Modeling Stirred Vessel Hydrodynamics

Using Large Eddy Simulation

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FLUENT

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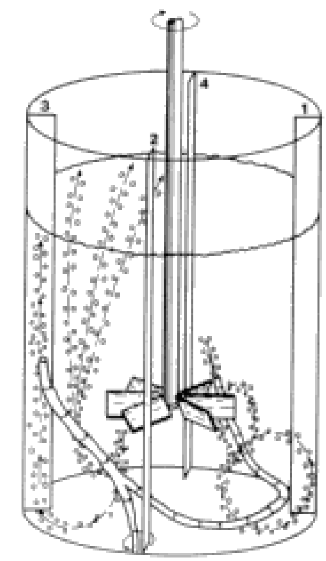
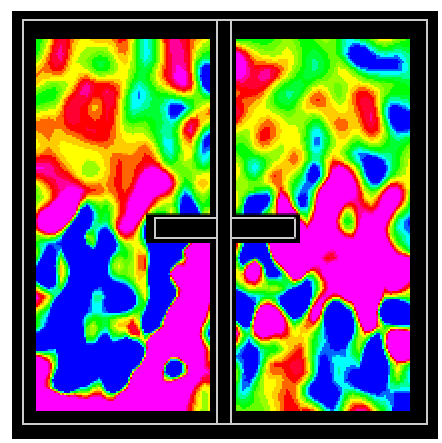
Flow Instabilities

- Experimental work suggests that large-scale, time-dependent structures, with periods much longer than the time of an impeller revolution, are involved in many of the fundamental hydrodynamic processes in stirred vessels.
- Local velocity data histograms may be bi-modal or tri-modal (Bakker and Van den Akker).
- The gas holdup distribution may be asymmetric and oscillating (Bakker and Van den Akker).
- In solids suspension processes, solids can be swept from one side of the vessel to the other in a relatively slow oscillating pattern, even in dilute suspensions.
- Digital particle image velocimetry experiments have shown large scale asymmetries with periods up to several minutes (Myers, Bakker and Ward).





The Turbulence Spectrum

- Many scales of turbulent eddies exist:
  - Large eddies contain most of the turbulent kinetic energy
  - 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

Reference for animations: 3D World Magazine, Issue 9, 2001, www.3dworldmag.com.

Direct Numerical Simulation (DNS)

- Navier-Stokes equations are solved on a fine grid using a small time-step.
- Goal is to capture the all turbulence scales.
- Result is accurate, 3D, transient behavior.
- Great 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:
  - *k*-ε: Robust, popular 2-equation model using constants taken from simple, high Re flows
  - Isotropic turbulence effects modeled through effective viscosity
    - μ_{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

Subgrid-Scale (SGS) Modeling

SGS Reynolds stresses are modeled by

$$\sigma_{ij}^{s} - \frac{1}{3}\delta_{ij}\,\sigma_{kk}^{s} = -2\mu_{t} S_{ij}$$

where μ_t is the subgrid-scale eddy viscosity and S_{ij} is the rate of strain tensor

Two models in FLUENT 5 are:

Smagorinsky SGS model

$$\mu_{t} = \rho L^{2}\sqrt{2S_{ij}S_{ij}}$$

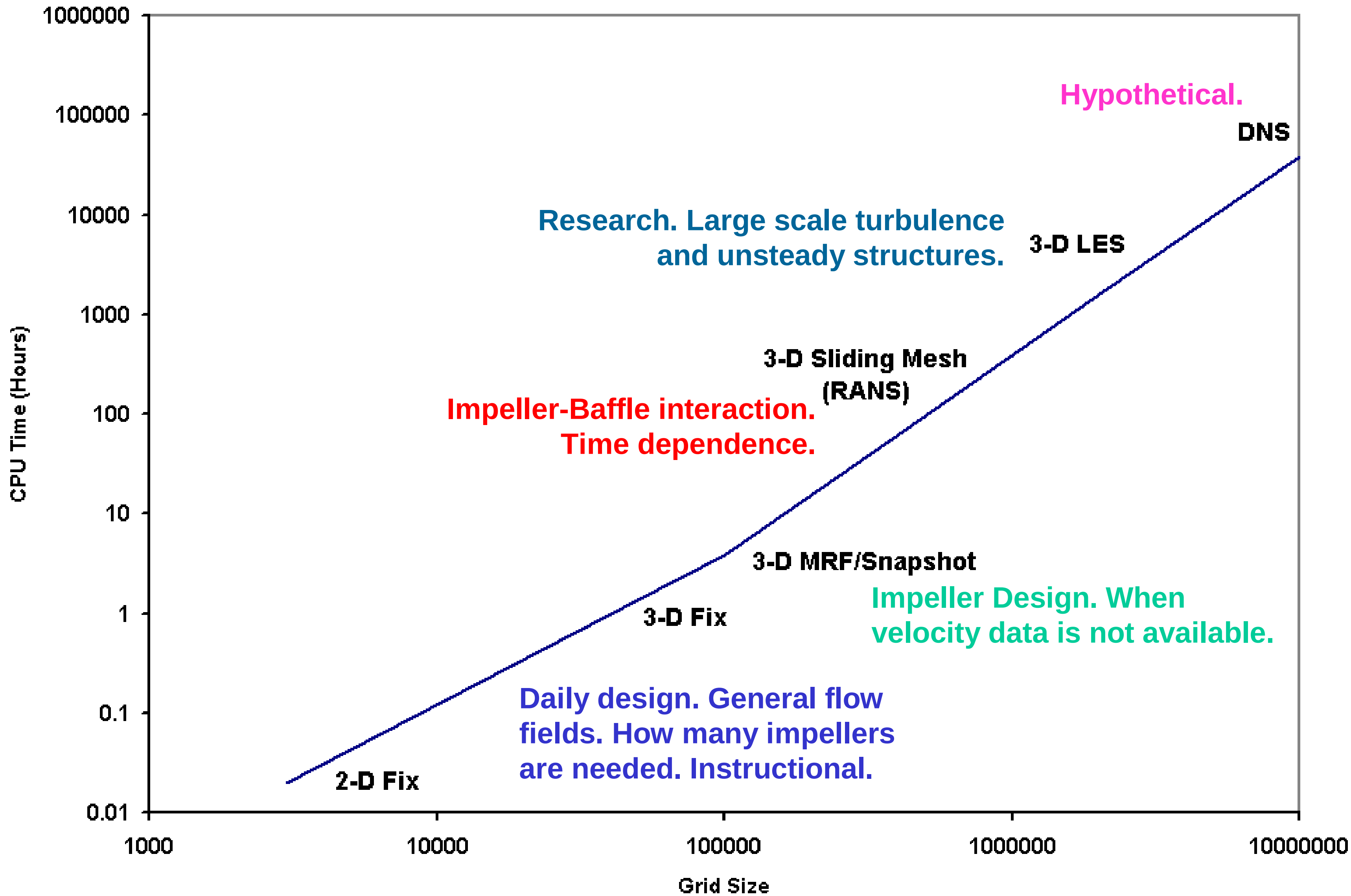
$$L = \min\left(\kappa\, d, C_{s}\, V^{\frac{1}{3}}\right)$$

RNG SGS model

$$\mu_{t} = \mu\left[1 + H\left(\frac{\mu_{s}^{2}\mu_{tot}}{\mu^{3}} - C\right)\right]^{1/3}$$

$$\mu_{s} = \left(0.157 V^{\frac{1}{3}}\right)^{2}\sqrt{2S_{ij}S_{ij}}$$

Stirred Tank Modeling Options



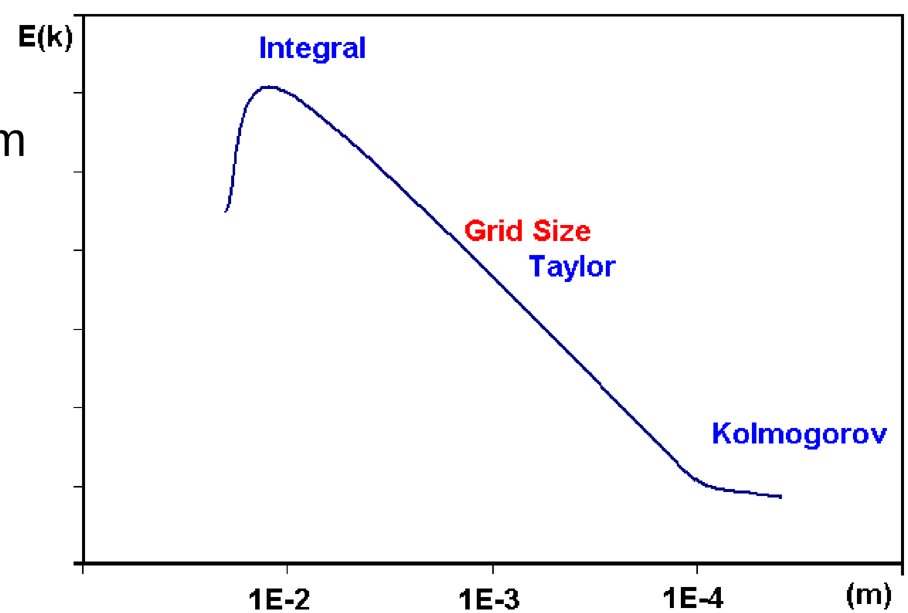
Stirred Tank Modeling

- 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., Standard k-ε, RNG k-ε, Reynolds Stress Model
  - Large Eddy Simulation or LES
- Three impeller styles were tested:
  - Hydrofoil impeller (HE-3)
  - Pitched blade turbine (PBT)
  - Rushton turbine (RT)

