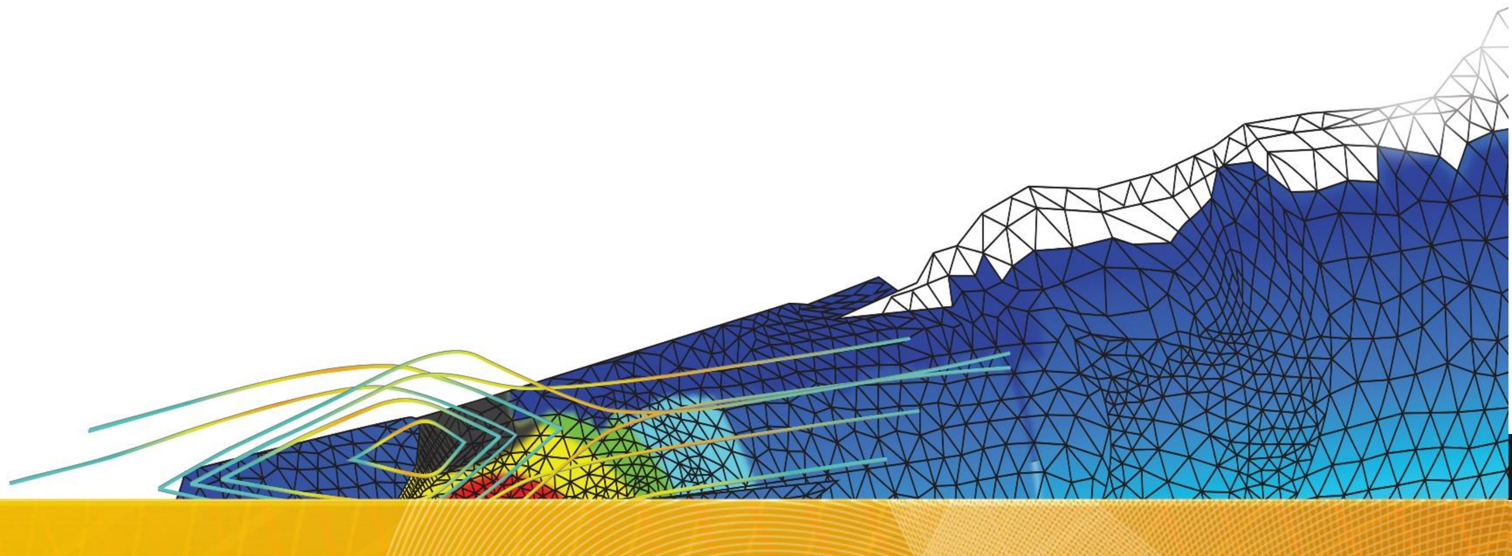
CFD simulation of stirred tank mixing processes using ANSYS

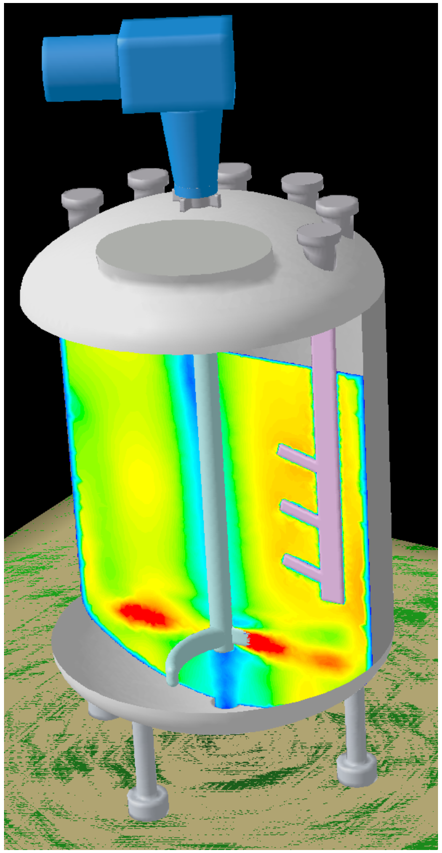
Sravan Kumar Nallamothu



Agenda

- Mixing in process industry
- Mixing Modeling
- Physics in Agitated Vessels
- Modeling tools
- Summary

Mixing in the Chemical Process Industry



- **Mixing in agitated vessels is part of the infrastructure of the chemical, petrochemical and biochemical industries**
- **Need to determine under- or over-mixing of processes**
  - Poor mixing leads to waste
- **Proper mixing is needed for chemical reaction**
  - Fast reactions (rates, selectivity and production) are controlled by the rate of mixing
- **Scale-up and scale-down is challenging**

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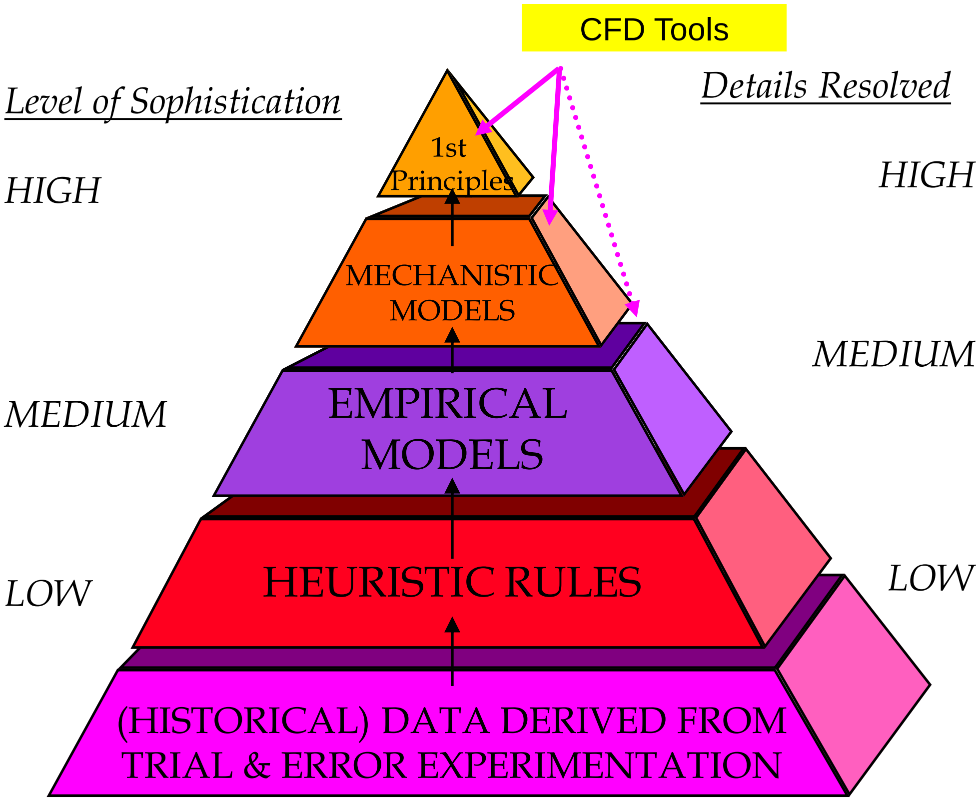
Mixing Modeling: CFD Approaches



CFD Modeling Approaches

1. **Comprehensive model including all physics**
   - **Computationally expensive**
   - **Used for new design of equipments**
   - **Use for in-depth analysis of final design**
2. **Focus only on key physics**
   - **Widely used method**
   - **Limit modeling to important physical processes**
   - **Quick solution for gaining engineering insight**

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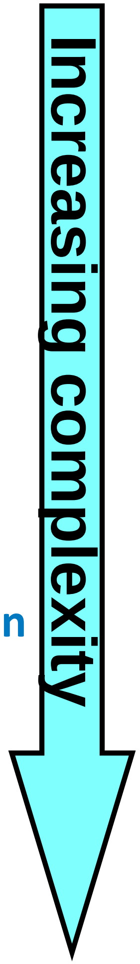
Physics in Agitated Vessels

- Single phase
  - Velocity field prediction
  - Turbulence prediction
  - Turbulence
- Gas liquid flows
  - Bubble size distribution
  - Mass transfer
  - Vortex prediction
- Liquid solid flows
  - Solid suspension
- ANSYS tools can model all above processes individually or in combination



Physics in Agitated Vessels

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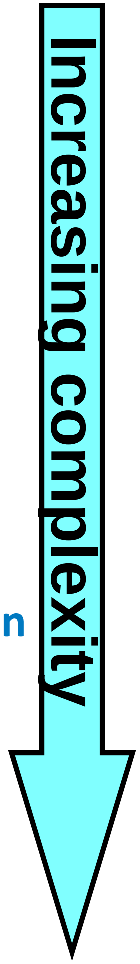
- **Liquid solid flows**
  - **Solid suspension**
- **ANSYS tools can model all above processes individually or in combination**

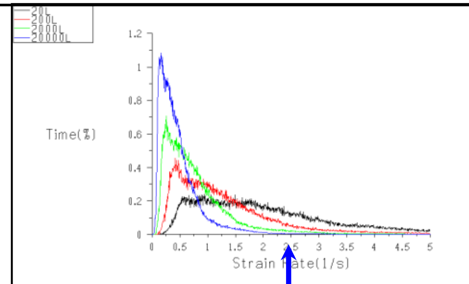


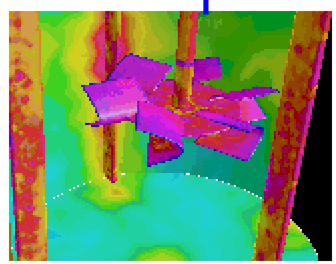
Single Phase Flow Analysis

Numerical data

- Dissipation rate
- Shear rate
- Power number
- Blend time
- Flow number
- Kolmogorov length

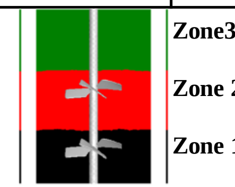
Shear rate characteristics of reactor



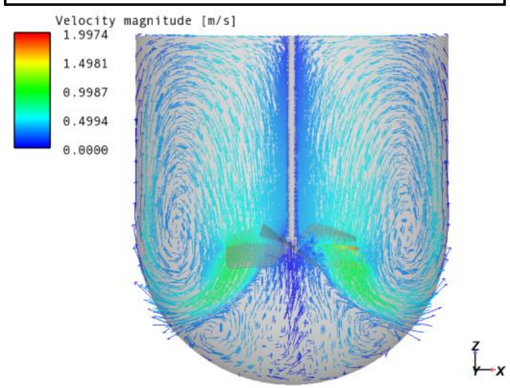


Zonal Residence Time Distribution

Quantity	Zone 1	Zone 2	Zone 3
Zone Ht (m)	1.01	2.20	3.37
Total Visit No,	109k	180k	71 K
Average RTD(s)	7.11	5.56	16.01

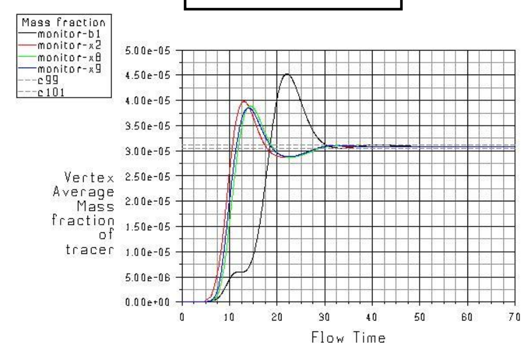


Field data at every location



Velocity vectors in an unbaffled reactor

Blend time



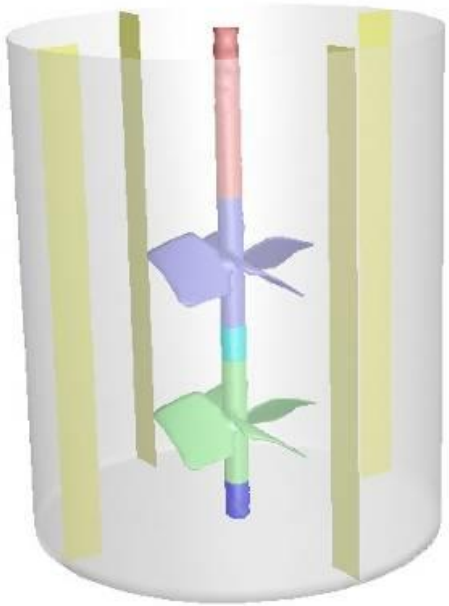
Blend time data at different locations in reactor

Output from single phase simulation?

