MODELING TURBULENCE IN STIRRED VESSELS
A Review and Recent Developments

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FLUID / THERMAL / CHEMICAL / STRESSED SYSTEMS
WITH INDUSTRIAL APPLICATIONS
Introduction

• Turbulence in stirred vessels: a historical perspective.
• Prediction methods and large eddy simulation models.
• Examples:
  – Straight blade and pitched blade turbines.
  – Hydrofoil impeller systems.
  – Glass lined vessel example.
• Turbulence modeling: a projection for the future.
1980’s view of stirred tank flow fields

- Relatively simple flow fields, with superimposed random turbulence. Vortices behind the impeller blades.


Early 1990’s

- Asymmetric, unstable flow fields observed.
- Multimodal velocity histograms.
Solids distribution and CFD flow fields - 1994

Issues

• Local velocity data histograms may be multimodal.
• In single-phase blending systems:
  – Blend time experiments are poorly reproducible.
  – Lots of scatter in literature data.
• In dilute multiphase systems:
  – Gas holdup distribution may be asymmetric and oscillating.
  – Solids can be swept from one side of the vessel to the other in a relatively slow oscillating pattern.
• Need a better description of the hydrodynamics to understand these issues.
Digital particle image velocimetry (DPIV)

- First usable commercial systems came on the market in the mid 1990s.
- Allows instantaneous measurement of full 2-D flow fields.
PBT system – velocity vectors and vorticity - 1
PBT system – velocity vectors and vorticity - 2
Time series of spatially averaged vorticity
Spectral analysis – PBT system

Period = 42 seconds = 42 impeller revolutions
DPIV analysis conclusions

• Visually observed asymmetric flow patterns were confirmed.
• Long time scale oscillations were found, typically on the order of tens to hundreds of impeller revolutions.
• Importantly: the oscillations have time scales longer than the blend time!
• What does this mean for the proper choice of turbulence modeling method?
Turbulence modeling objective

- The objective of turbulence modeling is to develop equations that will predict the time averaged velocity, pressure, and temperature fields without calculating the complete turbulent flow pattern as a function of time.
  - This saves us a lot of work!
  - Most of the time it is all we need to know.
  - We may also calculate other statistical properties, such as RMS values.

- Important to understand: the time averaged flow pattern is a statistical property of the flow.
  - It is not an existing flow pattern!
  - The flow never actually looks that way!!
Example: flow around a cylinder at \( \text{Re}=1\times10^4 \)

- The figures show:
  - An experimental snapshot.
  - Streamlines for time averaged flow field. Note the difference between the time averaged and the instantaneous flow field.
  - Effective viscosity used to predict time averaged flow field.
Prediction methods

\[ l = \eta / Re^{3/4} \]

- Direct numerical simulation (DNS)
- Large eddy simulation (LES)
- Reynolds averaged Navier-Stokes equations (RANS)
Kolmogorov energy spectrum

- Energy cascade, from large scale to small scale.
- $E$ is energy contained in eddies of wavelength $\lambda$.
- Length scales:
  - Largest eddies. Integral length scale $(k^{3/2}/\varepsilon)$.
  - Length scales at which turbulence is isotropic. Taylor microscale $(15\nu u'^2/\varepsilon)^{1/2}$.
  - Smallest eddies. Kolmogorov length scale $(\nu^3/\varepsilon)^{1/4}$. These eddies have a velocity scale $(\nu \varepsilon)^{1/4}$ and a time scale $(\nu / \varepsilon)^{1/2}$.

$\varepsilon$ is the energy dissipation rate (m$^2$/s$^3$)
$k$ is the turbulent kinetic energy (m$^2$/s$^2$)
$\nu$ is the kinematic viscosity (m$^2$/s)
Direct numerical simulation (DNS)

- Navier-Stokes equations are solved on a fine grid using a small time-step. Goal is to capture all the turbulence scales.
- Result is accurate, 3D, transient behavior.
- Great idea for simple flows, but computationally intensive.
- The overall cost, including time step, of the computational effort is $\sim Re_t^3$.
- Not suited to industrial applications with CPU resources available today.
RANS turbulence models

• Reynolds averaged Navier-Stokes equations.
• Many flavors exist, such as:
  – Mixing length model, Spalart-Allmaras model, standard k-ε model, k-ε RNG model, realizable k-ε model, k-ω model.
  – Isotropic turbulence effects modeled through effective viscosity:
    • $\mu_{\text{eff}}$ 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 and 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.
- LES models in FLUENT are: RNG-Smagorinsky, Smagorinsky-Lilly, dynamic Smagorinsky, WALE, dynamic subgrid kinetic energy transport model.
Required mesh resolution

- Suppose you want to resolve 80% of TKE.
- Then, we need to resolve the eddies whose sizes are larger than roughly half the size of the integral length scale ($\ell_0$).