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:

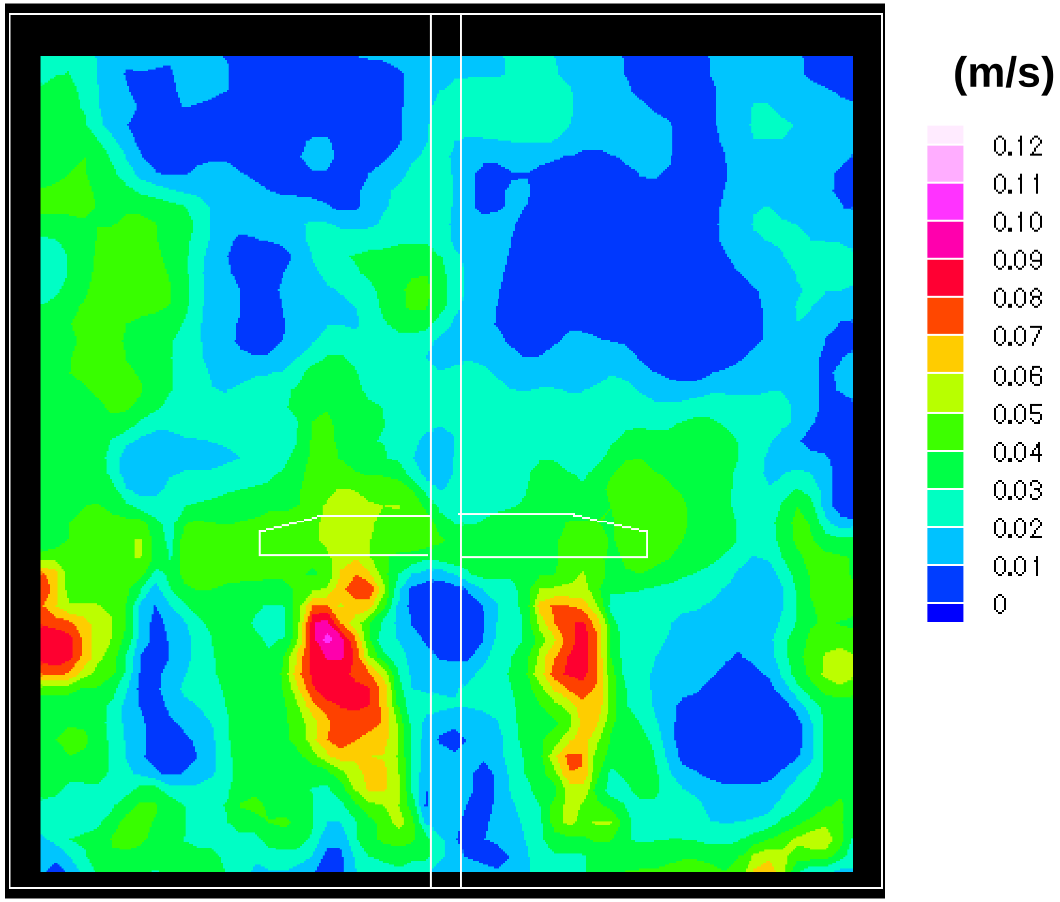
  - Integral length scale $(k^{3/2}/\varepsilon)$ ~ 10mm
  - Taylor length scale $(15\nu k/\varepsilon)^{0.5}$ ~ 1.3mm
  - Kolmogorov scale $(\nu^3/\varepsilon)^{1/4}$ ~ 0.06 mm.
  - E(k) is energy contained in eddies for given wavelength.



Hydrofoil Impeller (HE-3)

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

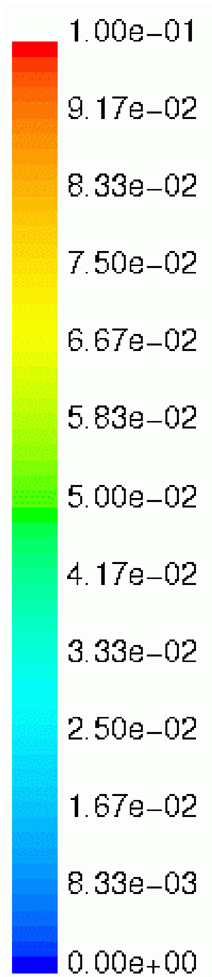
Reference: Myers K.J., Ward R.W., Bakker A. (1997) A Digital Particle Image Velocimetry Investigation of Flow Field Instabilities of Axial Flow Impellers, Journal of Fluids Engineering, Vol. 119, No. 3, page 623-632.

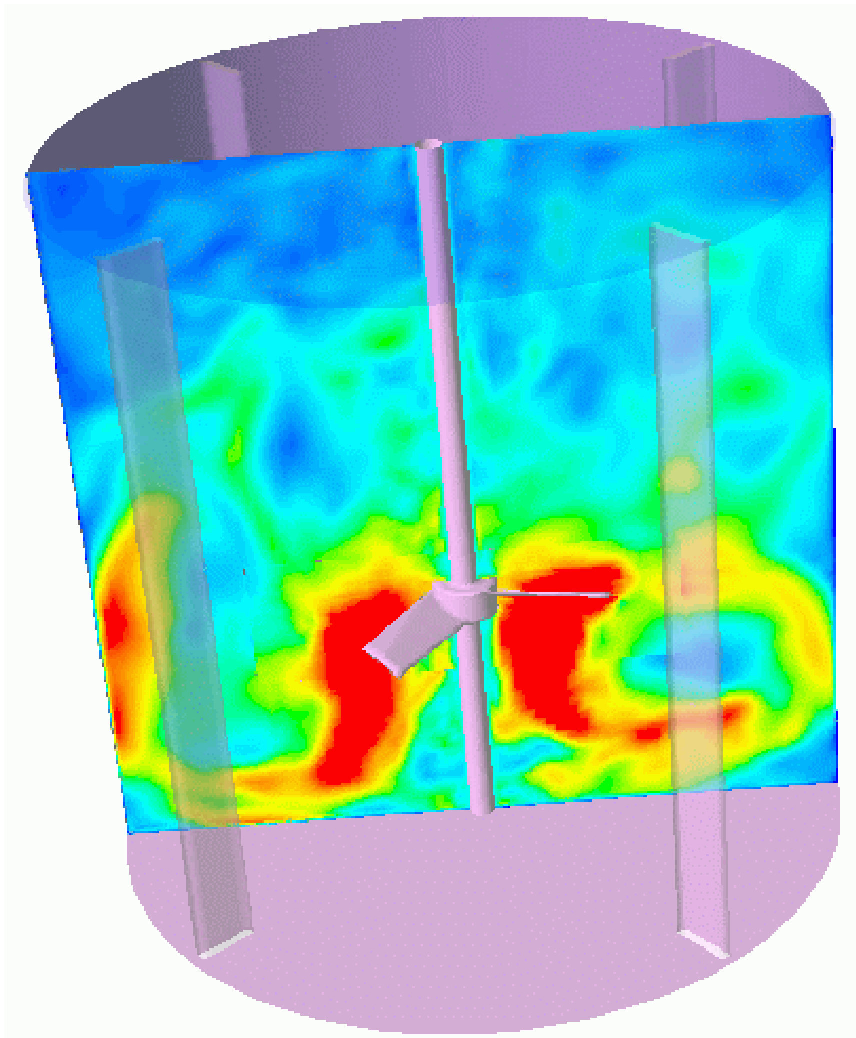


Experimental PIV data measured at *Chemineer Inc.* Animation has approximately one snapshot every five revolutions. Plays approximately 10 times faster than real time.

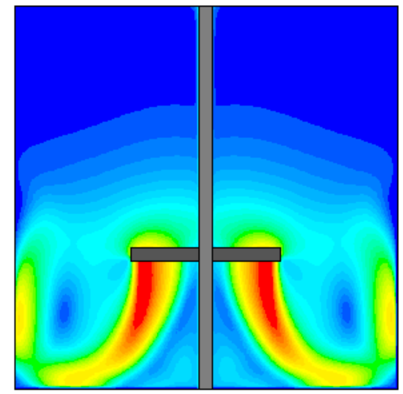
Time Dependent Velocity Magnitude

(m/s)