Case Study 1: Scale up analysis

(Ref: ACS BIOT 2008)

- **Objective: Evaluate local energy dissipation rate as scale up criterion for geometrically scaled vessels**
- **Number of reactors: 4**
  - **20, 200, 2000, 20000 liter**
- **Operating Conditions:**
  - **20Litre reactor is run at 63 rpm**
  - **RPM for other reactor selected such as to obtain same local energy dissipation rate**



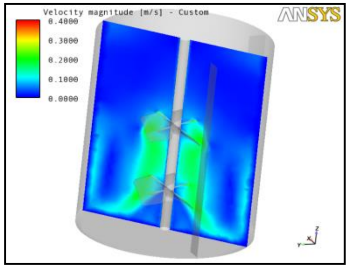
Baffled vessel with two A315 impellers

$$\text{Assume} \quad \varepsilon \propto \frac{P}{\rho V_{imp}} = \frac{P_o \rho N^3 D^5}{\rho \frac{\pi D^2}{4} D_w} = \frac{P_o N^3 D^5}{\frac{\pi D^2}{4} \alpha D} = \frac{P_o}{\frac{\pi \alpha}{4}} N^3 D^2 \quad \Rightarrow \quad \varepsilon \propto N^3 D^2$$

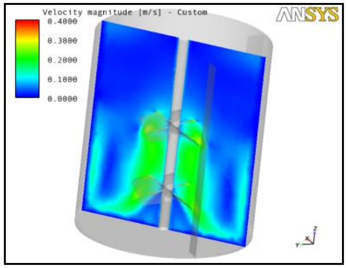
Case Study 1: Simulation Results – Flow and Blend Time

- **Types of simulations done**
  - **Flow**
  - **Blend Time**
  - **Exposure Analysis (TDR, Shear Rate)**
  - **Zonal Residence Time Distribution (RTD)**

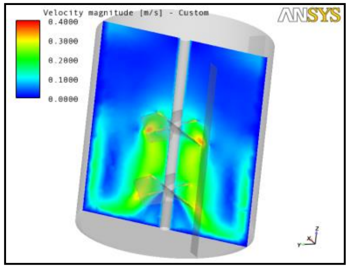
20-Liter



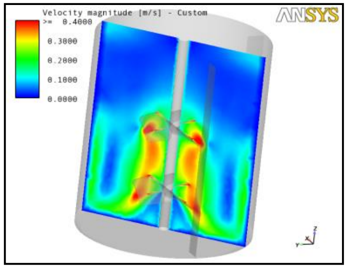
200-Liter



2000-Liter



20000-Liter



Power Numbers:

	20L	200L	2000L	20000L
RPM	63	37.7	22.6	13.6
CFD Upper Po	0.85	0.84	0.83	0.82
CFD Lower Po	0.5	0.49	0.48	0.48

Table 1: Power Number for both impellers

Blend Time

	20L	200L	2000L	20000L
Blend Time	25.8s	41.9	61.2s	111.8s

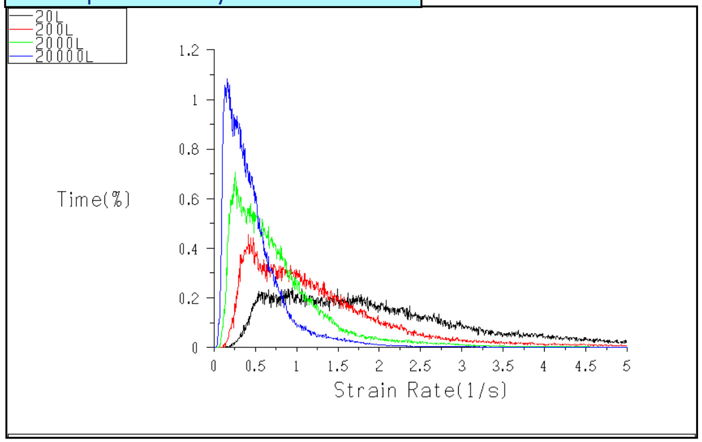
Table 2: Blend time for different sizes

Observations:

- **Vendor specified "single impeller" power number is 0.75**
  - Upper impeller close to that
  - Lower impeller draws lower power
- **Blend time increases with scale**

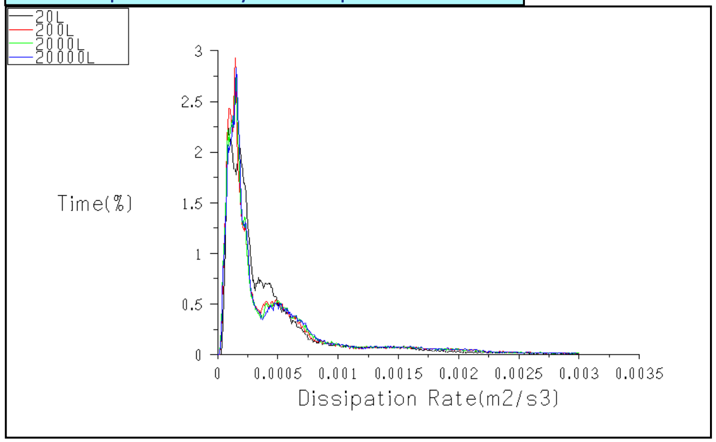
Case Study 1: Simulation Results – Exposure Analysis and Zonal RTD

Exposure Analysis: Shear Rate



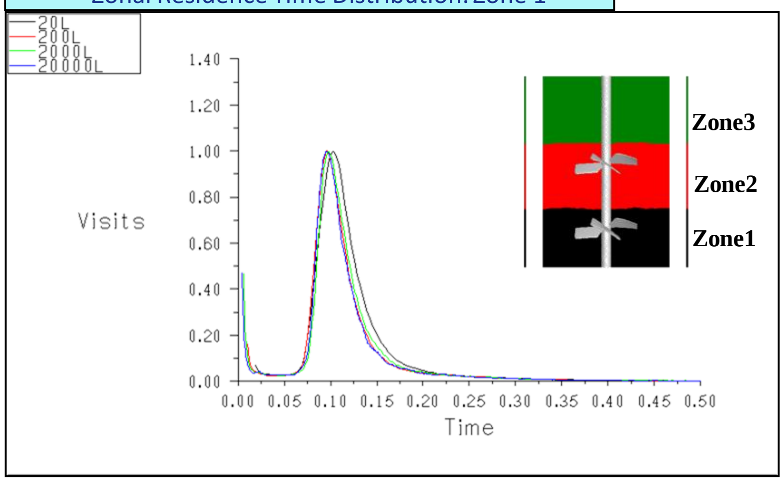
Low intensity at high reactor volumes

Exposure Analysis: Dissipation Rate



Dissipation Rate Exposure Analysis – Almost Identical environment

Zonal Residence Time Distribution: Zone 1



Zonal Residence Time Distribution – Similar distribution at different scales

Observations:

- **Cells/Particles exposure to high shear rate decreases with increase in reactor size**
- **Dissipation rate profiles are identical**
- **"Normalized" Zonal Residence Time behaviors similar for all reactor sizes**

- **At different scale particles/cells will experience similar environment**

Time taken for the study ~ 1.5 days

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Example: Fluid flow of shear thinning material in stirred tank

- **Venneker et al.[2],**
  - Flat bottom tank
  - 6 bladed Rushton turbine
  - Full baffled condition
- **Mesh**
  - Polyhedra cells with boundary layers
- **Operating conditions**
  - **T = 0.627 m**
  - **0.1% Blanose**
    - K = 13.2e-3, n = 0.85
  - **Rotational Speed**
    - 3.8 rev/sec
  - **Turbulent flow**
    - RKE model

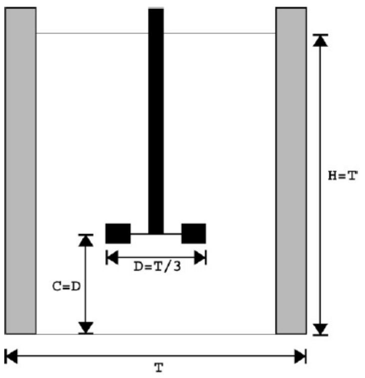
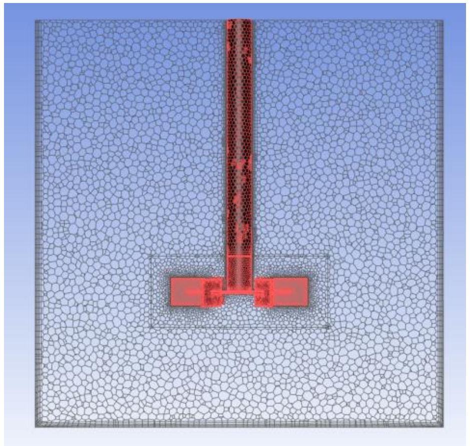


Fig. 1 – Geometry of the stirred vessel equipped with a Rushton turbine.



[2]Bart C.H. Venneker1, Jos J. Derksen2, Harry E.A. Van den Akker,Turbulent, *flow of shear-thinning liquids in stirred tanks—The effects of Reynolds number and flow index*, chemical engineering research and design 88 (2010) 827–843

Case files are available for this study and can be shared

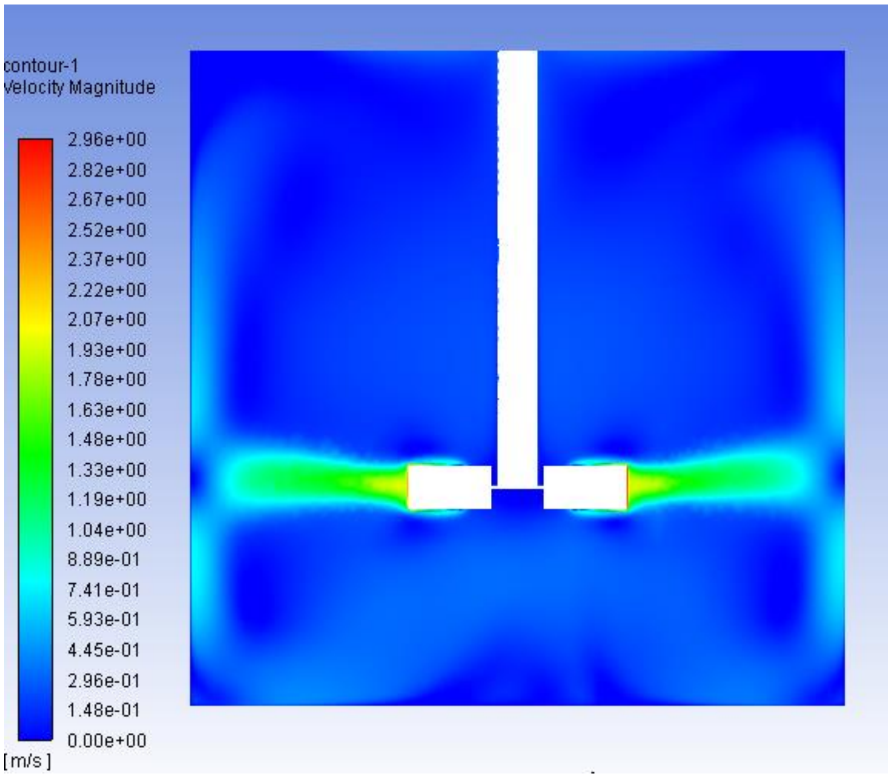
Case setup

- **Models**
  - Realizable K-epsilon with Standard wall functions
    - Enable non-Newtonian turbulent models

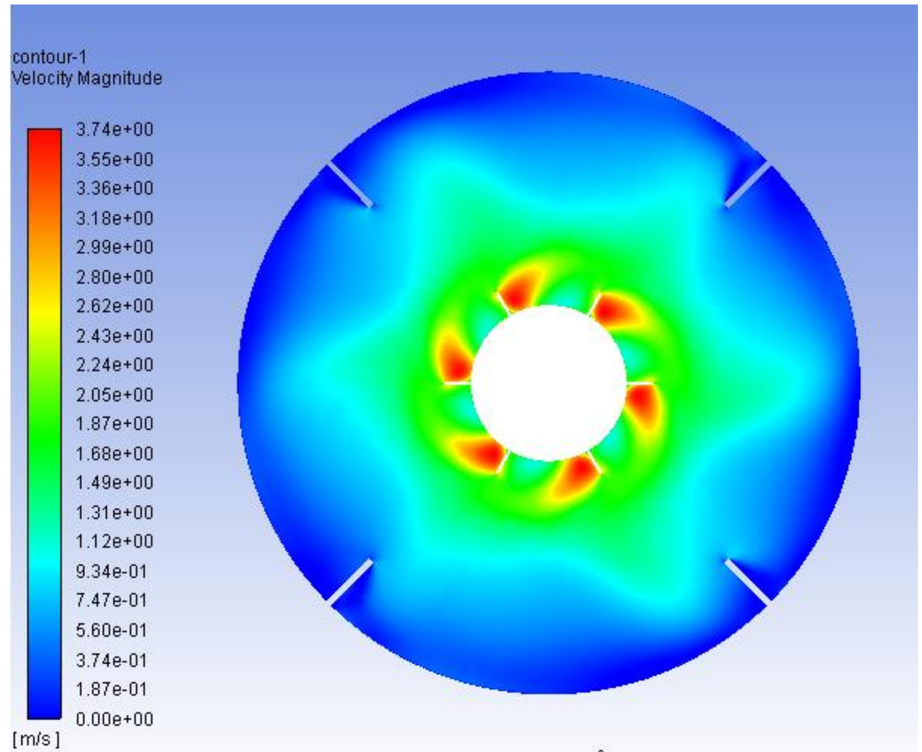
```
/define/models/viscous/turbulence-expert> turb-non-newtonian?
Enable turbulence for non-Newtonian fluids? [yes]
```

  - Non-Newtonian Power Law model for viscosity
- **Solver settings:**
  - Second order discretization for momentum
  - Second Order for Pressure discretization
  - SIMPLE for P-V coupling
  - Steady state solver for calculating solution

