k-E Standard

Cylindrical  Square Duct
HEV Results Discussion

- LES predicts unsteady vortex system including transient hairpin vortices, as also seen in experiments
- Interaction between vortices causes material exchange between tabs, and between the center and tabs
- Practical issues:
  - Calculation time for 1500 time steps on the order of a week on 350 MHz P2 PC
  - 500k node model requires 0.5 GB of RAM
  - Data files ~ 50MB each (compressed)

Summary

- LES is a transient turbulence model that falls midway between RANS and DNS models
- Time-averaged results better predicted the axial flow pattern in a bluff-body jet example
- Transient results showed hairpin and longitudinal vortices in an HEV mixer, the former long observed experimentally, but not predicted with CFD until now
- LES has potential benefit for engineering applications, and is within reach computationally