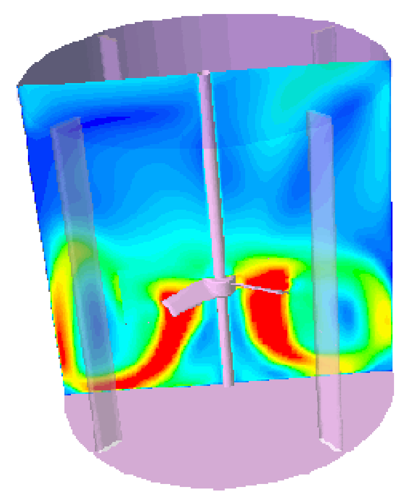




3-D LES

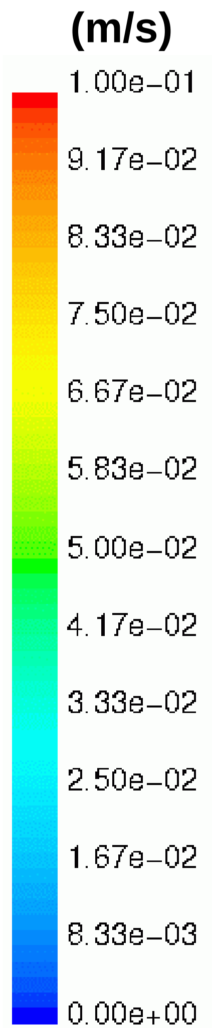


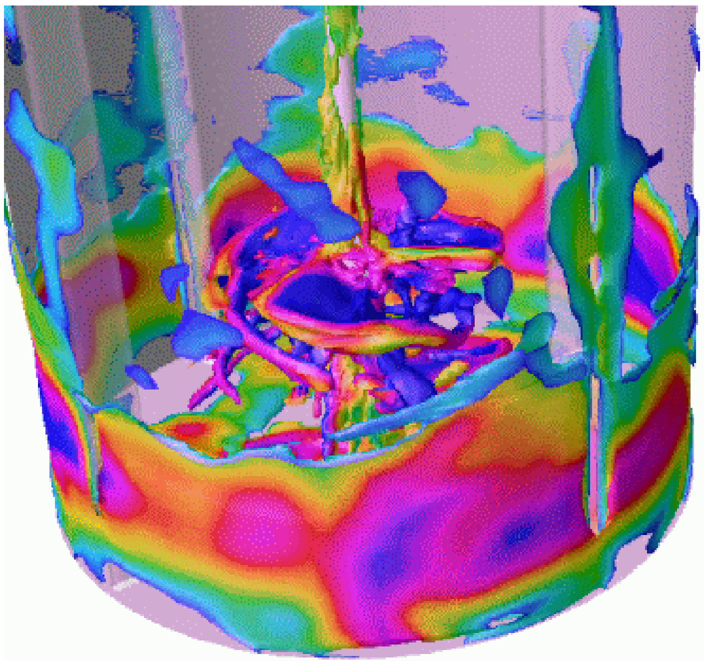
2-D Fix



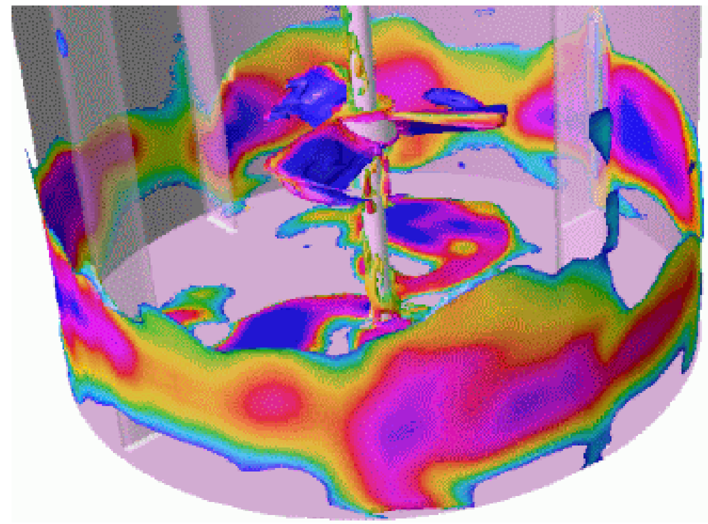
3-D MRF

Velocity on Vorticity Iso-Surfaces





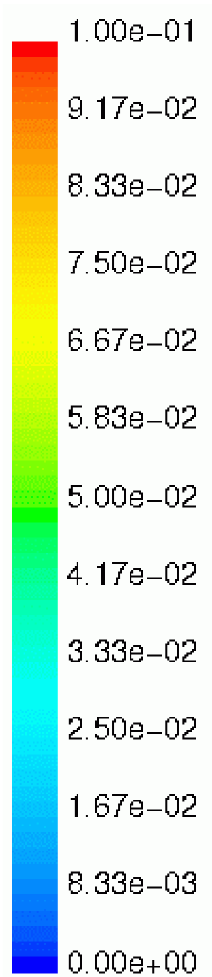
Iso-Surface of Vorticity Magnitude (15 s^{-1})

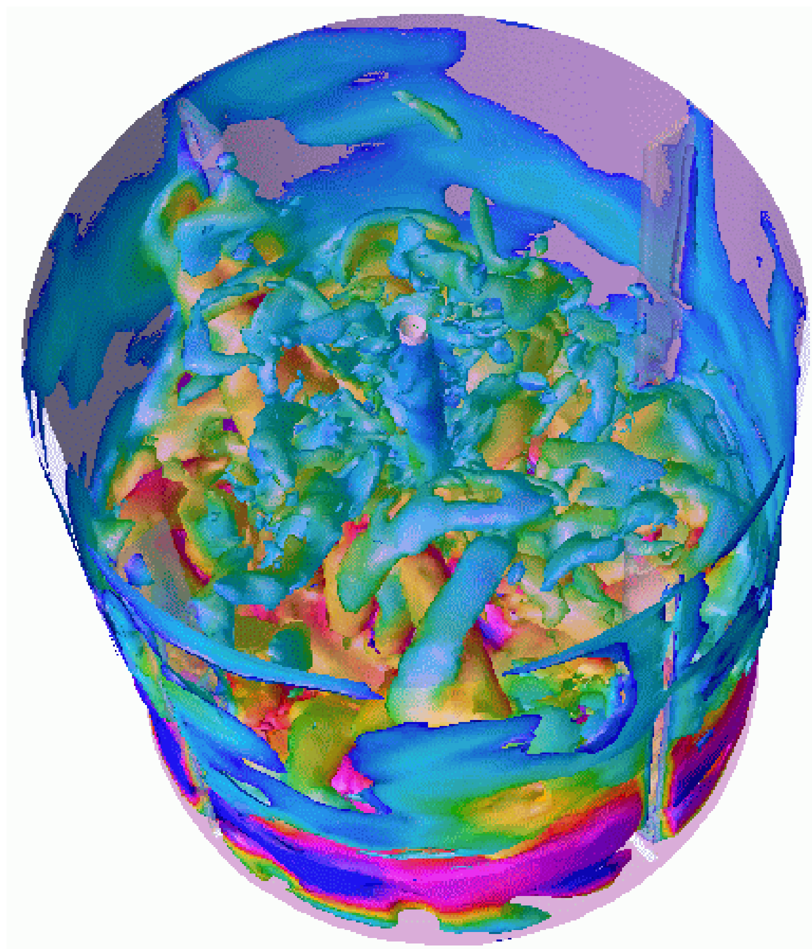


Iso-Surface of Vorticity Magnitude (30 s^{-1})

Velocity on Vorticity Iso-Surfaces

(m/s)

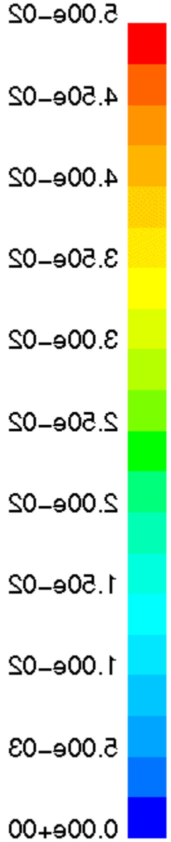


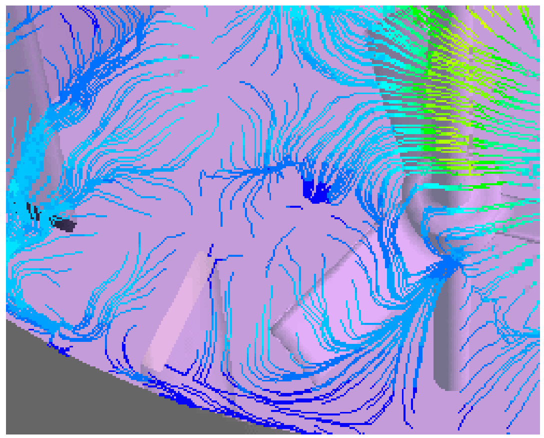


Iso-Surface of Vorticity Magnitude (5 s^{-1})

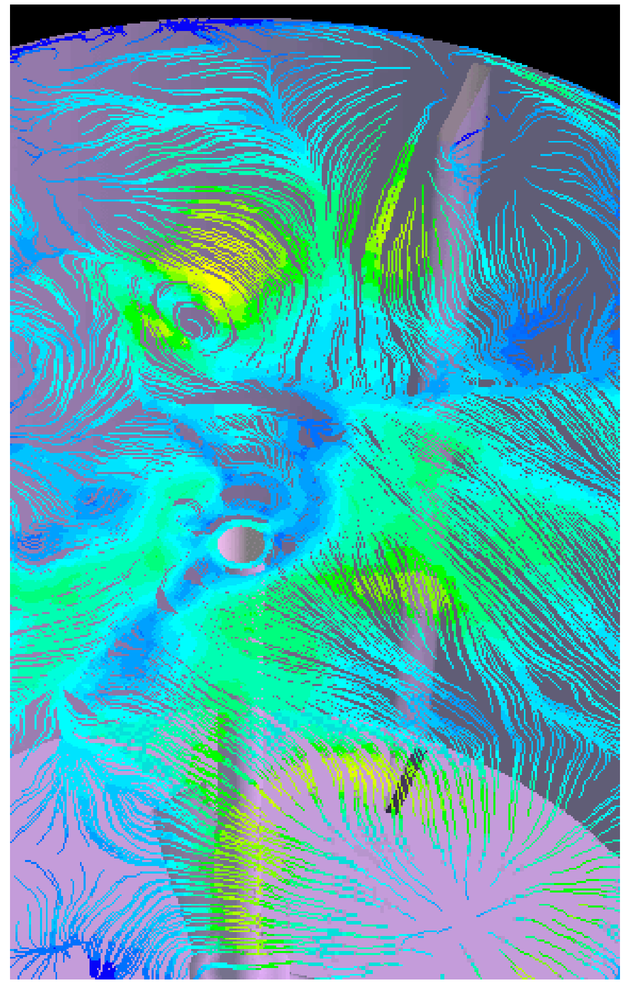
Flow at the surface

(m/s)