Flow patterns: Velocity distribution



Center Plane



Impeller Plane

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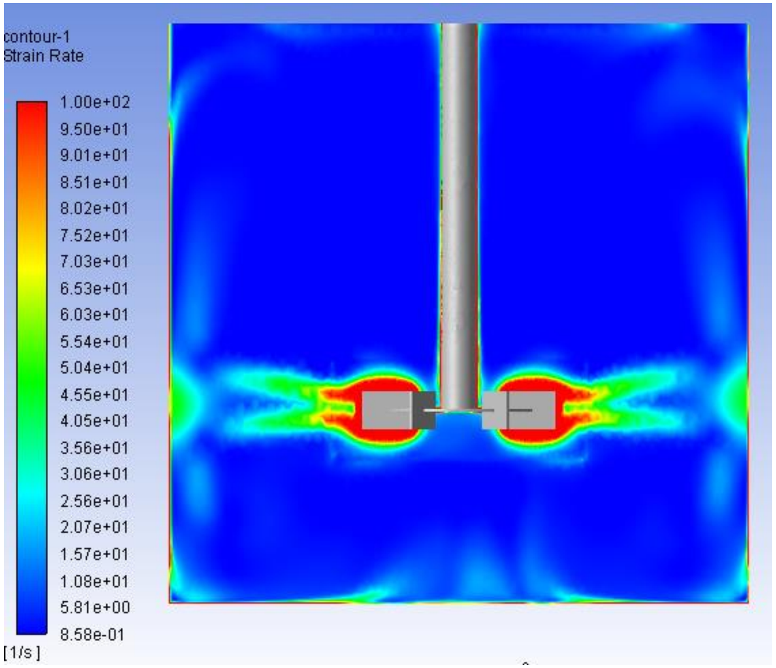
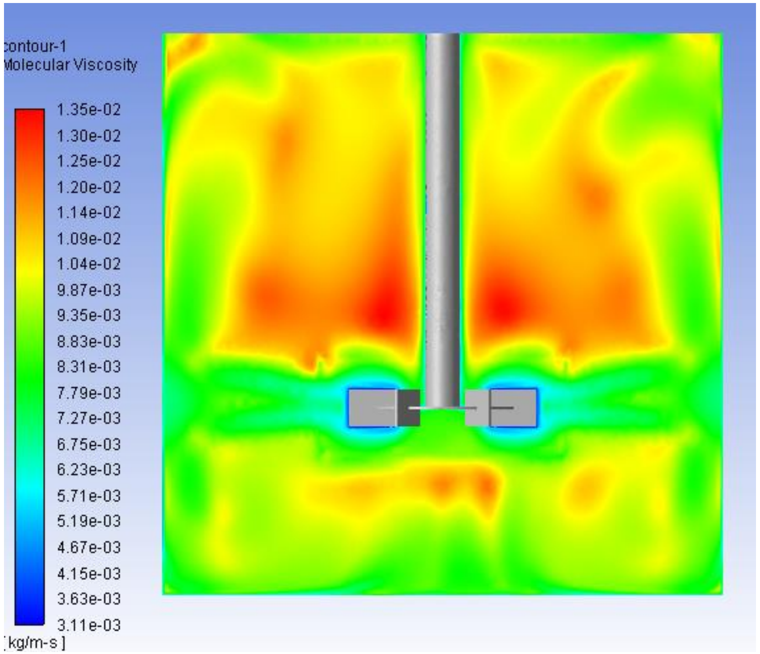
Flow patterns: Strain rate & Viscosity



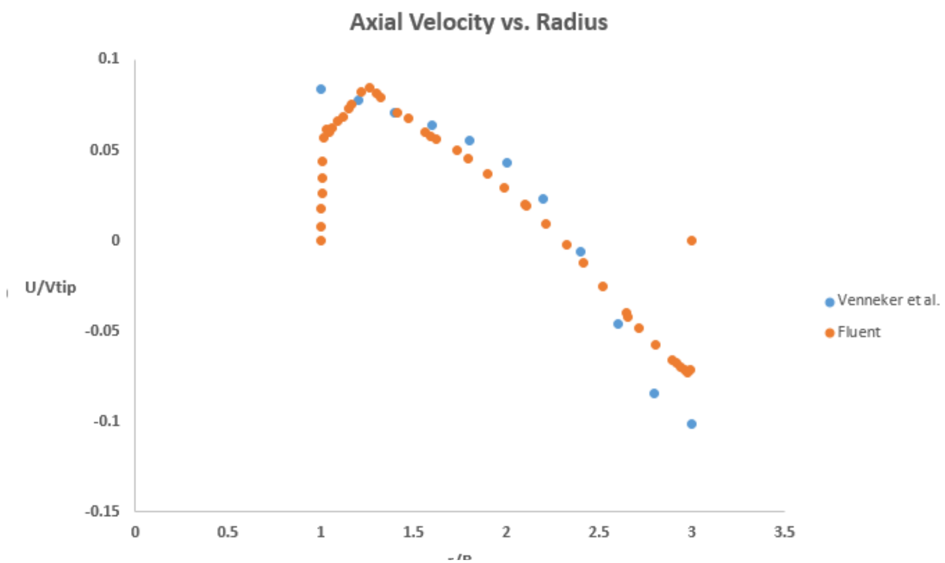
Strain rate distribution

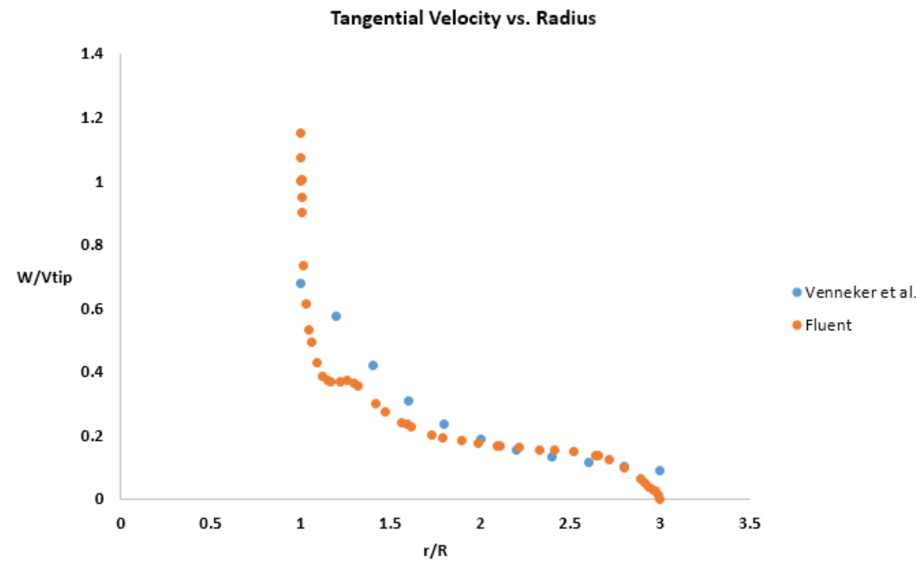


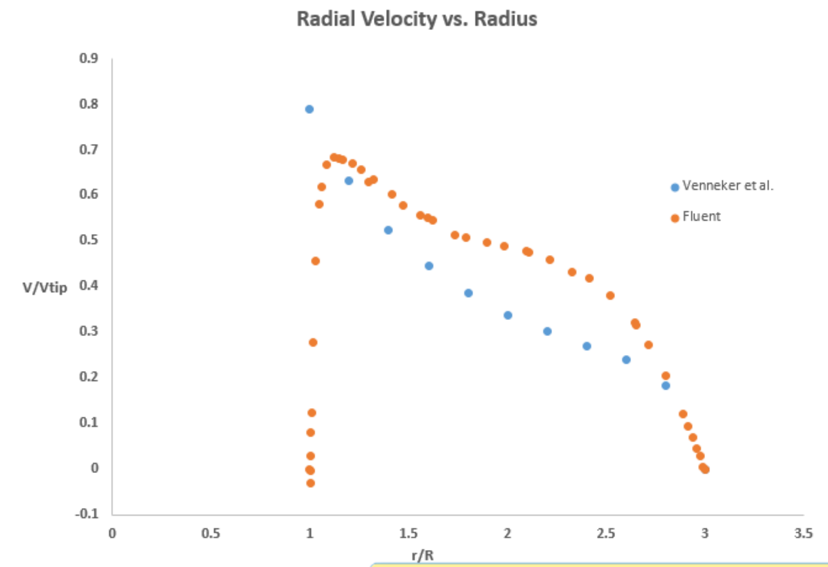
Viscosity distribution

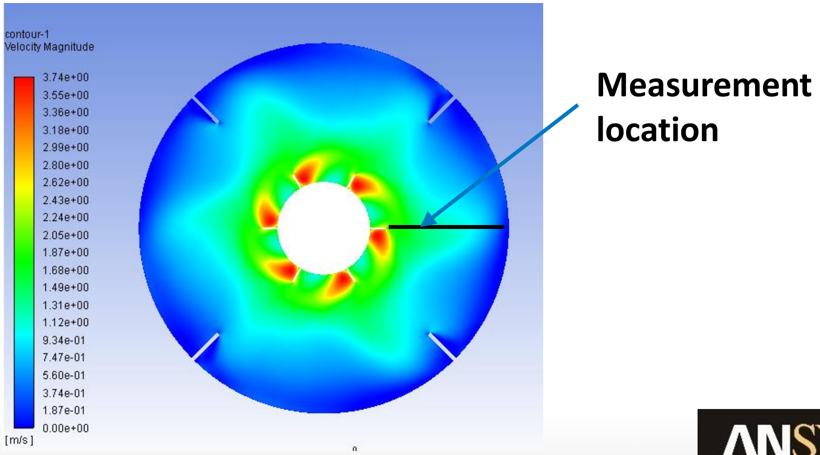
Case files are available for this study and can be shared

Velocity profile comparison









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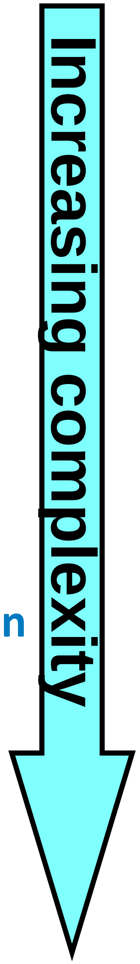
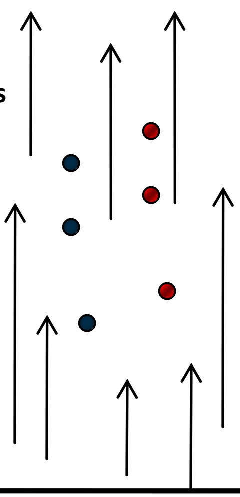


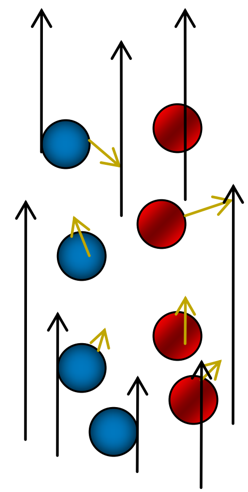
Modeling Approaches: Gas-phase Transport

Lagrangian frame models

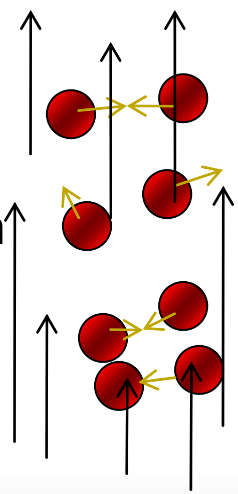
- **Liquid driving the gas flow**
  - Effect of gas bubbles on liquid flow is absent
  - Bubbly flow with small bubble sizes
  - Hold up < 0.1
- **DPM with one-way coupling**
- **Bubble diameter predefined**



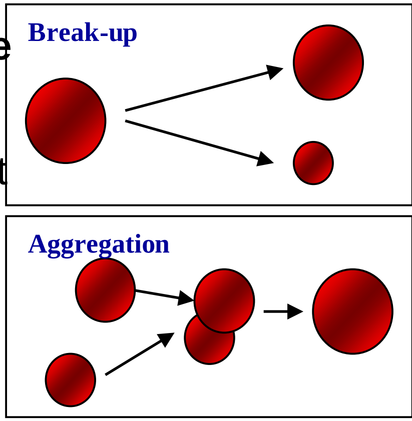
- **Gas-liquid momentum exchange**
  - Gas movement affects liquid flow
  - Bubbly flow with Large bubbles
  - Hold up < 0.1
- **DPM coupled simulation**
- **Bubble diameter predefined**



- **Gas-liquid and gas-gas interaction**
  - Important for high gas volume fraction flows
- **Pre defined constant diameter Eulerian frame**



- **Breakup and coalescence modeling**
  - Important when a pre-defined diameter is not adequate
  - Expensive model
- **Population balance Eulerian frame**