Cumulative TKE against length-scale of eddies based on the Kolmogorov’s energy spectrum

<table>
<thead>
<tr>
<th>$k(\ell)$</th>
<th>$\ell/\ell_0$</th>
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<tbody>
<tr>
<td>0.1 $k$</td>
<td>6.10</td>
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<tr>
<td>0.5 $k$</td>
<td>1.6</td>
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<tr>
<td>0.8 $k$</td>
<td>0.42</td>
</tr>
<tr>
<td>0.9 $k$</td>
<td>0.16</td>
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</tbody>
</table>
Numerics - spatial discretization

- The central-differencing scheme has much lower numerical diffusion than high-order upwind schemes.

Taylor's inviscid vortex flow – 2-D periodic array of vortices

Evolution of total kinetic energy

- $\frac{q}{q_0}$
- Time (sec)

Central differencing

Second-order upwind
Numerics: CD vs. QUICK Scheme

Separation and reattachment points predicted by FLUENT and others

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<thead>
<tr>
<th></th>
<th>$X_F$</th>
<th>$X_R$</th>
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<tbody>
<tr>
<td>Exp. (Martinuzzi and Tropea (1993))</td>
<td>1.04</td>
<td>1.61</td>
</tr>
<tr>
<td>FLUENT (LES + CD)</td>
<td>1.18</td>
<td>1.78</td>
</tr>
<tr>
<td>FLUENT (LES + QUICK)</td>
<td>1.26</td>
<td>2.40</td>
</tr>
<tr>
<td>Breuer et al. LES</td>
<td>1.23</td>
<td>1.70</td>
</tr>
</tbody>
</table>

Time-averaged streamlines on the mid-plane
Stirred tank modeling

• The sliding mesh model was used to set up the transient motions of the impeller in the tank.
• Two turbulence model approaches were evaluated:
  – Reynolds-Averaged Navier-Stokes turbulence model, i.e., $k-\varepsilon$ style and Reynolds Stress Models.
  – Large Eddy Simulation or LES.
• The following impeller systems were modeled:
  – Hydrofoil impeller (HE-3).
  – Pitched blade turbine (PBT).
  – Multiple hydrofoil system (A310).
  – Rushton turbine (RT).
  – Glass lined impeller system (RCI).
Hydrofoil Impeller (HE-3)

- Flat bottom vessel with four baffles:
  - T=0.292m
  - Z/T=1
  - Water
- HE-3:
  - Three blades
  - D/T=0.39
  - C/T=0.33
  - 60 RPM
  - Reynolds ~ 1.3E4


Experimental PIV data measured at Chemineer Inc. Animation has approximately one snapshot every five revolutions. Plays approximately 12 times faster than real time.
Stirred Tank Models - LES Grid Size

- Grid size used was on the order of 800k cells.
- This corresponded to an average grid size of 2E-3m.
- From RANS simulations it was determined that:
  
  - Integral length scale \((k^{3/2}/\varepsilon)\) \(\sim 10\)mm
  
  - Taylor length scale \((15\nu k/\varepsilon)^{0.5}\) \(\sim 1.3\)mm
  
  - Kolmogorov scale \((\nu^3/\varepsilon)^{1/4}\) \(\sim 0.06\) mm.
  
  - \(E(k)\) is energy contained in eddies for given wavelength.
  
  - Modeling \(\sim 85\%\) of TKE.
Time Dependent Velocity Magnitude

2-D Fix

3-D MRF

3-D LES (14.5 revs.)
Velocity on Vorticity Iso-Surfaces

Iso-Surface of Vorticity
Magnitude (15 s$^{-1}$)

Vorticity is: $\nabla \times \mathbf{V}$
Shear rate is: $\nabla \mathbf{V}$
Velocity on Vorticity Iso-Surfaces

Iso-Surface of Vorticity Magnitude (5 s⁻¹) 3.9 revs.
Flow at the surface

HE-3 “oilflow” lines at liquid surface (8.8 revolutions)

“Oilflow” lines are pathlines constrained to the surface from which they are released.
HE-3 “oilflow” lines at liquid surface (12.3 revolutions)
HE-3 “oilflow” at vessel wall (18 revolutions)

(m/s)

- 5.00e-02
- 4.50e-02
- 4.00e-02
- 3.50e-02
- 3.00e-02
- 2.50e-02
- 2.00e-02
- 1.50e-02
- 1.00e-02
- 5.00e-03
- 0.00e+00
Pitched Blade Turbine

- Flat bottom vessel with four baffles:
  - $T=0.292\text{m}$
  - $Z/T=1$
- Pitched-blade turbine (PBT):
  - Four blades at 45°
  - $D/T=0.35$
  - $W/D=0.2$
  - $C/T=0.46$
  - 60 RPM
- Water
- Reynolds number $\sim 1E4$. 
Time Series of Axial Velocity - 1

(a) \(x = 0.185\text{m} \ y = -0.04\text{m}, \ z = -0.04\text{m}\) (below impeller)

PBT from 168.13306 (2500 time steps) to 178.12756s (3500 time steps) after start-up from a zero-velocity field.
Time Series of Axial Velocity - 2

(c) $x=0.25m, y=0.05m, z=0.05m$ (vessel bottom)

(d) $x=0.05m, y=0.05m, z=0.05m$ (liquid surface)
Rushton Turbine Model

- Flat-bottom tank with four flat baffles:
  - $T = 0.2 \text{ m}$
  - $Z/T = 1$
- Impeller:
  - Six blades
  - $D/T = 1/3$
  - $W/D = 0.2$
  - $C/T = 1/3$
  - 290 RPM
- Water.
- Reynolds number $\sim 2E4$. 