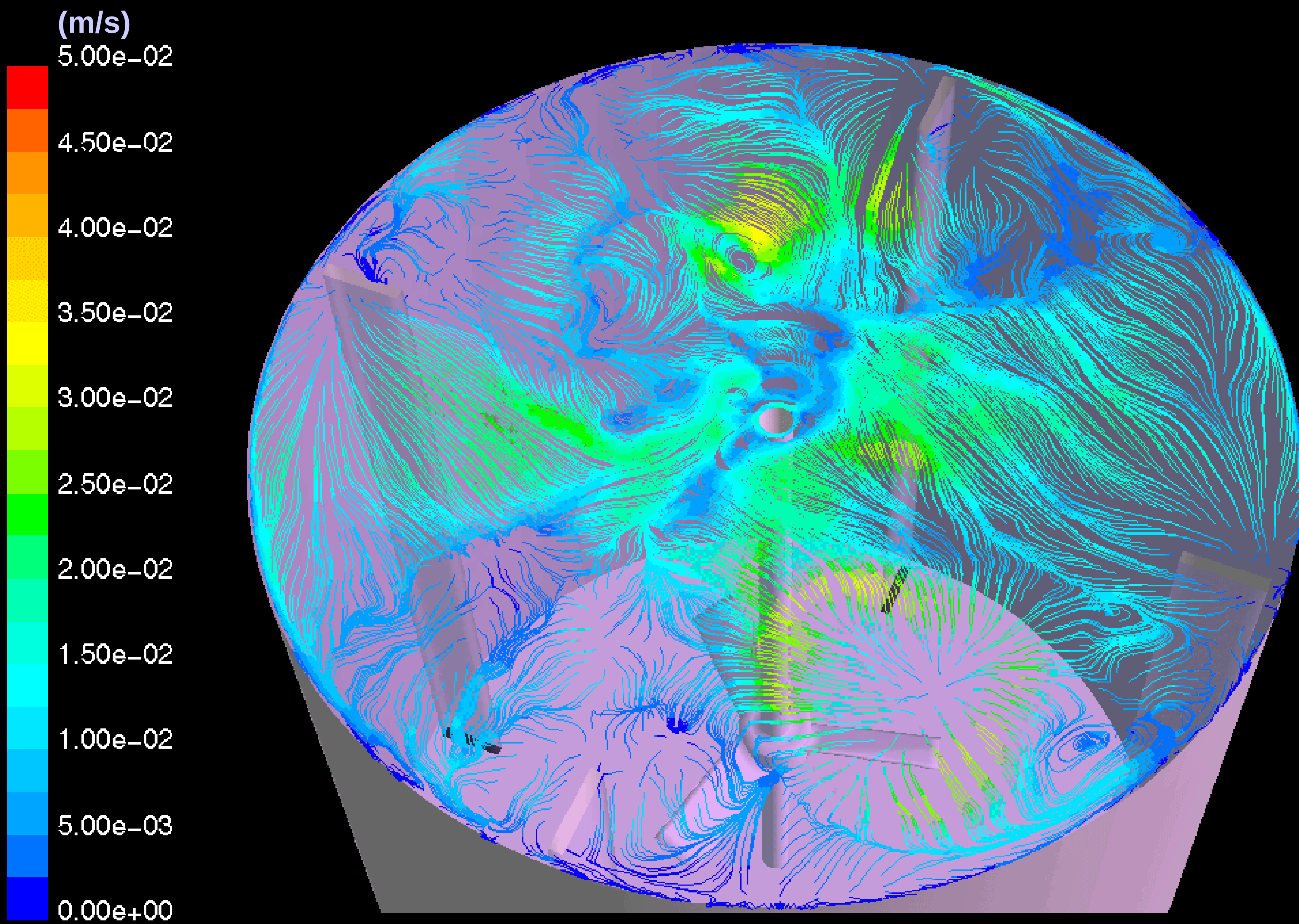


HE-3 "oilflow" lines at liquid surface (8 revolutions)

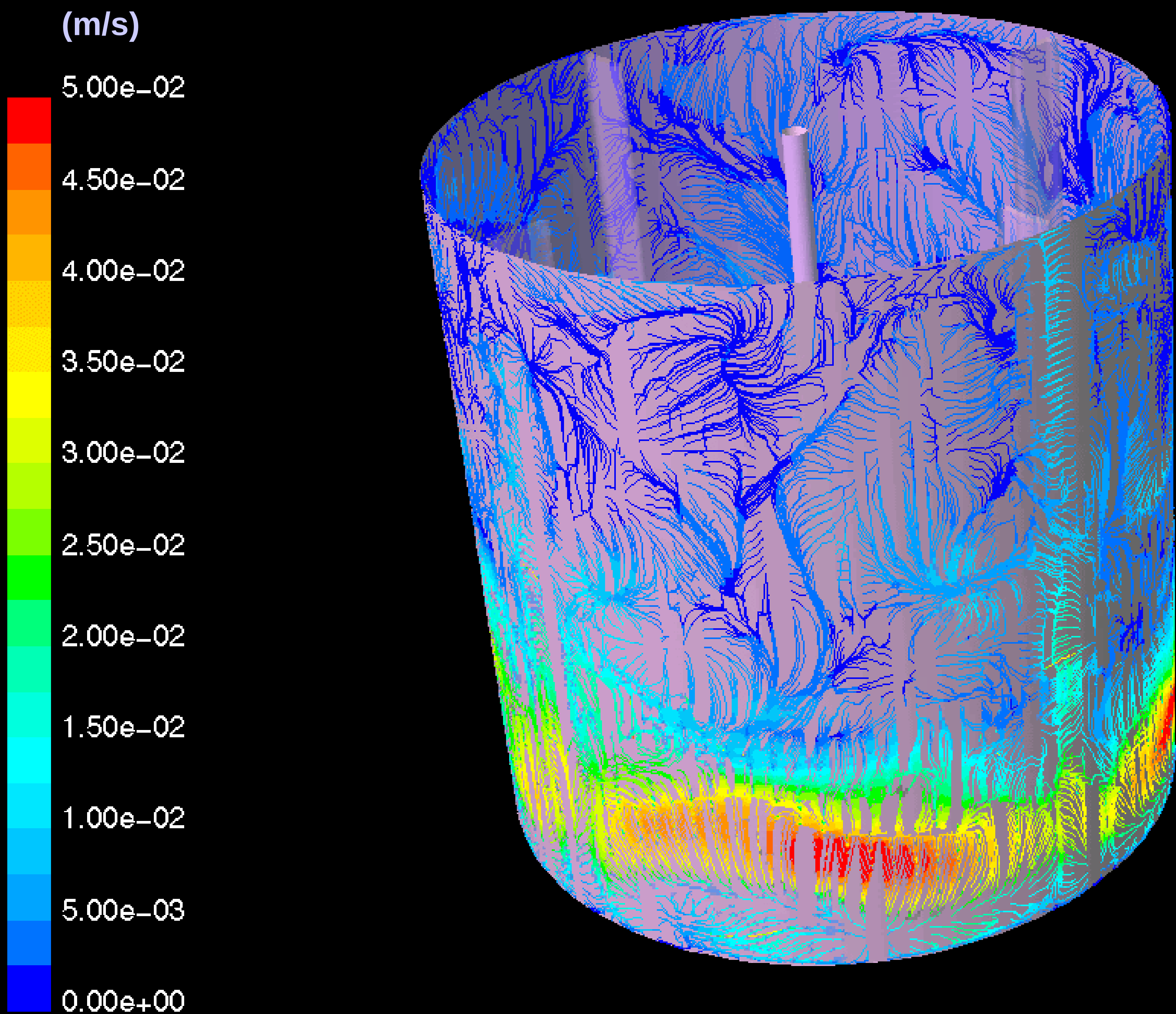


"Oilflow" lines are pathlines constrained to the surface from which they are released.