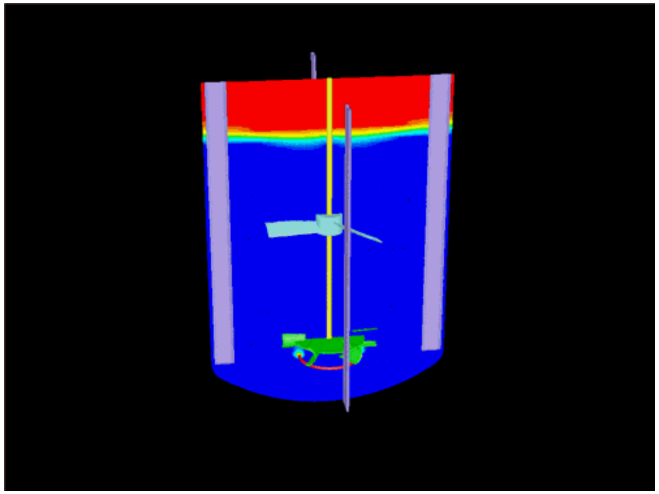


Eulerian frame models

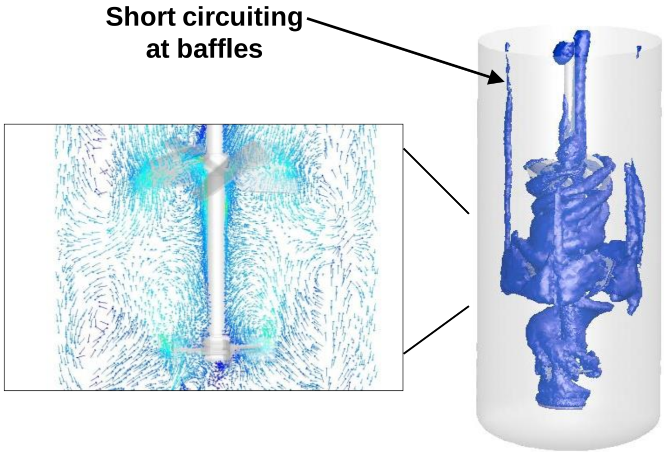
Gas-liquid Flows: Fermentor Modeling

Challenges

– Prediction of efficient mass transfer
– Gas distribution throughout the tank
– Power draw by impeller for sparging
– Limiting maximum shear rates
– Scale-up process to large reactor



Gas dispersion by Lightnin CD-6 impeller



Velocity vectors (left) Gas distribution (right) calculated in a tall fermentor

Benefits of CAE

– Detailed information for the flow field and shear rate characteristics
– Prediction of gas holdup
– Mass transfer quantities:
    – Estimation of local and global Kla
    – Interfacial area
– Power dissipation can be obtained to study effect of gas
– Gas distribution thought the vessel
– Simulate different conditions for scale up studies

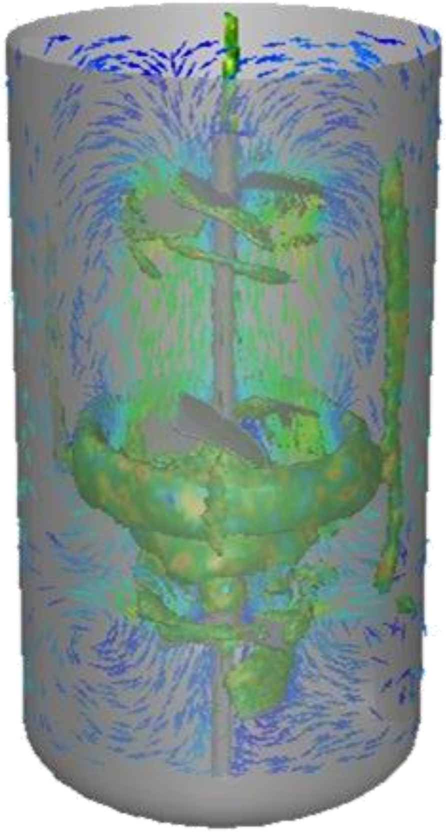
Case Study 2: Industrial Fermentor Modeling (courtesy Wyeth Vaccines, USA)

- **Problem statement:**
  - Analyze gas sparging in a three impeller bacterial fermentor
- **Fermentor details**
  - Baffled vessel
  - Partial ring sparger
  - Three impellers
    - Pitched blade turbine acting as sparging impeller
    - Two A315 impellers
- **Analysis:**
  - CFD simulation models: Velocity field, particle tracking (via the DPM model), Eulerian population balance

ANSYS

Case Study 2: Gas Distribution

- **Two A315s are working harmoniously**
  - **Top impeller discharges into middle impeller suction**
- **Short circuiting observed near baffles**
  - **Possible cause - complete ring, instead of partial one could resolve channeling**

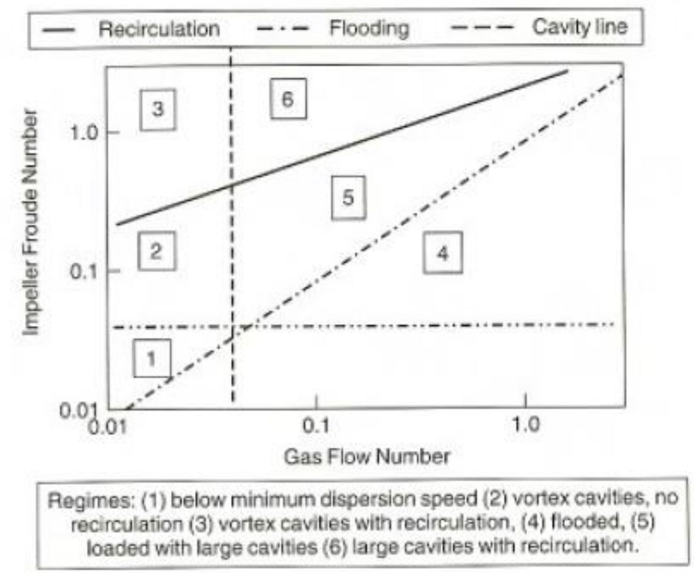


(courtesy of Wyeth USA)

Velocity and gas distribution in the fermentor

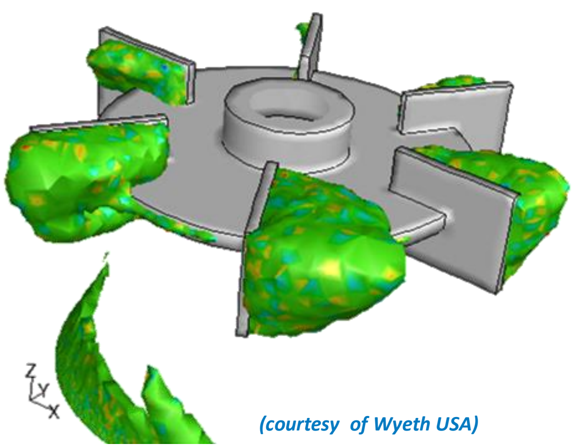
Case Study 2: Results - Gas Distribution near the Sparging Impeller

- **Gas cavity formation is observed behind RT blades**
  - **RT is one of the widely used sparging impeller**
  - **Cavities may exist in wake of any impeller**
  - **Depends on Gas Flow number and impeller Froude number**

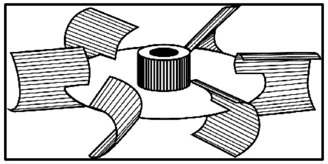


Ref: Chapter 11, Handbook of Industrial Mixing

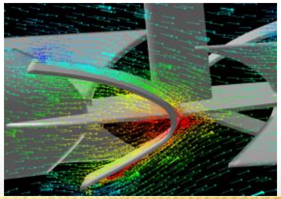
Iso-surfaces of gas volume fraction = 0.417



(courtesy of Wyeth USA)

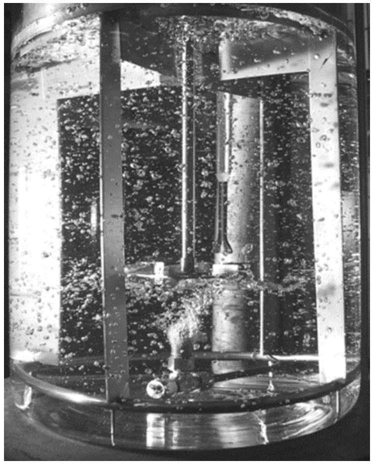


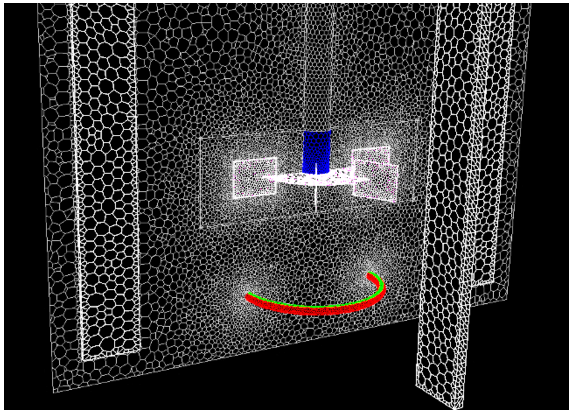
Curved Blade RT, an alternative ?



Gas holdup in stirred gas-liquid tank: Experiment

- **Experiments were done by Laakkonen[1]**
  - Performed CFX simulations as well
- **Geometry:**
  - Reactor volume: 194 Lit
  - 6 blade Rushton-Turbine
- **Operating conditions**
  - Angular velocity: 390 rpm
  - Gas flow rate: 0.7 vvm
- **Mesh**
  - Polyhedra mesh



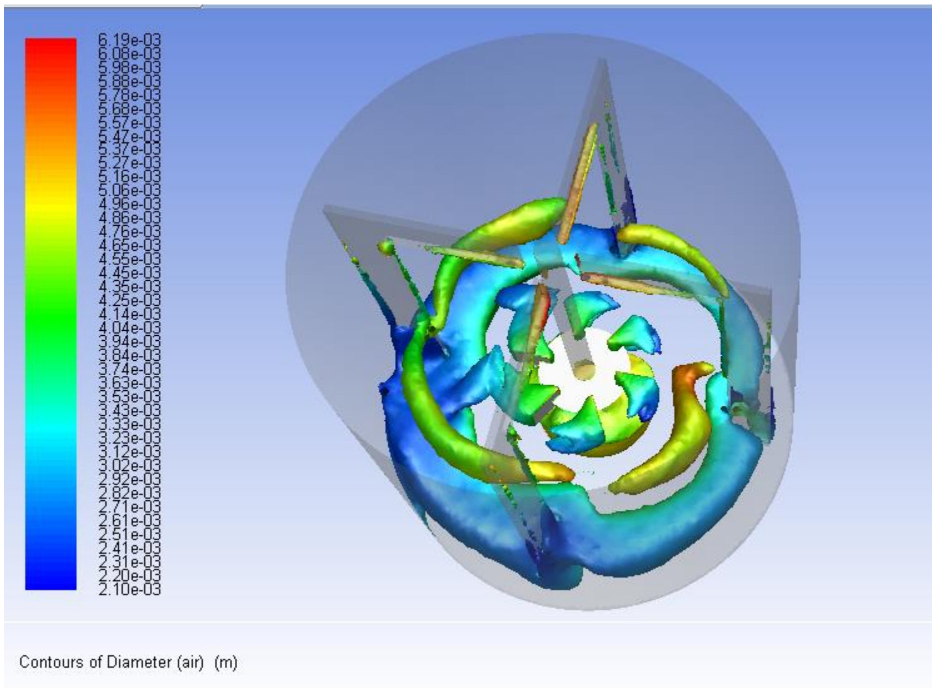


1. Laakkonen M, Alopaeus V, Aittamaa J. Modelling local bubble size distributions in agitated vessels. Chem Eng Sci. 2007;62;721-740

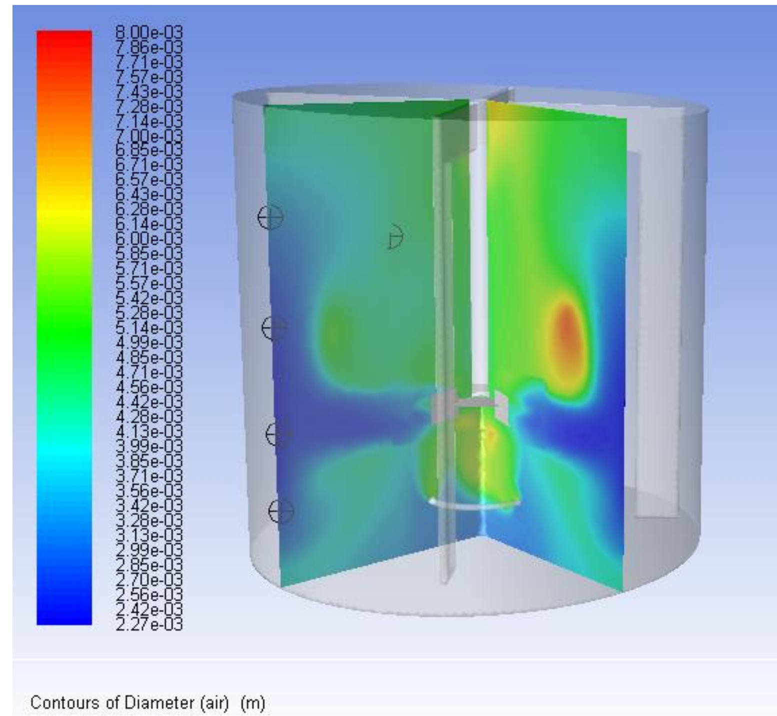
Case Setup

- **Models**
  - Eulerian multiphase model
  - Population balance model for modeling bubble size distribution
    - QMOM method
    - 6 moments
  - Ishii-zuber drag model with turbulent drag correction
- **Solution methods**
  - Least square cell based gradient method
  - First order discretization