2-D simulation
Rushton turbine - axial velocity

Iso-surface of axial velocity of 0.1m/s. The velocity is directed upwards in the regions enclosed by the iso-surface. The surface is colored by strain rate on a scale of 0 to 100 1/s.
Rushton Turbine - Trailing Vortices

Iso-Surface of Vorticity Magnitude (550 and 80 s\(^{-1}\))
Colored by velocity magnitude
Example: multiple hydrofoil impellers

- Vessel diameter $T = 0.232$ m.
- Vessel height $H/T = 4.1$.
- Impeller diameter $D/T = 0.41$.
- Center-to-center distance between impellers is $1.02T$.
- Liquid is water.
- Impeller speed is 300 RPM.
- Impeller $Re = 4.7E4$.
- Solution initialized with MRF.
- Continued for 118 revolutions with sliding mesh, LES-RNG subgrid model, and central differencing for momentum.
- Time step of 5 ms; 40 steps/rev.
Multiple A310 system

Velocity Magnitude (m/s)

<table>
<thead>
<tr>
<th>Value</th>
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<tbody>
<tr>
<td>5.50e-01</td>
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<td>5.32e-01</td>
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<tr>
<td>5.13e-01</td>
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</tr>
<tr>
<td>1.83e-02</td>
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<tr>
<td>0.00e+00</td>
</tr>
</tbody>
</table>

MRF with k-ε Turbulent viscosity ratio ~ 157

LES. Smagorinsky-RNG Subgrid viscosity ratio ~ 10
Multiple A310 system

Velocity Magnitude (m/s)

- 5.50e-01
- 5.32e-01
- 5.13e-01
- 4.95e-01
- 4.77e-01
- 4.58e-01
- 4.40e-01
- 4.22e-01
- 4.03e-01
- 3.85e-01
- 3.67e-01
- 3.48e-01
- 3.30e-01
- 3.12e-01
- 2.93e-01
- 2.75e-01
- 2.57e-01
- 2.38e-01
- 2.20e-01
- 2.02e-01
- 1.83e-01
- 1.65e-01
- 1.47e-01
- 1.28e-01
- 1.10e-01
- 9.17e-02
- 7.33e-02
- 5.50e-02
- 3.67e-02
- 1.83e-02
- 0.00e+00
Multiple A310 system

Velocity Magnitude
(m/s)

5.50e-01
5.32e-01
5.13e-01
4.95e-01
4.77e-01
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2.02e-01
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1.65e-01
1.47e-01
1.28e-01
1.10e-01
9.17e-02
7.33e-02
5.50e-02
3.67e-02
1.83e-02
0.00e+00
Glass lined equipment

- Glass lined equipment is characterized by the fact that all angles have to be rounded to prevent cracking of the glass coat.
- Vessels are typically equipped with either a classic retreat curve impeller or a combination of a radial flow impeller on the bottom and an axial flow impeller on the top.
- Glass lined vessels usually have one baffle and a diptube, which can have instrumentation.

- 8 m³ vessel at 5.8 m³ fill level.
- 180 RPM with water. Re=3E6.
- RCI at D/T=0.49.
- Fin baffle and diptube.
- LES. Smagorinsky-RNG subgrid model.
Diptube suspended from here

Baffle suspended from here

Liquid surface

Diptube

Fin baffle

Retreat curve impeller
Flow field at liquid surface

Vortex precesses around shaft approximately once per 40 revolutions.
Flow field behind baffle

- Flow field visualized by means of “oilflow” lines.
- Oilflow lines are trajectories of flow following particles that are constrained to the surface of which they are released, in this case the liquid surface.
- The animation covers 8.4s real time, which corresponds to ~25 impeller revolutions.
Velocity magnitude at plane through baffle

Animation covers ~ 25 revs.
Stirred tank modeling options - 2004

- Daily design. General flow fields. How many impellers are needed. Instructional.
- Impeller design. When velocity data is not available.
- Impeller-baffle interaction. Time dependence.
- Research. Large scale turbulence and unsteady structures.
- Hypothetical. DNS
- 3-D LES
- 3-D Sliding Mesh (RANS)
- 3-D MRF/Snapshot
- 3-D Fixed Impeller Velocities
- 2-D Fixed Impeller Velocities
- Daily design. General flow fields. How many impellers are needed. Instructional.
Turbulence modeling for different users

• Researchers, analysts.
• FLUENT:

• Designers.
• FloWizard:
Availability for different user categories

Predictions are difficult, especially those of the future!
Summary

• LES has potential benefit for engineering applications, and is within reach computationally.
• However, steady state models models are much faster computationally, and still have their place.
• There will be a progression over time, with researchers, analysts, and designers adopting different turbulence modeling methods with intervals spanning ~15 years.