HE-3 “oilflow” lines at liquid surface (25 revolutions)

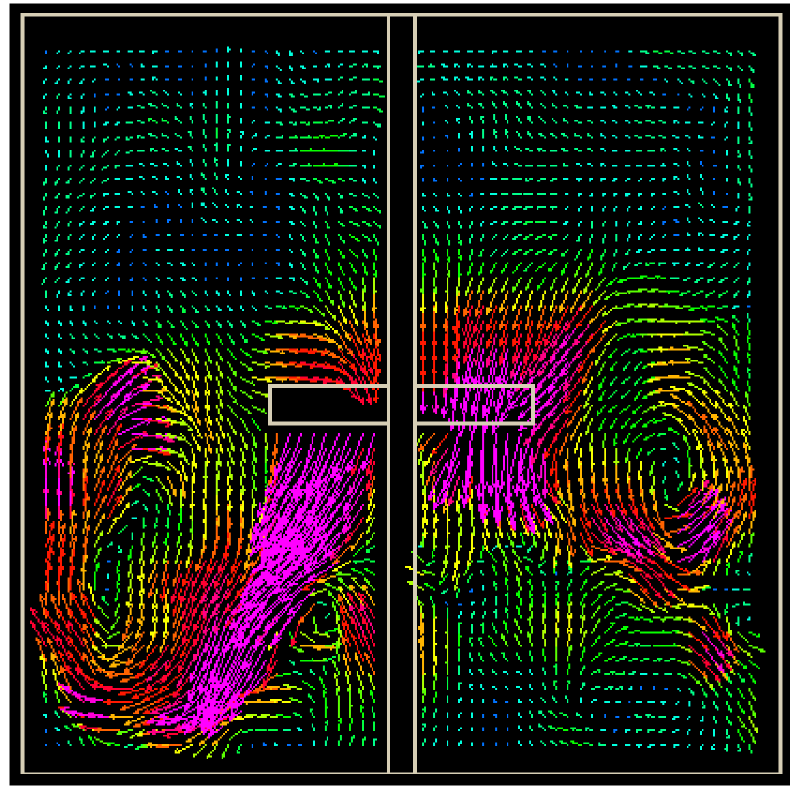


HE-3 “oilflow” at vessel wall (18 revolutions)



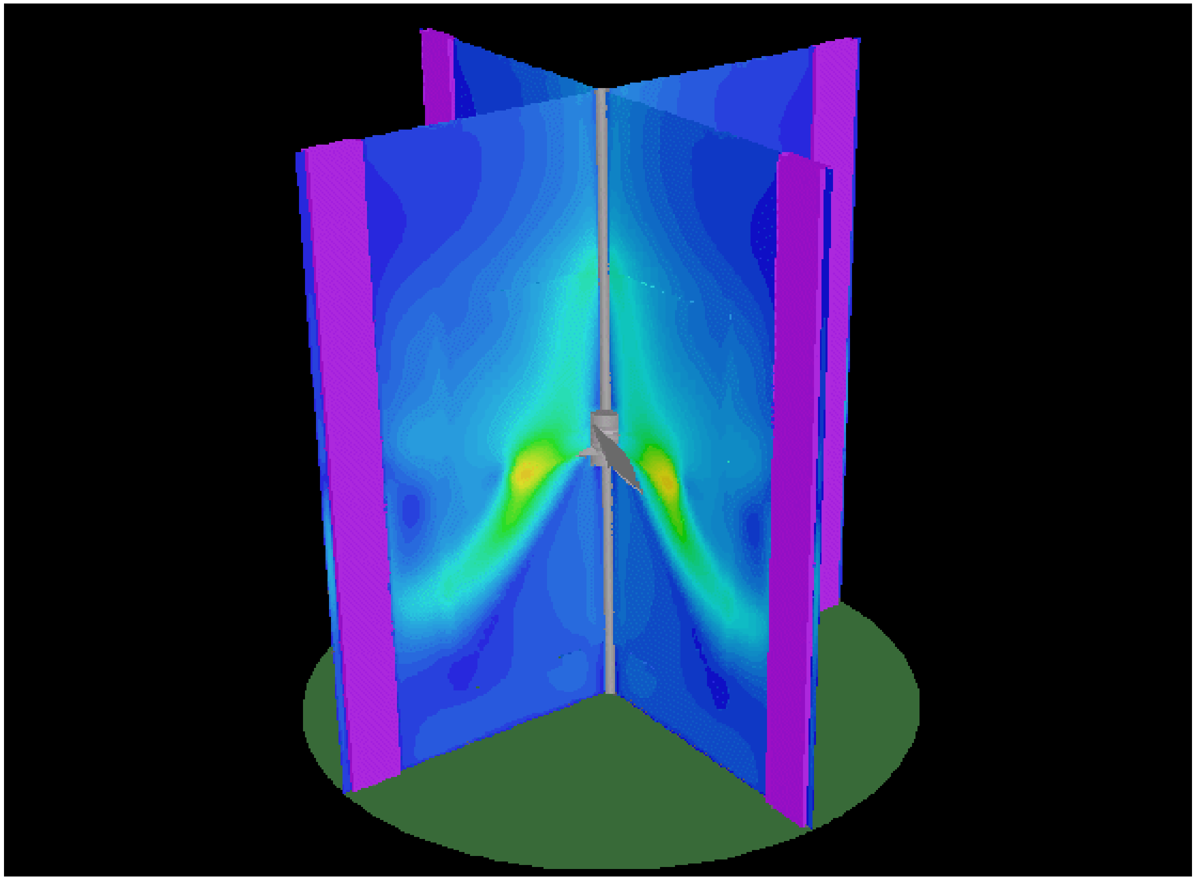
Pitched Blade Turbine

- 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.