Gas volume fraction & bubble diameter



Bubble size distribution on Isosurface of gas volume fraction 10%

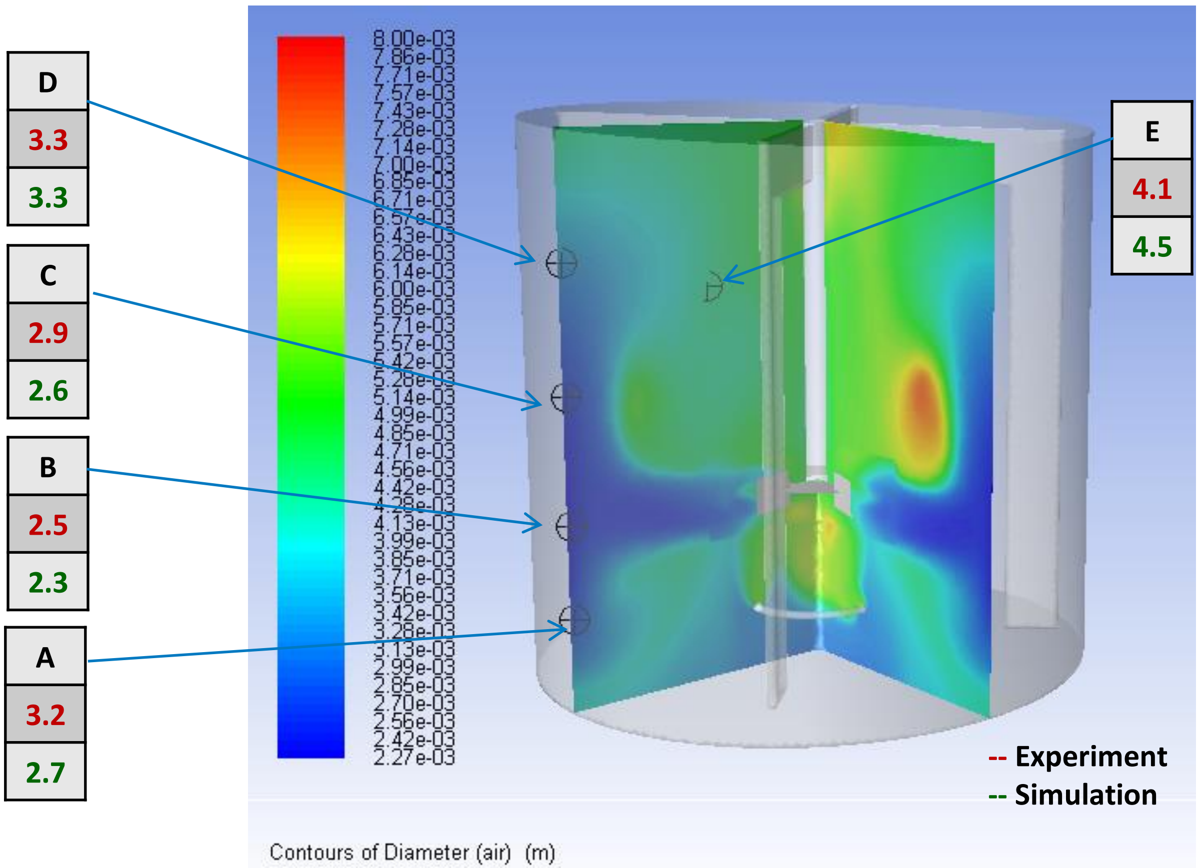


Bubble size distribution on planes between baffles

Case files are available for this study and can be shared

Bubble size distribution

390 rpm, 0.7 vvm



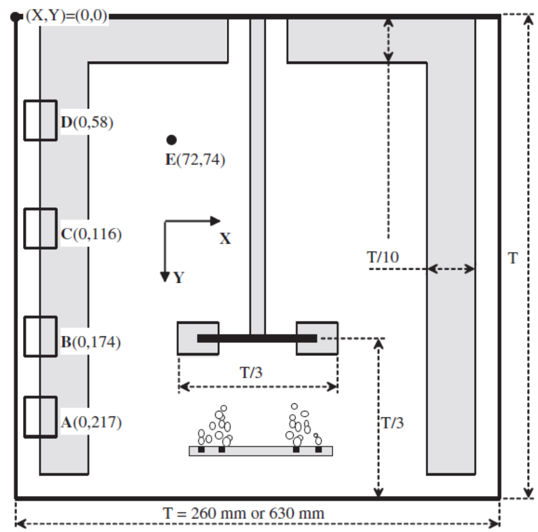
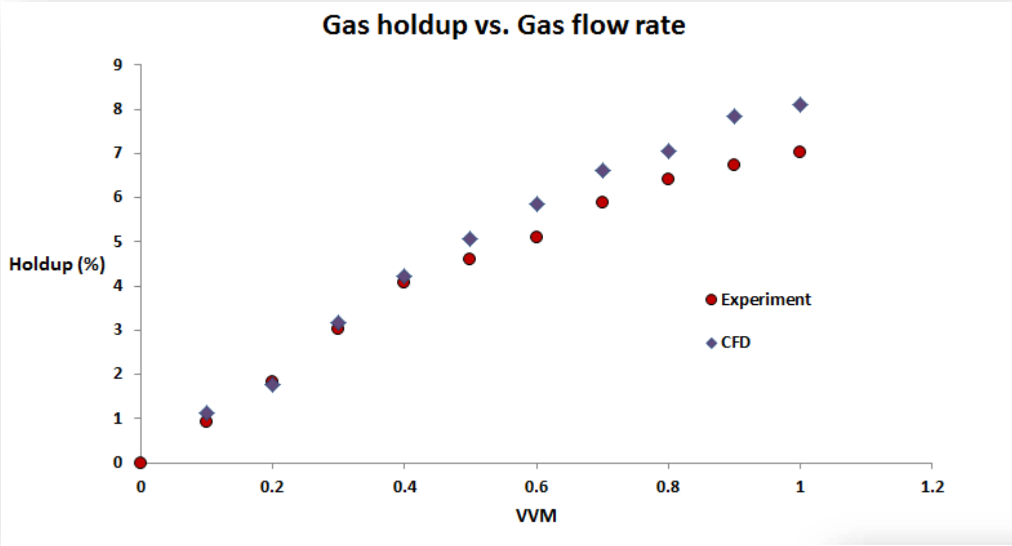


Fig. 1. The dimensions of agitated vessel and the locations of bubble size experiments (A–E) in the 200 L tank in millimetres.

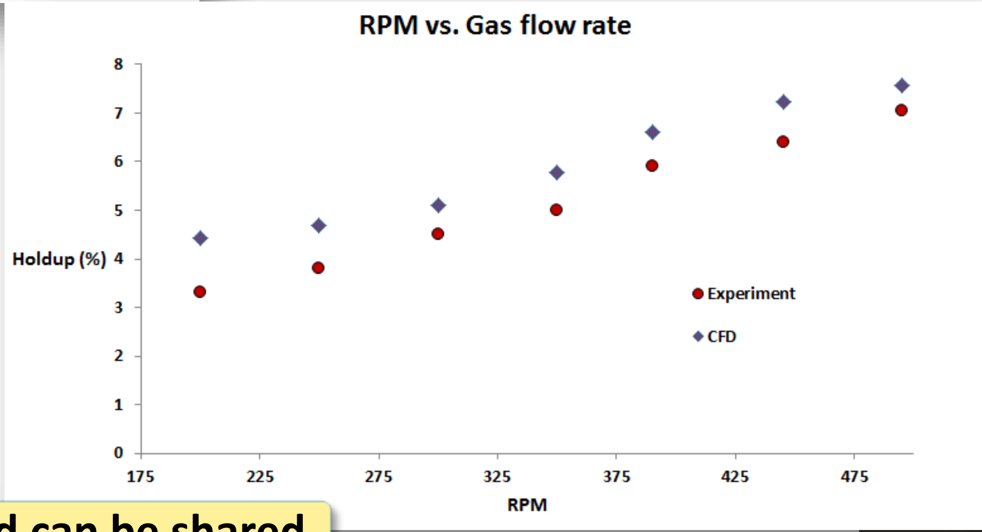
Case files are available for this study and can be shared

Gas holdup comparison



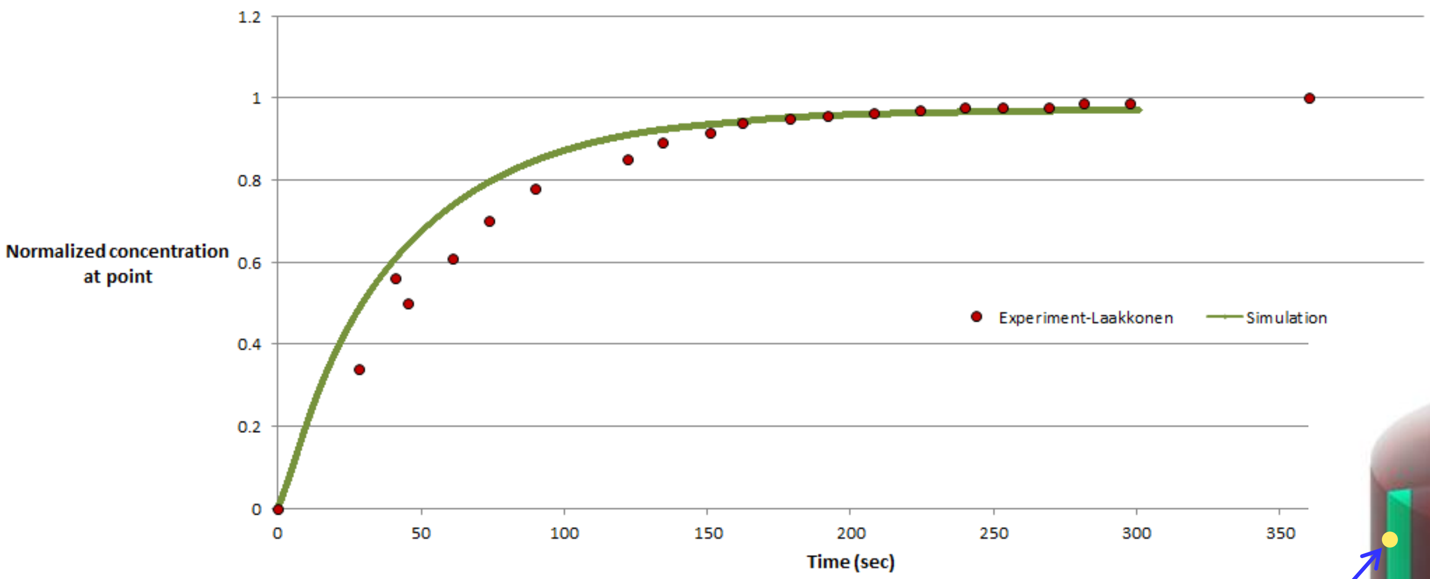
Simulation results match very well with experimental measurements

Simulations slightly over-predicted gas holdup at higher gas flow rates

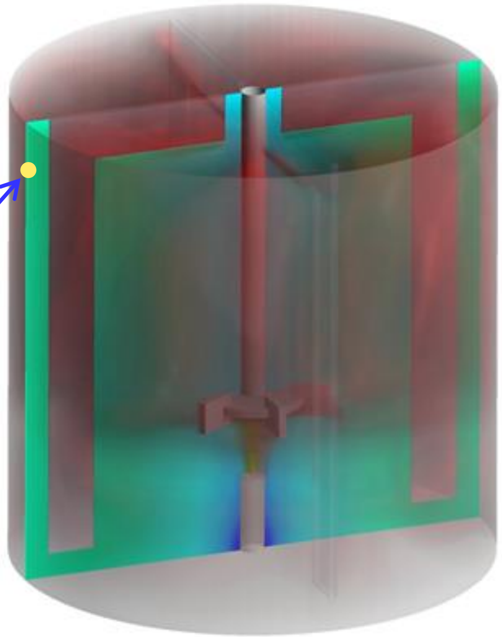


Case files are available for this study and can be shared

Dissolved Oxygen



Normalized dissolved oxygen concentration at a point near the liquid level



Contours of oxygen mass fraction on center plane along with gas volumetric distribution

Case files are available for this study and can be shared

Physics in Agitated Vessels

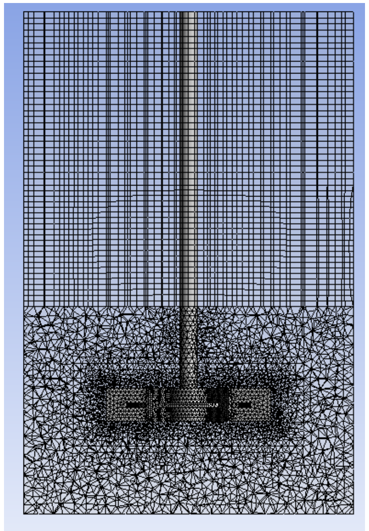
- Single phase
  - Velocity field prediction
  - Turbulence prediction
  - Turbulence
- Gas liquid flows
  - Bubble size distribution
  - Mass transfer
  - **Vortex prediction**
- Liquid solid flows
  - Solid suspension
- **ANSYS tools can model all above processes individually or in combination**

Increasing complexity

ANSYS

Geometry

- **Mixing tank geometry[1]:**
  - Cylindrical tank
  - 6 bladed Rushton Turbine impeller
- **Mesh: ~400K elements**
  - Tetrahedral mesh near the impeller
  - Prism layers in the upper half of the tank



