# MODELING TURBULENCE IN STIRRED VESSELS

### A Review and Recent Developments

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Presented at 5th International Bi-Annual ASME/JSME Symposium on COMPUTATIONAL TECHNOLOGY FOR FLUID / THERMAL / CHEMICAL / STRESSED SYSTEMS WITH INDUSTRIAL APPLICATIONS July 25-29, 2004, San Diego



### **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.



Flow pattern generated by disk turbine or radial flow impeller.

Flow pattern generated by propeller.

Joshi, Pandit, Sharma. Chem. Eng. Sci. Vol. 37, No. 6, pp. 813-844, 1982.

#### Warmoeskerken, 1984.



## Early 1990's

- Asymmetric, unstable flow fields observed.
- Multimodal velocity histograms.





### Solids distribution and CFD flow fields - 1994



Bakker A., Fasano J.B., Myers K.J. (1994) *Effects of Flow Pattern on the Solids Distribution in a Stirred Tank.* 8th European Conference on Mixing, September 21-23, 1994, Cambridge, U.K. IChemE Symposium Series No. 136, ISBN 0 85295 329 1, page 1-8.



### <u>Issues</u>

- 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





### **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?



0.005

0.01

0.015



0.025

0.02

Frequency (1/s)

## Turbulence modeling objective

- The objective of turbulence modeling is to develop equations that will predict the <u>time averaged</u> 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 Re=1E4

- 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.





### **Experimental Snapshot**



### **Effective Viscosity**



### Prediction methods





### Kolmogorov energy spectrum

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



 $\varepsilon$  is the energy dissipation rate (m<sup>2</sup>/s<sup>3</sup>) k is the turbulent kinetic energy (m<sup>2</sup>/s<sup>2</sup>) V is the kinematic viscosity (m<sup>2</sup>/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 ~ Ret<sup>3</sup>.
- 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:
    - $\mu_{eff}$  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  $(\ell_0)$ .





### 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







### Numerics: CD vs. QUICK Scheme

### Central-differencing



Separation and reattachment points predicted by FLUENT and others

	X <sub>F</sub>	X <sub>R</sub>
Exp. (Martinuzzi and Tropea (1993)	1.04	1.61
FLUENT (LES + CD)	1.18	1.78
FLUENT (LES + QUICK)	1.26	2.40
Breuer <i>et al</i> . LES	1.23	1.70

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-ε 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

Reference: Myers K.J., Ward R.W., Bakker A. (1997) A Digital Particle Image Velocimetry Investigation of Flow Field Instabilities of Axial Flow Impellers, Journal of Fluids Engineering, Vol. 119, No. 3, page 623-632.



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  $(k^{3/2}/\epsilon) \sim 10$ mm
- Taylor length scale  $(15vk/\epsilon)^{0.5} \sim 1.3mm$
- Kolmogorov scale  $(v^{3}/\epsilon)^{1/4} \sim 0.06$  mm.
- E(k) is energy contained in eddies for given wavelength.
- Modeling ~85% of TKE.





### Time Dependent Velocity Magnitude







2-D Fix



### Velocity on Vorticity Iso-Surfaces

#### (m/s)







Iso-Surface of Vorticity Magnitude (30 s<sup>-1</sup>)

> Vorticity is:  $\nabla x V$ Shear rate is:  $\nabla V$

### Velocity on Vorticity Iso-Surfaces

(m/s)		
	1.00e-01	
	9. <b>1</b> 7e–02	
	8. <b>33</b> e–02	
	7.50e-02	
	6.67e-02	
	5.83e-02	
	5.00e-02	
	4. <b>1</b> 7e–02	
	3.33e-02	
	2.50e-02	
	1.67e-02	
	8.33e-03	
	0.00e+00	
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Iso-Surface of Vorticity Magnitude (5 s<sup>-1</sup>) 3.9 revs.

### Flow at the surface



"Oilflow" lines are pathlines constrained to the surface from which they are released.









### Pitched Blade Turbine

- Flat bottom vessel with four baffles:
  - T=0.292m
  - 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 ~ 1E4.







### Time Series of Axial Velocity - 1

(a) x = 0.185 m y = -0.04 m, z = -0.04 m (below impeller)







PBT from 168.13306 (2500 time steps) to 178.12756s (3500 time steps) after start-up from a zero-velocity field.



### <u>Time Series of Axial Velocity - 2</u>

(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 m
  - -Z/T=1
- Impeller:
  - Six blades
  - D/T=1/3
  - W/D=0.2
  - C/T=1/3
  - 290 RPM
- Water.
- Reynolds number ~ 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<sup>-1</sup>) 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



**MRF** with k-ε **Turbulent viscosity #FLUENT** ratio ~ 157



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



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

**FLU** 



### 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

**FLU** 



### 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 m<sup>3</sup> vessel at 5.8 m<sup>3</sup> fill level.
- 180 RPM with water. Re=3E6.
- RCI at D/T=0.49.
- Fin baffle and diptube.
- LES. Smagorinsky-RNG subgrid model.





# Baffle suspended from here

Diptube suspended from here

Liquid surface —

Fin baffle

Diptube-

- 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.



#### (m/s) 1.70e+00.64e+00 .59e+00 .53e+00 .47e+00 1.42e+00 1.36e+00 .30e+00 1.25e+00 1.19e + 001.13e+00 1.08e+00 1.02e+00 9.63e-01 9.07e-01 8.50e-01 7.93e-01 7.37e-01 6.80e-01 .23e-01 5.67e-01 5 10e–01 53e-01 3.97e-01 3.40e-01 2.83e-01 2.27e-01 1 70e\_01 1.13e-01

5.67e-02 0.00e+00



### Velocity magnitude at plane through baffle







### Stirred tank modeling options - 2004



### Turbulence modeling for different users

- Researchers, analysts.
- FLUENT:

- Designers.
- FloWizard:

#### 🔏 Flow Type Guide

Refer to the pictures and descriptions to decide which type of flow you are interested in simulating

C Laminar: Choose this option if the Reynolds number (defined as density\*velocity\*size/viscosity) is low. This is usually the case for low-speed or highly viscous flows. For laminar flow, the flowlines will be smooth.



- Turbulent: Choose this option if the Reynolds number (defined above) is high (see also the description of "Turbulent with strong swirl", below). This is usually the case for high-speed or low-viscosity flows. Turbulent flow is unstable and the flowlines have an irregular look.
- Turbulent with strong swirl: Choose this option for turbulent flow in devices that are purposely designed to create a strong swirl, such as cyclones and swirl combustors. (If you are not sure if this is the case for your application, choose the "Turbulent" option above. If you choose "Turbulent with strong swirl" for turbulent flows without strong swirl, the accuracy of the simulation results will not be affected, but the calculation time will be unnecessarily increased.)

Unknown: Choose this option if you do not know if the flow will be laminar or turbulent. FloWizard will determine this for you as part of the simulation. Note that choosing this option may increase your calculation time, but it will not reduce the accuracy of the results (with the exception of turbulent flows with strong swirl).

0K



### Availability for different user categories



### <u>Summary</u>

- 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.