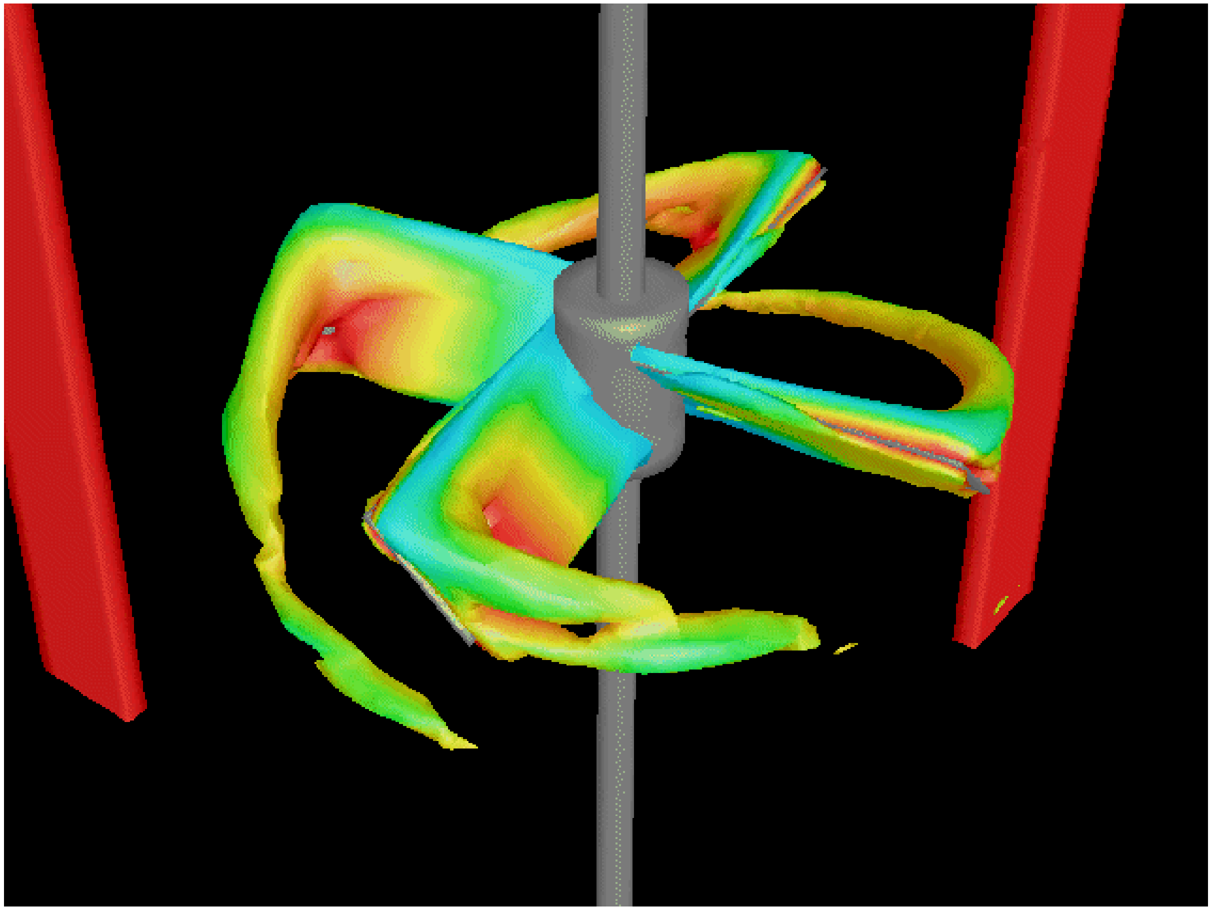
Experimental DPIV Data

Unsteady RANS (RSM) Flow Field



Pitched Blade Turbine - Velocity Magnitude

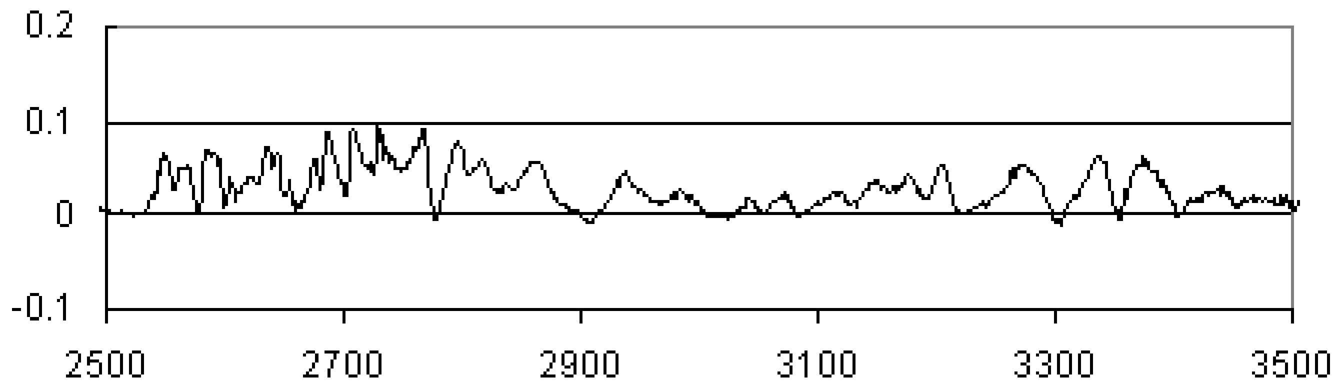
Unsteady LES Flow Field



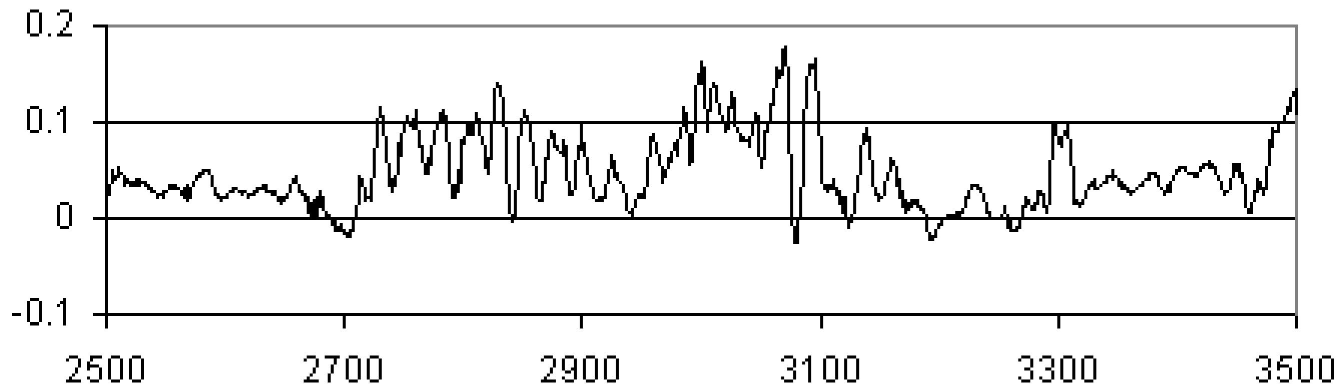
Iso-surface of Vorticity Magnitude

Time Series of Axial Velocity - 1

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



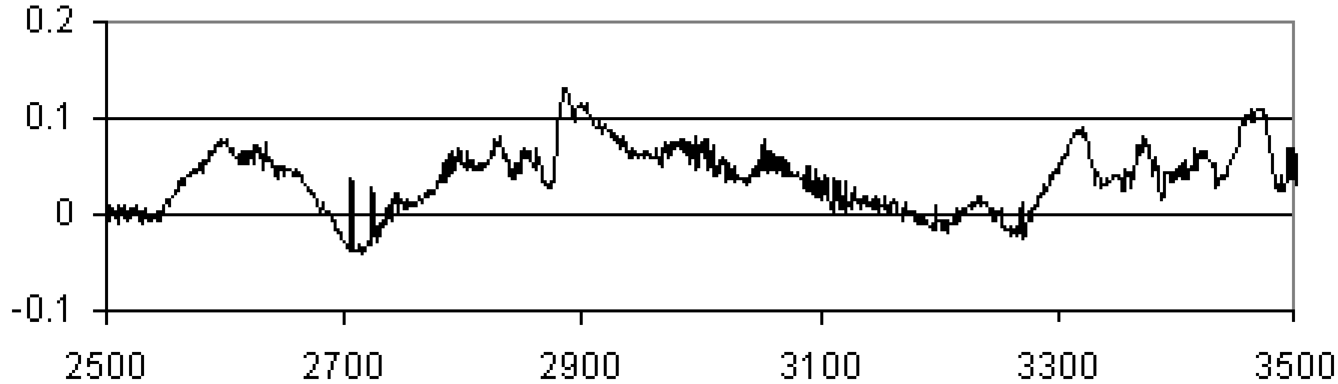
(b) x = 0.185m y = 0.04m z = 0.04m



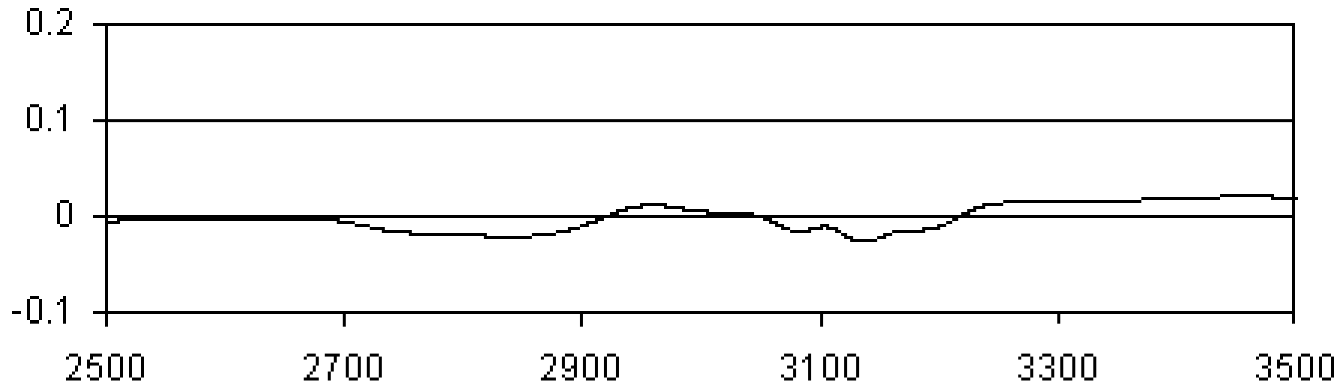
PBT from 168.13306 (2500 time steps) to 178.12756s (3500 time steps) after start-up from a zero-velocity field.