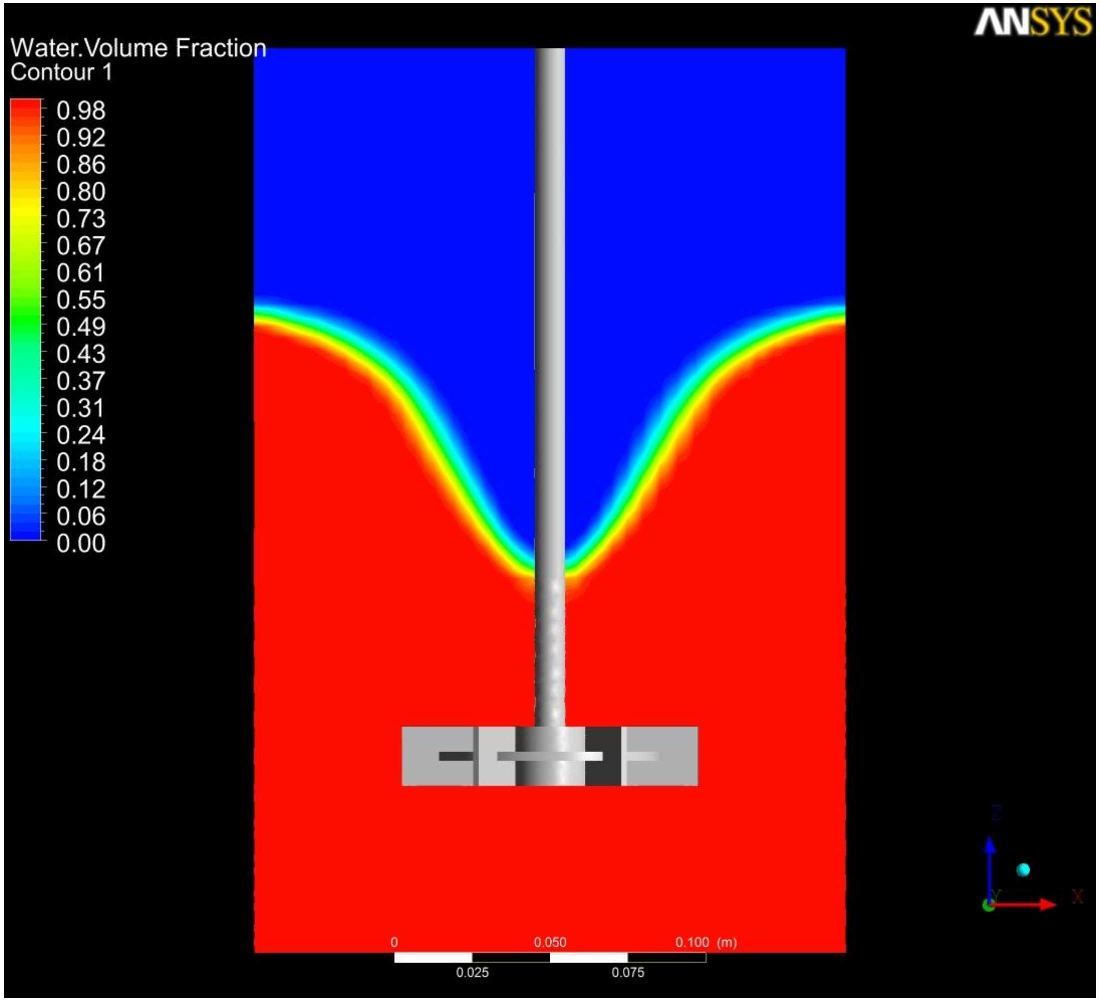
vessel geometry	Rushton turbine[15]
vessel diameter (*T*)	0.19 m
impeller diameter (*D*)	0.095 m (*T*/2)
impeller clearance (*C*)	0.063 m (*T*/3)
blade height (*b*)	0.019 m
blade width (*a*)	0.023 m
initial liquid height (*H*)	0.19 m (1*T*)

1. Jennifer N. Haque, Tariq Mahmud, Kevin J. Roberts, and Dominic Rhodes, ***Modeling Turbulent Flows with Free-Surface in Unbaffled Agitated Vessels*** *Ind. Eng. Chem. Res.*, ***2006, 45 (8), 2881-2891***

Case Setup

- **Models**
  - VOF multiphase model to track the gas-liquid freesurface position
  - Realizable k-epsilon model with standard wall functions
- **Solution Methods**
  - Transient solver
  - PISO for pressure-velocity coupling
  - Cell based gradients
  - Compressive scheme for volume fraction discretization
  - Second order upwind for momentum and turbulence

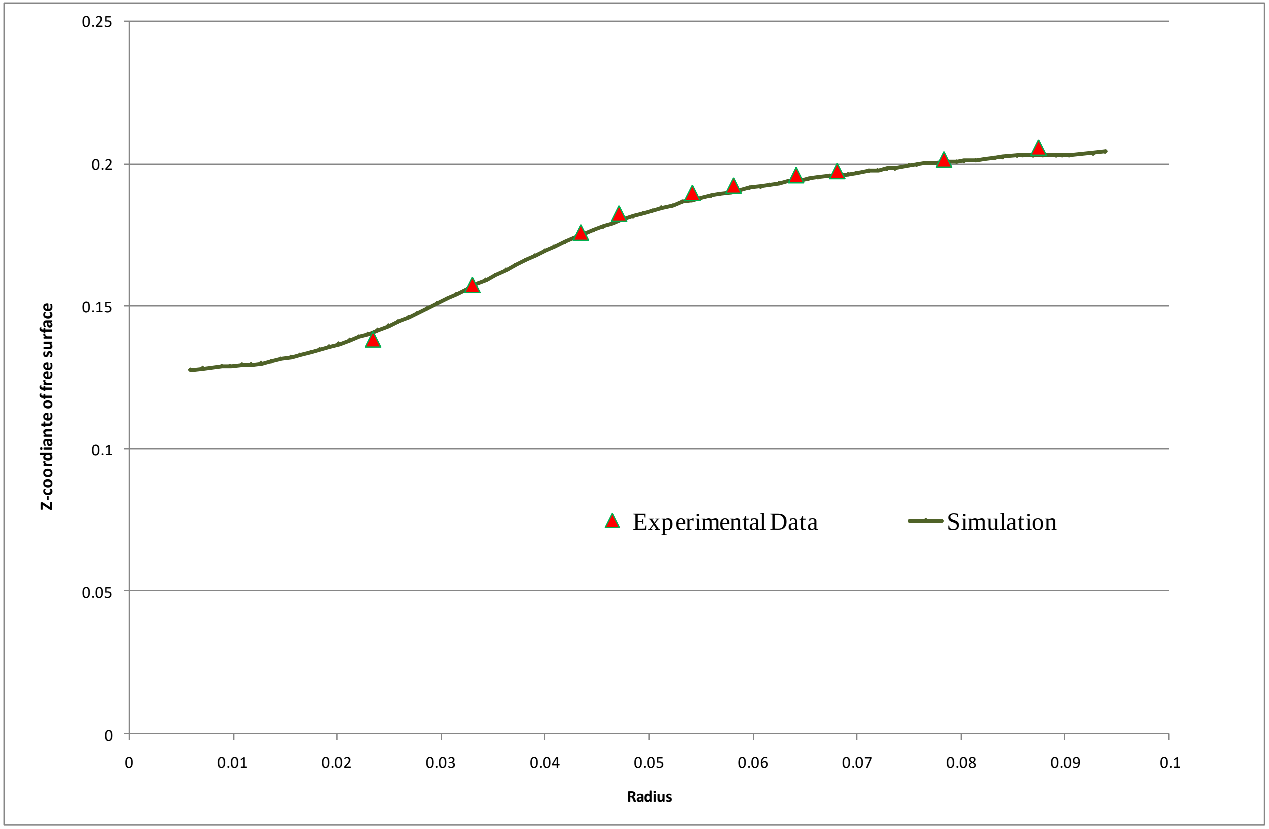
Results: Volume fraction contour of water on center plane

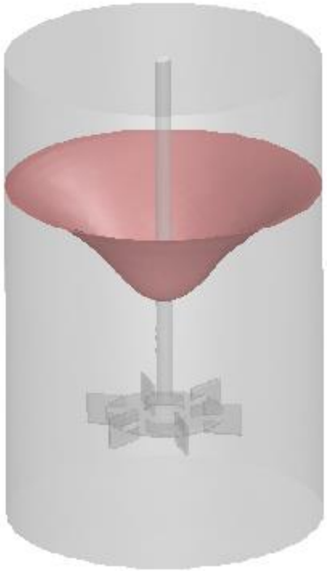


Case files are available for this study and can be shared

Free surface profile: Comparison

Experimental Data are approximately measured from haque et. al. paper.

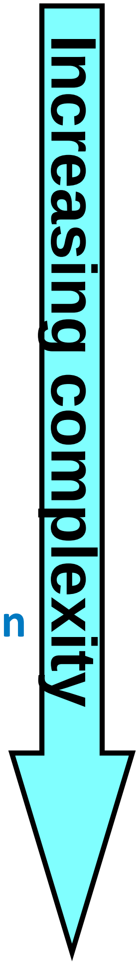




Case files are available for this study and can be shared

Physics in Agitated Vessels

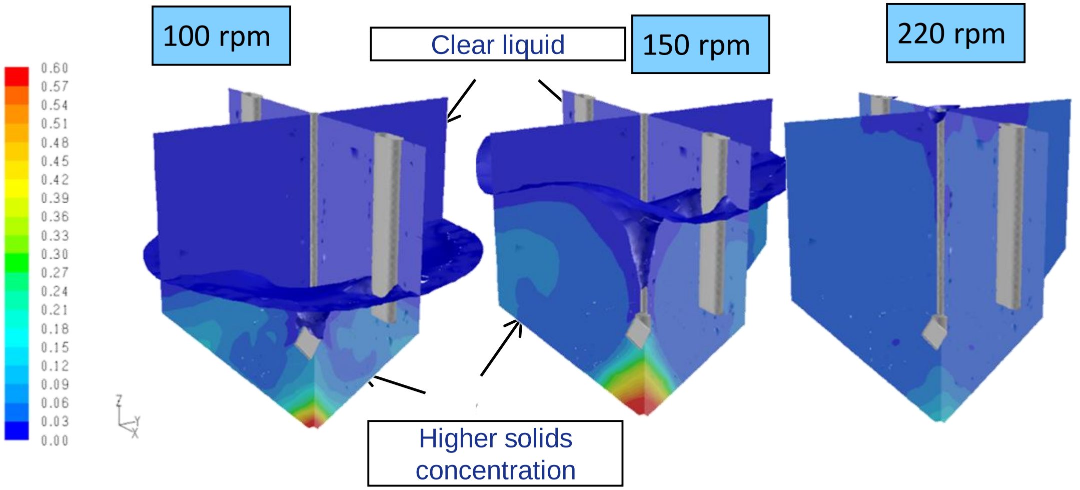
- Single phase
  - Velocity field prediction
  - Turbulence prediction
  - Turbulence
- Gas liquid flows
  - Bubble size distribution
  - Mass transfer
  - Vortex prediction
- **Liquid solid flows**
  - **Solid suspension**
- **ANSYS tools can model all above processes individually or in combination**



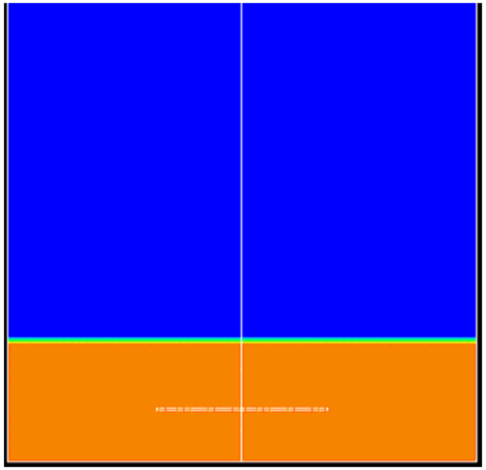
Solid Suspension Modeling

Challenges

- Solid suspension is a key concern for:
  - Solid catalyzed reactions
  - Crystal growth
  - Dissolution
- Uniform solid suspension
- Power prediction with the presence of solids



Solid profile at different agitation speeds. Ref: IchemE, 2008



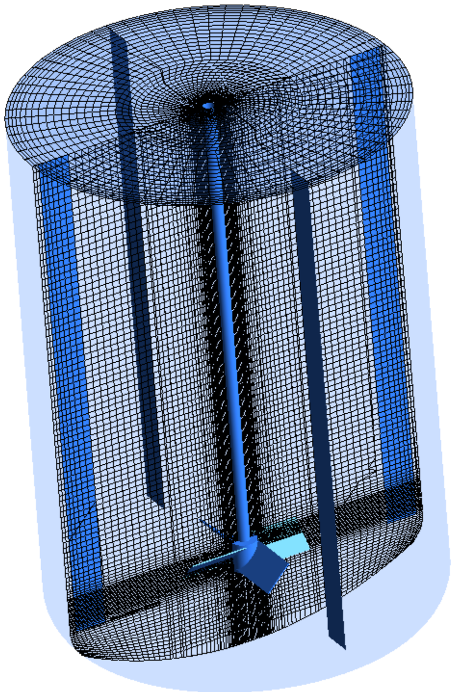
Iso surface and contours showing solid distribution and cloud height in a conical based vessel