Time Series of Axial Velocity - 2

(c) x=0.25m y=0.05m z=0.05m

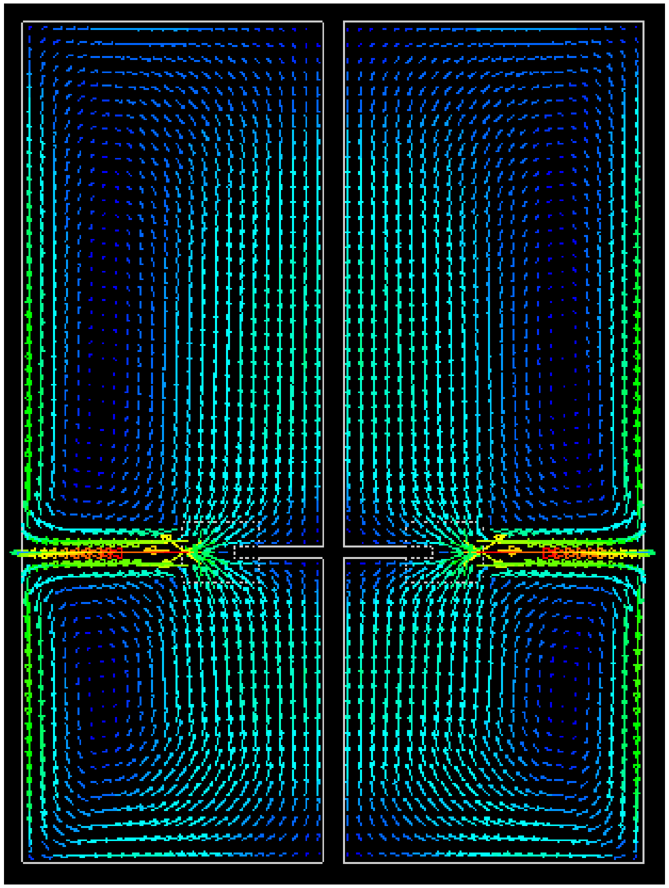


(d) x=0.05m y=0.05m z=0.05m



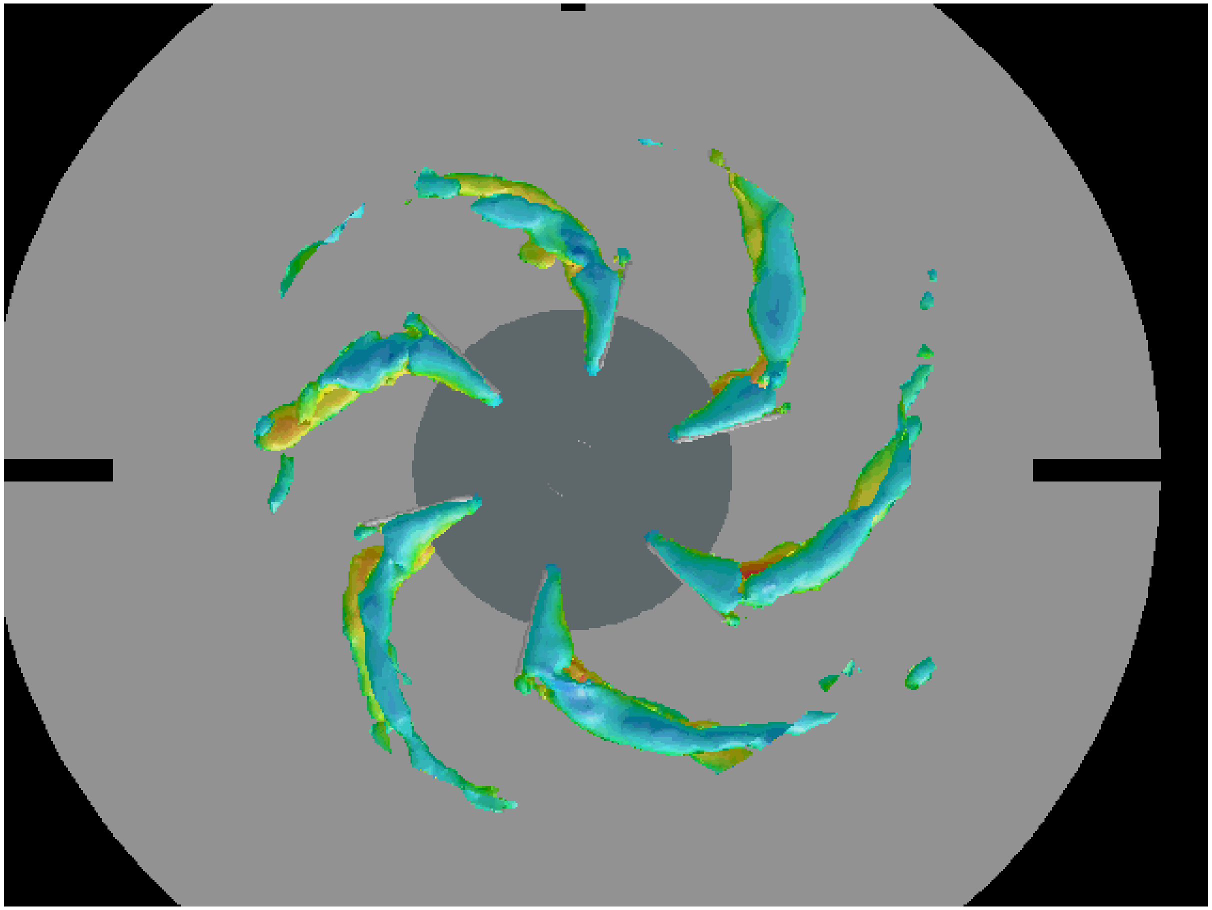
Rushton Turbine Model

- 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

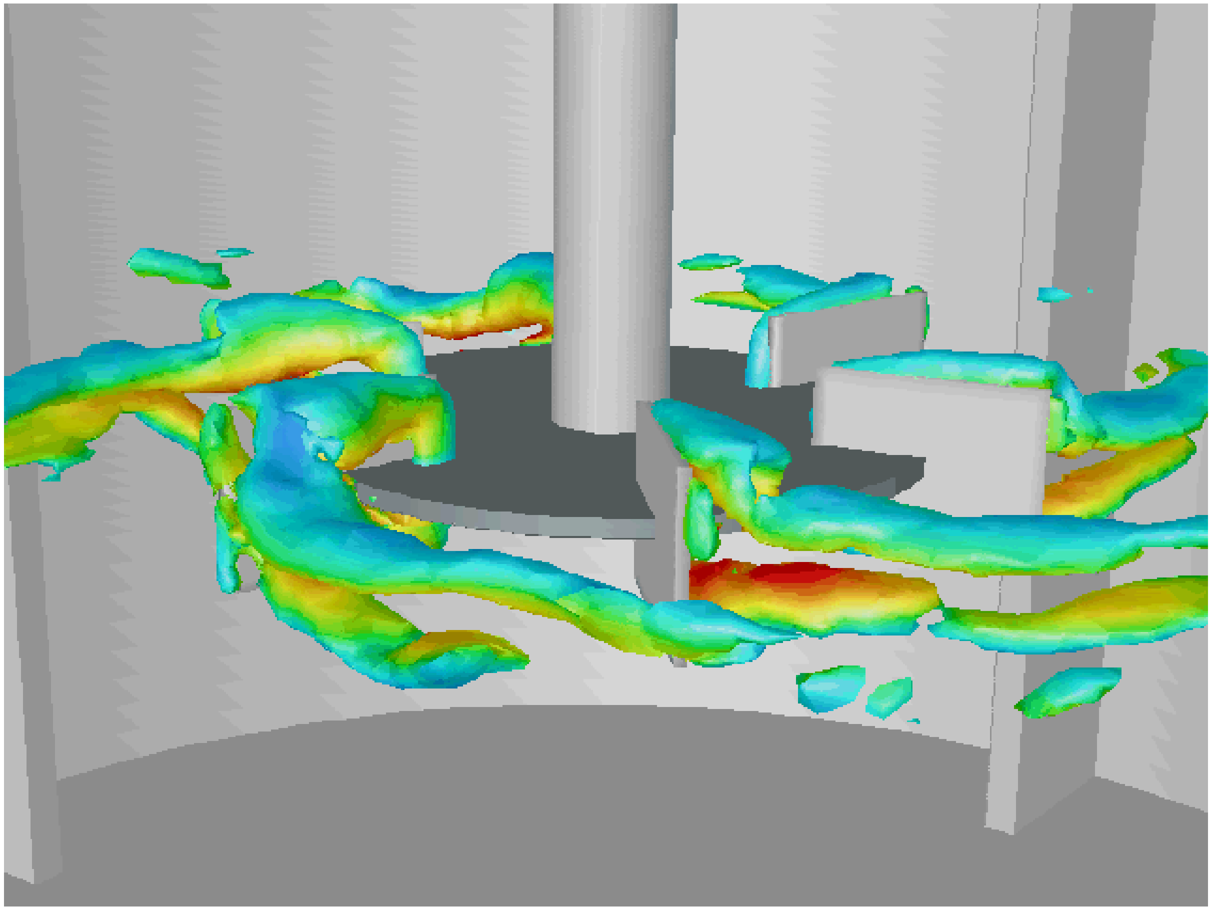
Rushton Turbine - Trailing Vortices



Iso-Surface of Vorticity Magnitude (550 s^{-1})

Colored by velocity magnitude

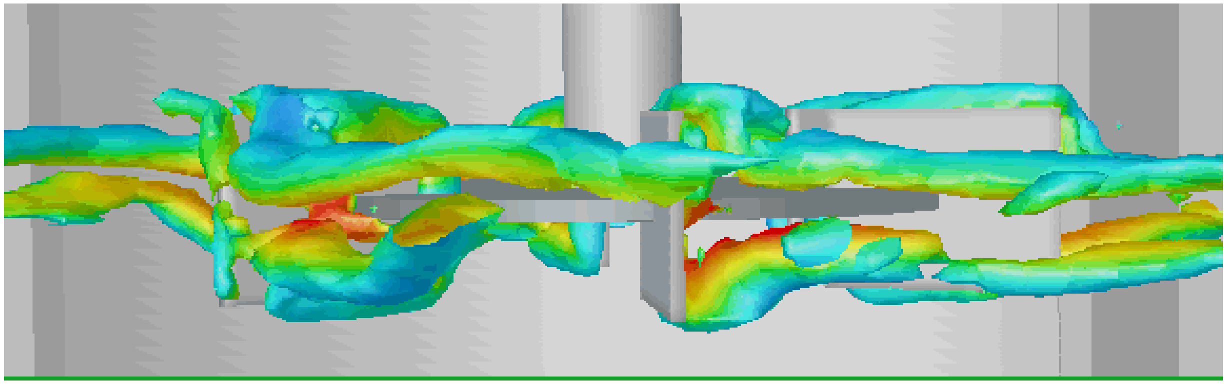
Rushton Turbine - Trailing Vortices



Iso-Surface of Vorticity Magnitude (550 s^{-1})