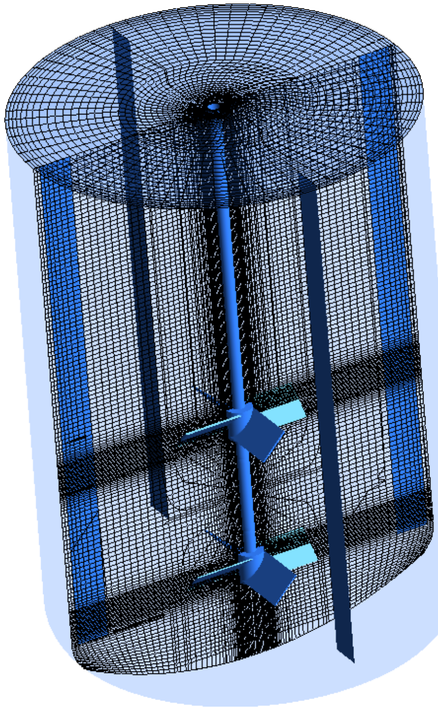
Benefits of CAE

- Detailed information for the flow field
- Shear rate characteristics
  - Many crystals can be damaged by exposure to regions of high shear
- Predict Just Suspension Velocity
- Predict the solids concentration profile through out the vessel

Problem Description

- **Reactor details**
  - Vessel Diameter: 0.61m
  - Liquid Level: 0.915m
  - Impeller Diameter: 0.2m
  - Clearance from Bottom: 0.15m and 0.39 m
  - Tank Bottom: Torispherical
- **Material Properties**
  - Liquid Density: 1000 kg/m3
  - Liquid Viscosity: 0.001 Pa-s
  - Solid Density: 2630 kg/m3
  - Particle Diameter: 180 micron
- **Operating Conditions**
  - Solid Concentration: 10% wt and 15% wt
  - Agitation Rate: 150 RPM to 450 RPM in the steps of 50 RPM



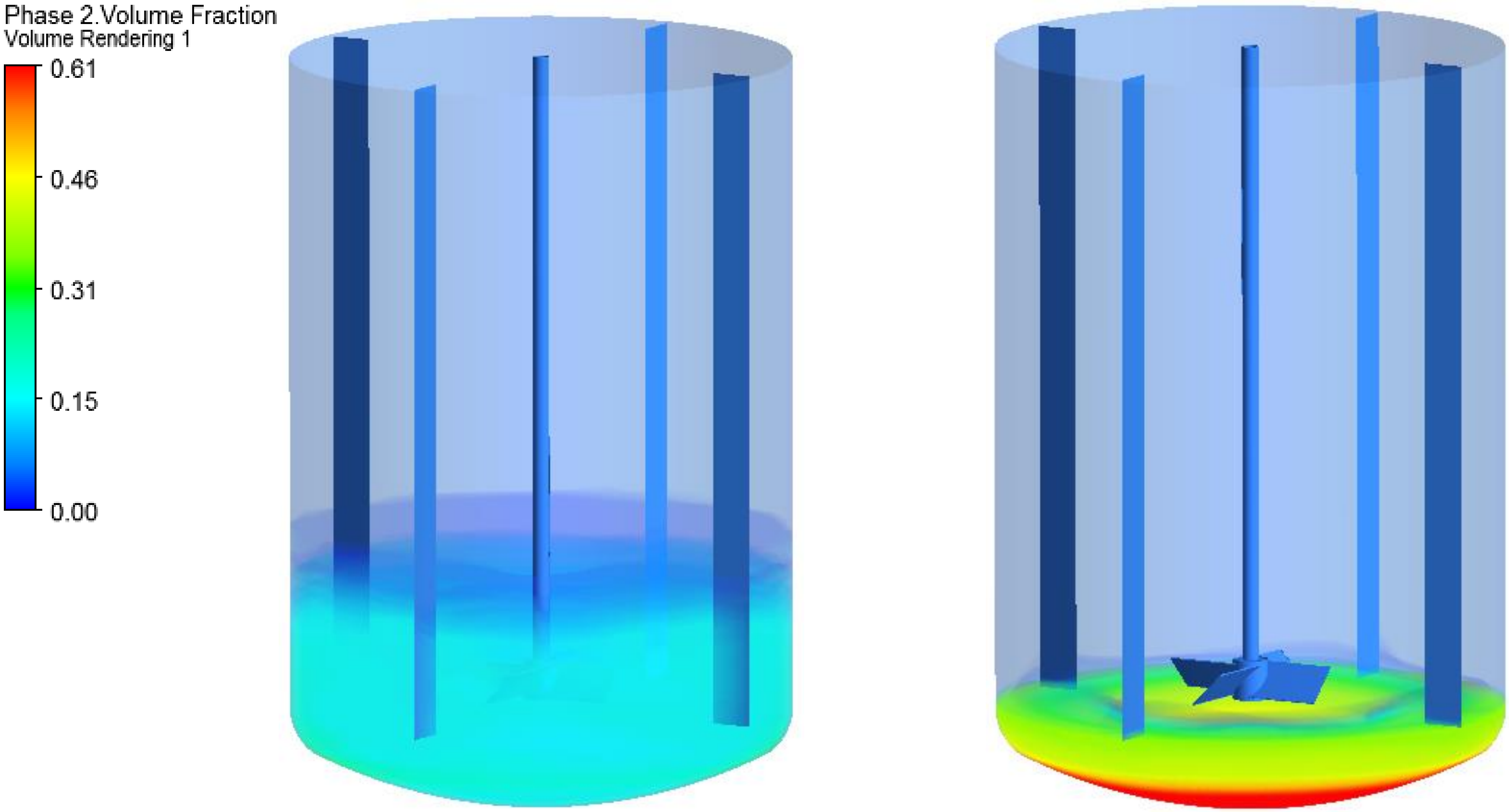


Experimental Details from BHR Group, UK

Case setup

- **Models**
  - **Eulerian Multiphase model**
    - Granular secondary phase
    - Gidaspow drag model
    - Simonin turbulent dispersion model
  - **Realizable k-epsilon turbulence model**
    - Mixture turbulence
- **Methods**
  - Node based gradient method
  - QUICK discretization method for momentum, volume fraction and turbulence