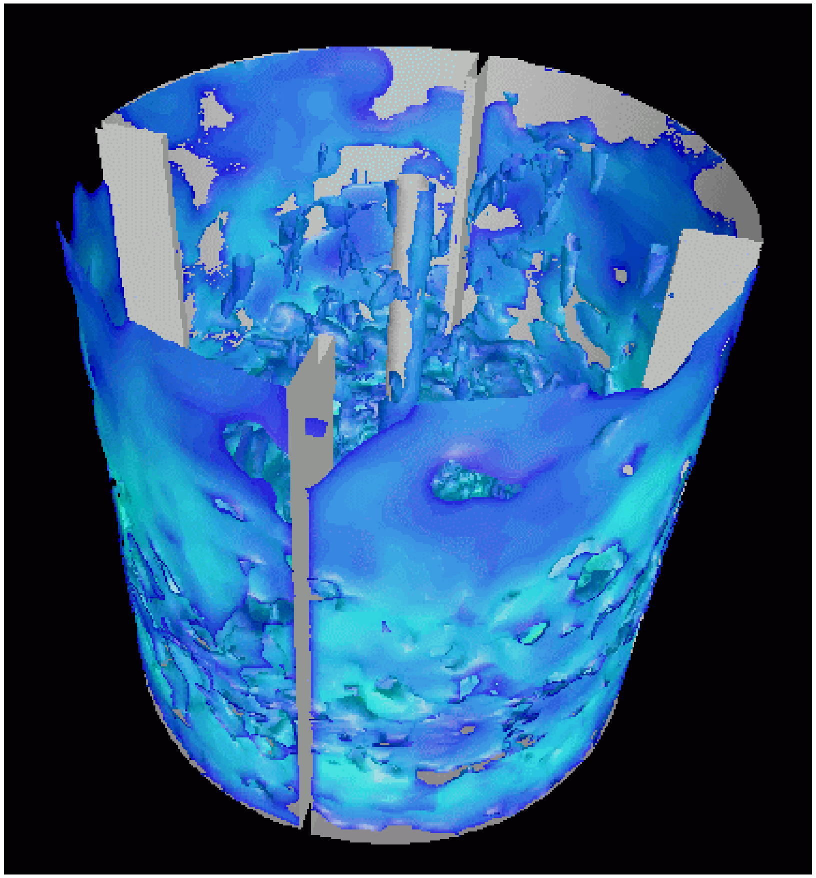
Colored by velocity magnitude

Rushton Turbine - Trailing Vortices



Iso-Surface of Vorticity Magnitude (550 s^{-1})
Colored by velocity magnitude

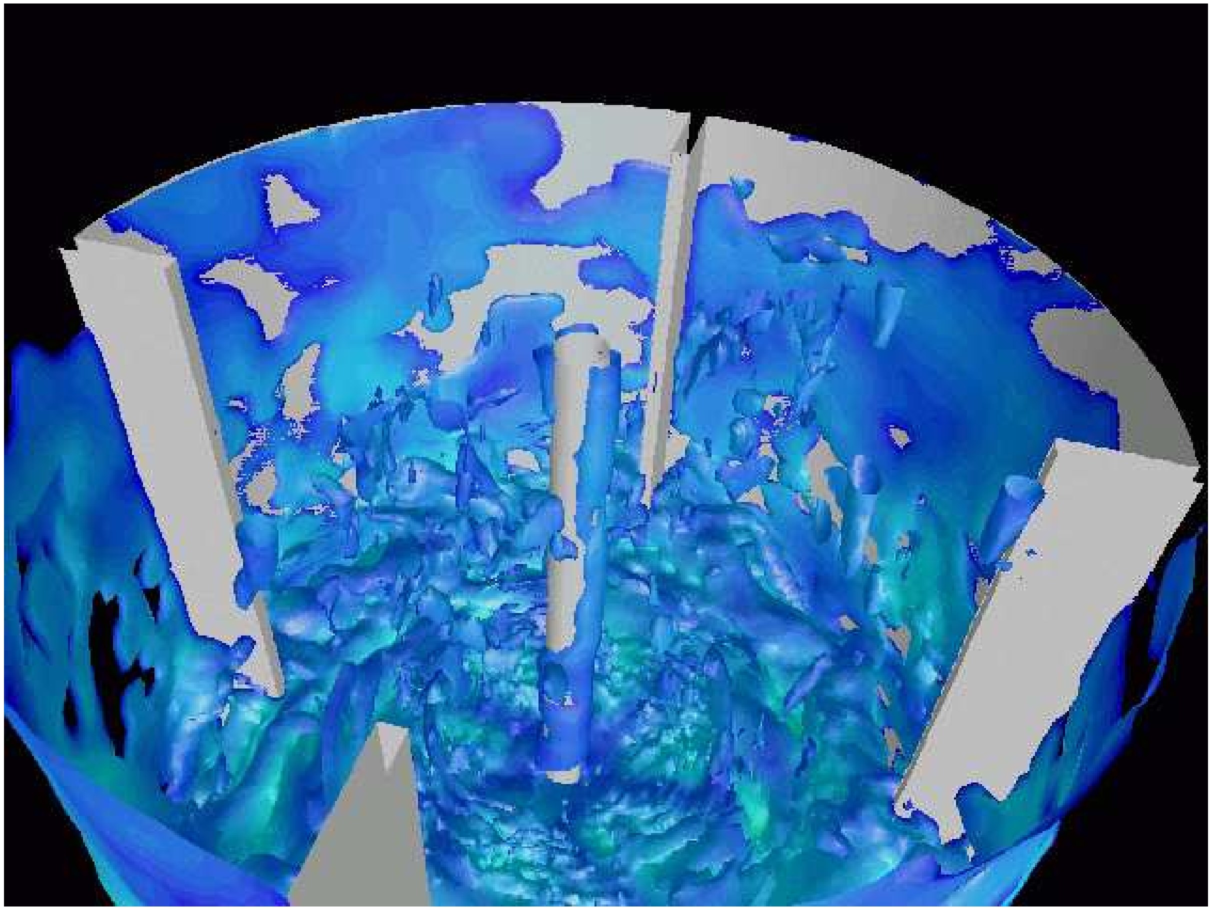
Rushton Turbine - Vorticity



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

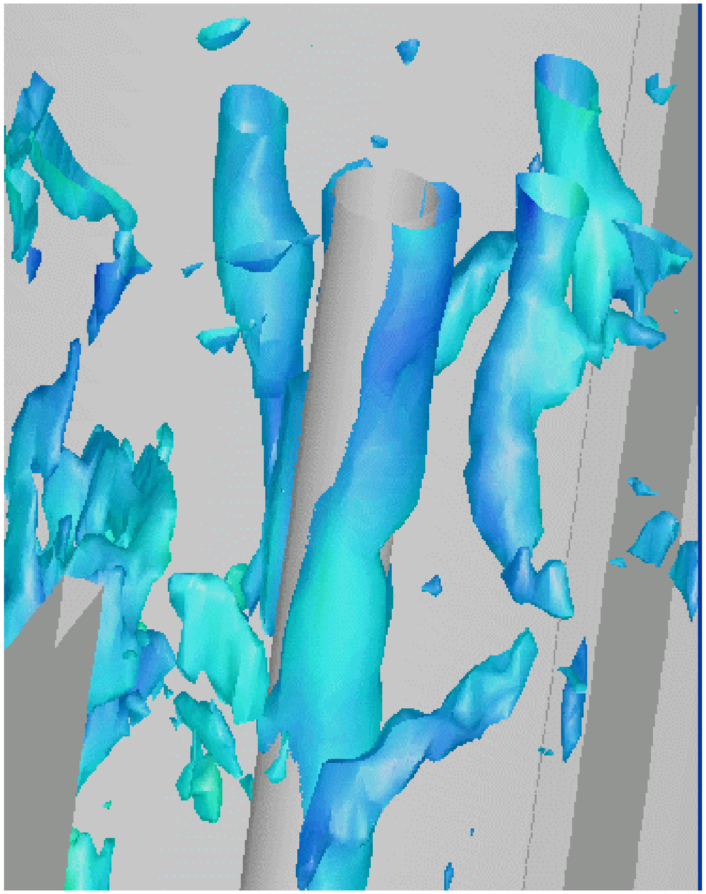
Rushton Turbine - Vorticity



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

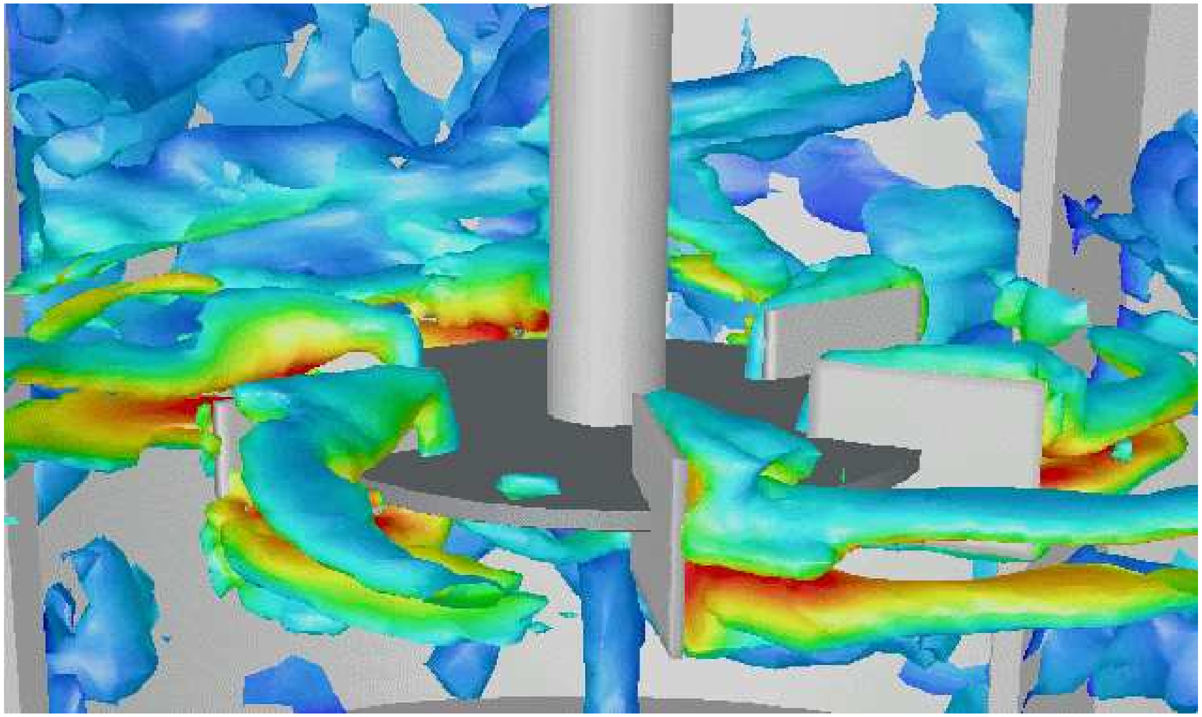
Rushton Turbine - Vortices at Surface



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

Rushton Turbine - Trailing Vortices



Iso-Surface of Vorticity Magnitude (550 and 80 s^{-1})
Colored by velocity magnitude

Summary

- LES is a transient turbulence model that falls midway between RANS and DNS models.
- The differences between predicted mixing patterns with RANS and LES are clear.
- LES has potential benefit for engineering applications, and is within reach computationally.
- However, 2-D fix, 3-D fix, and MRF models are much faster computationally, and still have their place.
- The predicted flow patterns for the HE-3 and PBT compared well with digital particle image velocimetry data reported in the literature, and exhibited the long time scale instabilities seen in the experiments. The results for the Rushton turbine compared well with LES simulations reported previously (e.g. Eggels, Derksen).
- The results of these studies open the way to a renewed interpretation of many previously unexplained hydrodynamic phenomena that are observed in stirred vessels.