Effect of Turbulent Dispersion Force



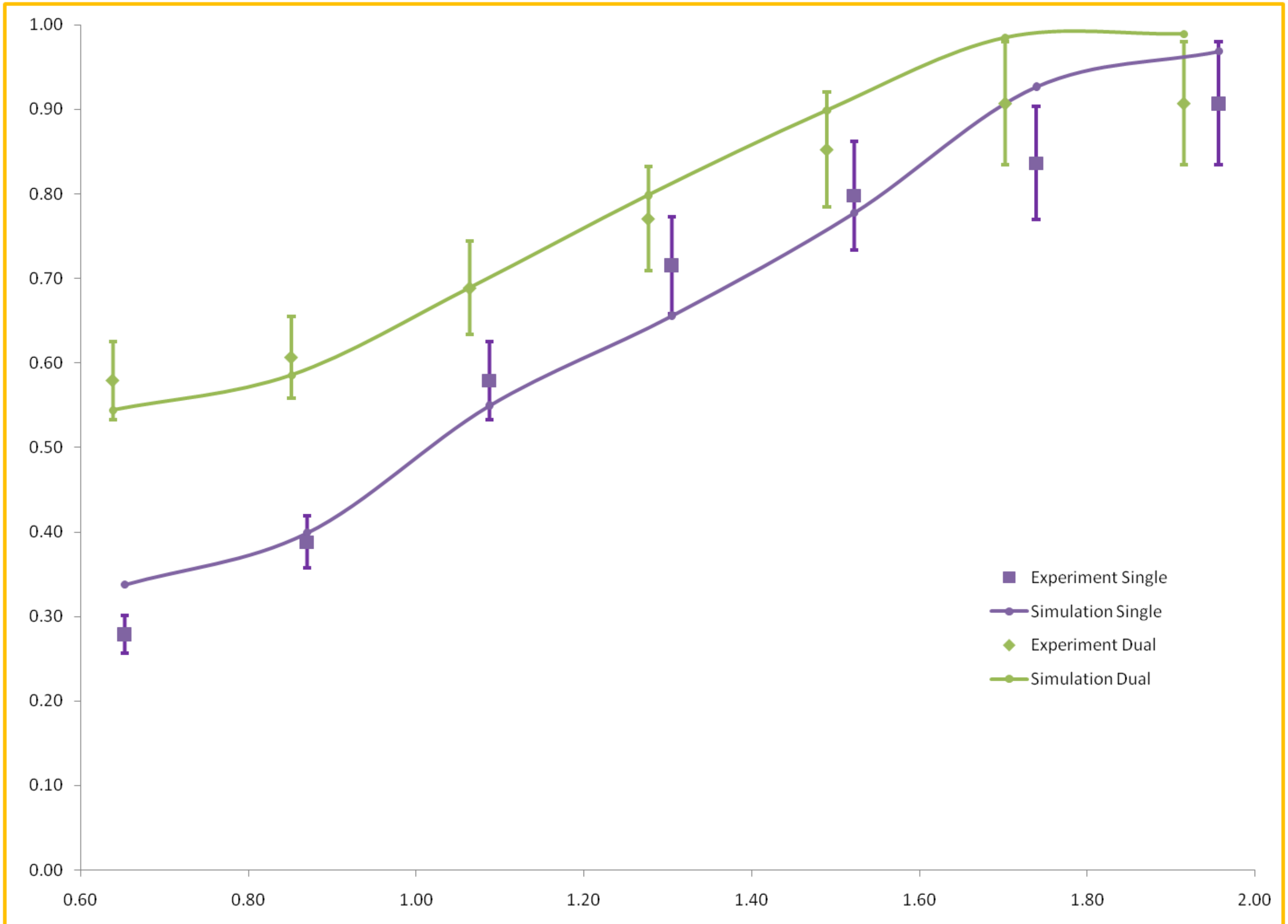
With TDF

Without TDF

Single Impeller, 150 RPM, 10% wt Loading

Case files are available for this study and can be shared

Plot for 10% wt loading

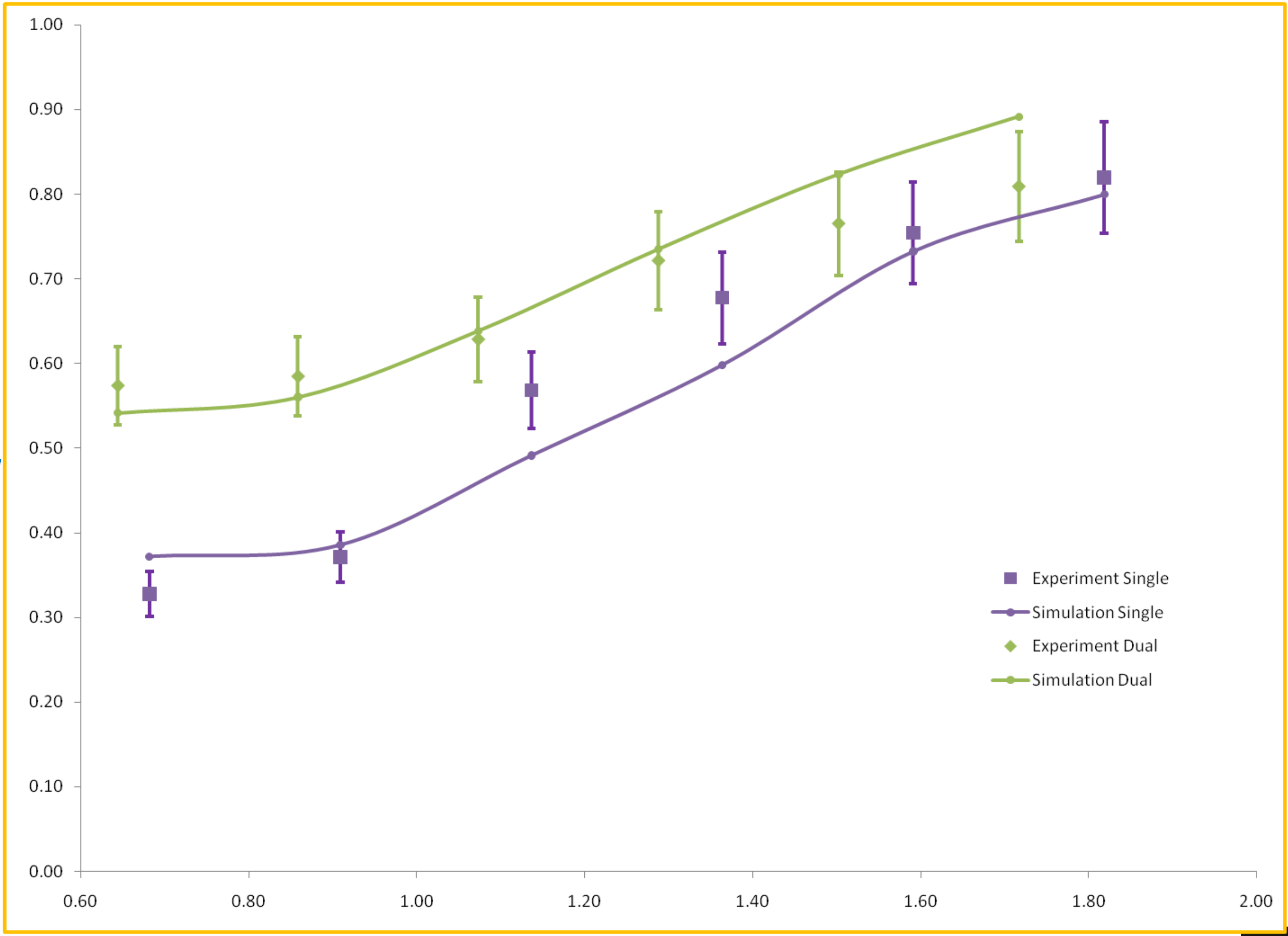


H_c/H

N/N_{is}

Case files are available for this study and can be shared

Plot for 15% wt Loading



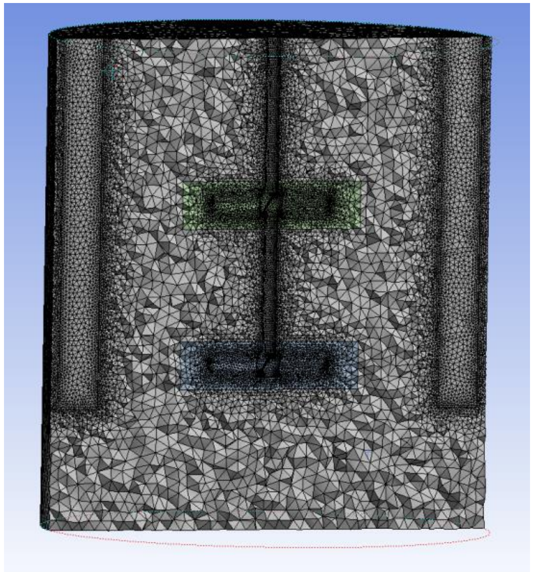
H_c/H

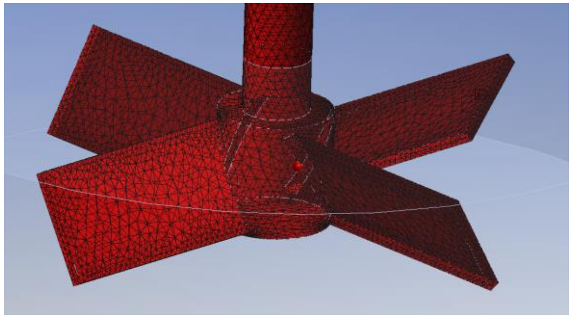
N/N_{is}

Case files are available for this study and can be shared

Meshing Guidelines

- **Mesh**
  - **Hexahedral cells if possible**
  - **Tetra/Polyhedra cells**
    - Polyhedra to reduce cell count with minimum/negligible loss of accuracy
  - **1-2 cells across impeller blade thickness is preferred**
  - **Boundary layers are needed for laminar flow regime**



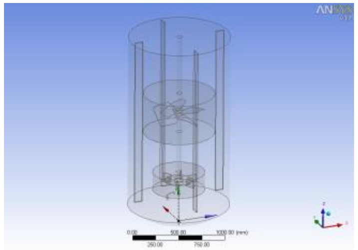


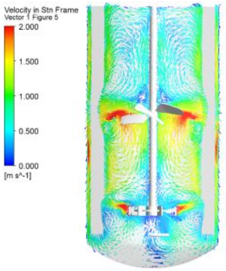
Agenda

- Mixing in process industry
- Mixing Modeling
- Physics in Agitated Vessels
- **Modeling tools**
- Summary

Modeling Options

Geometry & Meshing

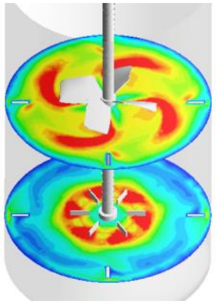




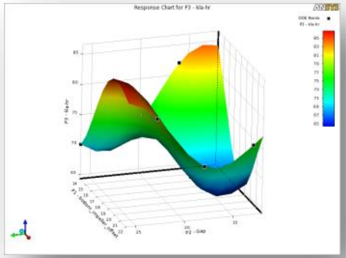
Solver

Mixing modeling tool

Post processing



Design space study



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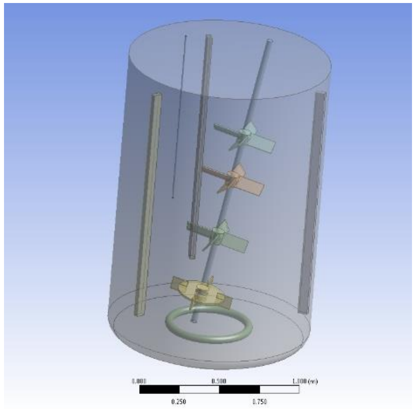
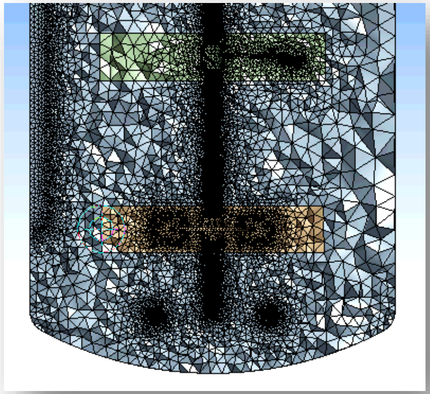
17.0 Release

MixingWizard

Mixing Wizard

- **ACT based customization tool for mixing**
  - **Automation of**
    - Geometry
    - Meshing
    - Solution setup
    - Postprocessing





MixingWizard: Postprocessing

A customized HTML Mixing Report is generated as part of post processing

Tabulated data for several parameters
- Torque, power, Froude number etc

Contours
- Flow, turbulence, Kolmogorov mixing length

Plots
- Blend time, RTD, Exposure

Animation
- Blend time

Mixing Report

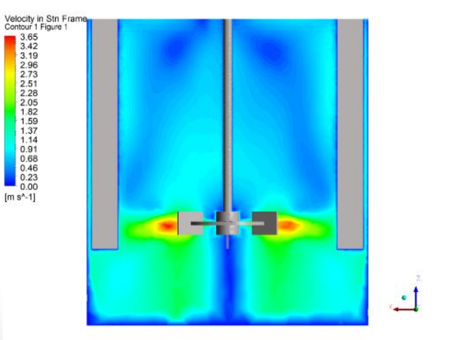
2. User Data

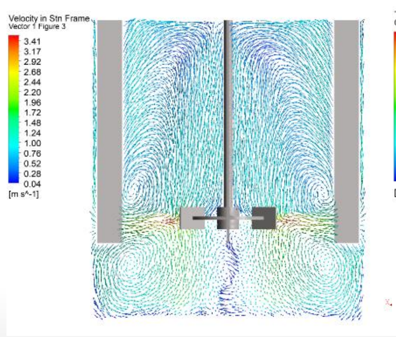
Table 2. Geometry Inputs

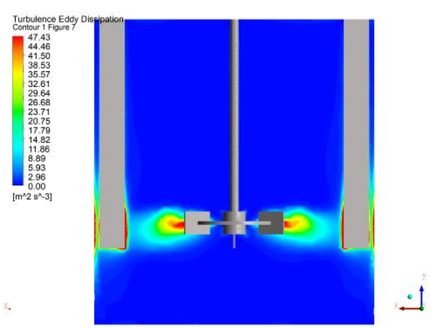
Tank Details										
Tank Shape	**Diameter**	**Height**	**Liquid Level**	**Bottom Type**	**Continuous Stirred Tank**					
Cylindrical	1.1m	1.3m	1.2m	Flat	No					
Shaft Details										
Diameter	**X Offset**	**Y Offset**	**Z Offset**	**Direction**	**Type**	**Shaft Inclined**	**Inclination Type**	**Alpha Angle**	**Beta Angle**	
0.035m	0m	0m	0.4m	Clockwise	Top Mounted	Yes	User Defined	0degree	0degree	
Impeller Details										
Diameter	**Z-Offset Type**	**Z Offset**	**Angular Offset**	**Type**	**Create Type**	**Pumping Direction**				
0.45m	User Defined	0.4m	0degree	Create Impeller	6RBT	Downward				
Baffle Details										
Number of Baffles	**Z Offset**	**Clearance from Wall**	**Height**	**Angular Offset (Anticlockwise)**	**Type**	**Width**	**Thickness**			
4.000e+00	0.3m	0.02m	1.05m	0degree	Flat	0.1m	0.01m			
Monitors Details										
Monitor Definition										
Automatic										
Feeds Details										
Feed Definition										
Automatic										

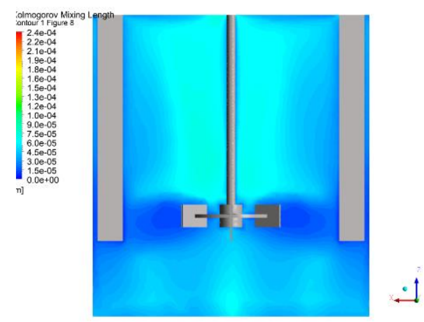
Variable	Value
	Impeller 1
Angurlar Velocity (RPM)	200.00
Tip Speed	4.71 [m s^-1]
Reynold's Number	703757.00
Torque [N-m]	117.30 [J]
Power	2456.64 [W]
Power Number	3.60
Froude Number	0.51
Overall Quantities	
Total Power	2456.640 [W]
Power/Volume	2169.730 [W m^-3]
Average Strain Rate	11.578 [s^-1]
Average Eddy Dissipation Rate	1.747 [m^2 s^-3]
Average Kolmogorov Mixing Length	4.402e-05 [m]
Average Micromixing Time Scale	0.036 [s]
Average Mesomixing Time Scale	0.147 [s]

Contours of flow variables

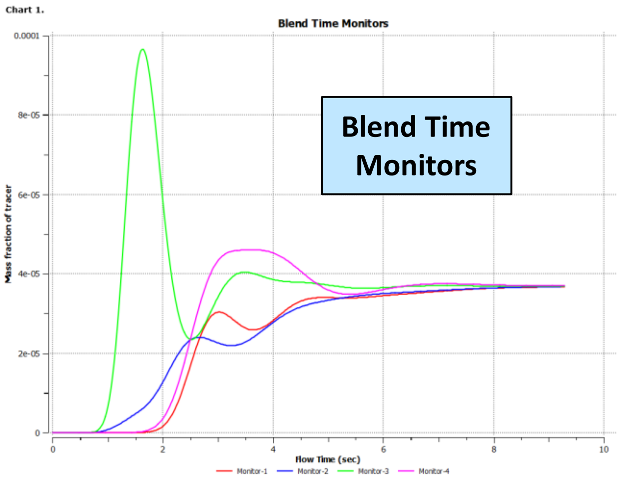








MixingWizard: Postprocessing



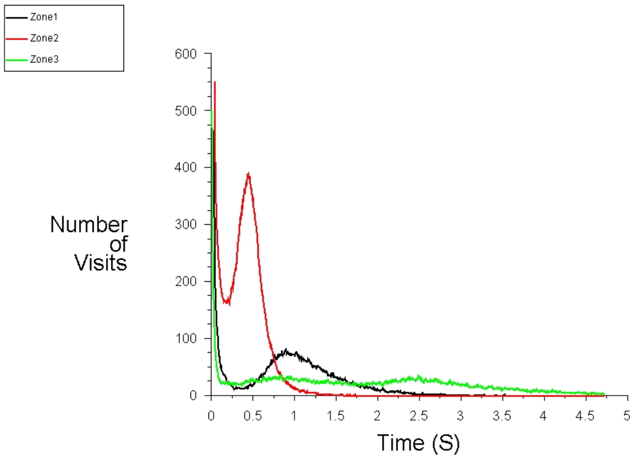
Blend Time Monitors

Quantitative Data

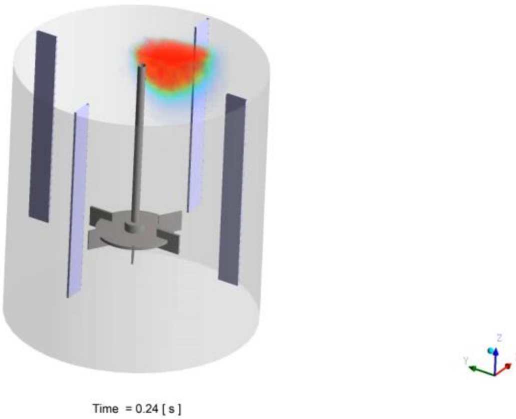
Table 3. Mixing Tank Quantitative Data

Mixing Tank Quantitative Data	
Variable	**Value**
	Impeller 1
Angurlar Velocity (RPM)	200.00
Tip Speed	4.71 [m s^-1]
Reynold's Number	703757.00
Torque [N-m]	117.30 [J]
Power	2456.64 [W]
Power Number	3.60
Froude Number	0.51
Overall Quantities	
Total Power	2456.640 [W]
Power/Volume	2169.730 [W m^-3]
Average Strain Rate	11.578 [s^-1]
Average Eddy Dissipation Rate	1.747 [m^2 s^-3]
Average Kolmogorov Mixing Length	4.402e-05 [m]
Average Micromixing Time Scale	0.036 [s]
Average Mesomixing Time Scale	0.147 [s]

Zonal Residence Time



Blend Animation



Agenda

- Mixing in process industry
- Mixing Modeling
- Physics in Agitated Vessels
- Downstream processes
- Study of Design Space
- Modeling tools
- **Summary**

Summary

- Simulation with CFD
  - is now an established method in process design.
  - helps planning and reducing experimentation and provides physical insight about particular behavior.
  - allows for the evaluation of new equipment prior to purchase.
- ANSYS tools can simulate the physical processes that need to be understood for process improvement, scale-up and design
- Advancements in interface design and solver technology are minimizing the knowledge/experience required to benefit from CFD.
- Mixing Wizard is a tool designed to provide automated workflows and results generation
- Different levels of simulation (single-phase, multi-phase, etc.) can be simulated based on required accuracy and insights needed into the physical process.

