# Validation Challenges in Industrial Computational Fluid Dynamics

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Computational Fluid Dynamics (CFD):
simulations to provide knowledge and understanding of gas, liquid, particulate and thermal flow

# Structure

- A few words about verification
- Validation
- What's special about validation of CFD simulations?
- What options do we have?
- Industrial case examples

# Definitions of Verification

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- In ‘How to Understand CFD Jargon’, NAFEMS defines verification as
  - The process of determining if a simulation accurately represents the conceptual model. A verified simulation does not make any claim relating to the representation of the real world by the simulation.
- Further, in the NAFEMS publication ‘What is Verification and Validation’, verification is defined as
  - The process of determining that a computational model accurately represents the underlying mathematical model and its solution
- In the ERCOFTAC Best Practise Guidelines, verification is defined as
  - The procedure to ensure that the program solves the equations correctly

# Validation or Verification

- We need to start from a verified solution
  - A mathematically acceptable solution
  - Converged
  - Mesh independent
  - Higher order schemes may be required

# Definitions of Validation

- In ‘How to Understand CFD Jargon’, NAFEMS defines validation as
  - The process of determining how accurately a simulation represents the real world.
- Further, in the NAFEMS publication ‘What is Verification and Validation’, validation is determined as
  - The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
- In the ERCOFTAC Best Practise Guidelines, validation is defined as
  - The procedure to test the extent to which the model accurately represents reality

# What is Validation?

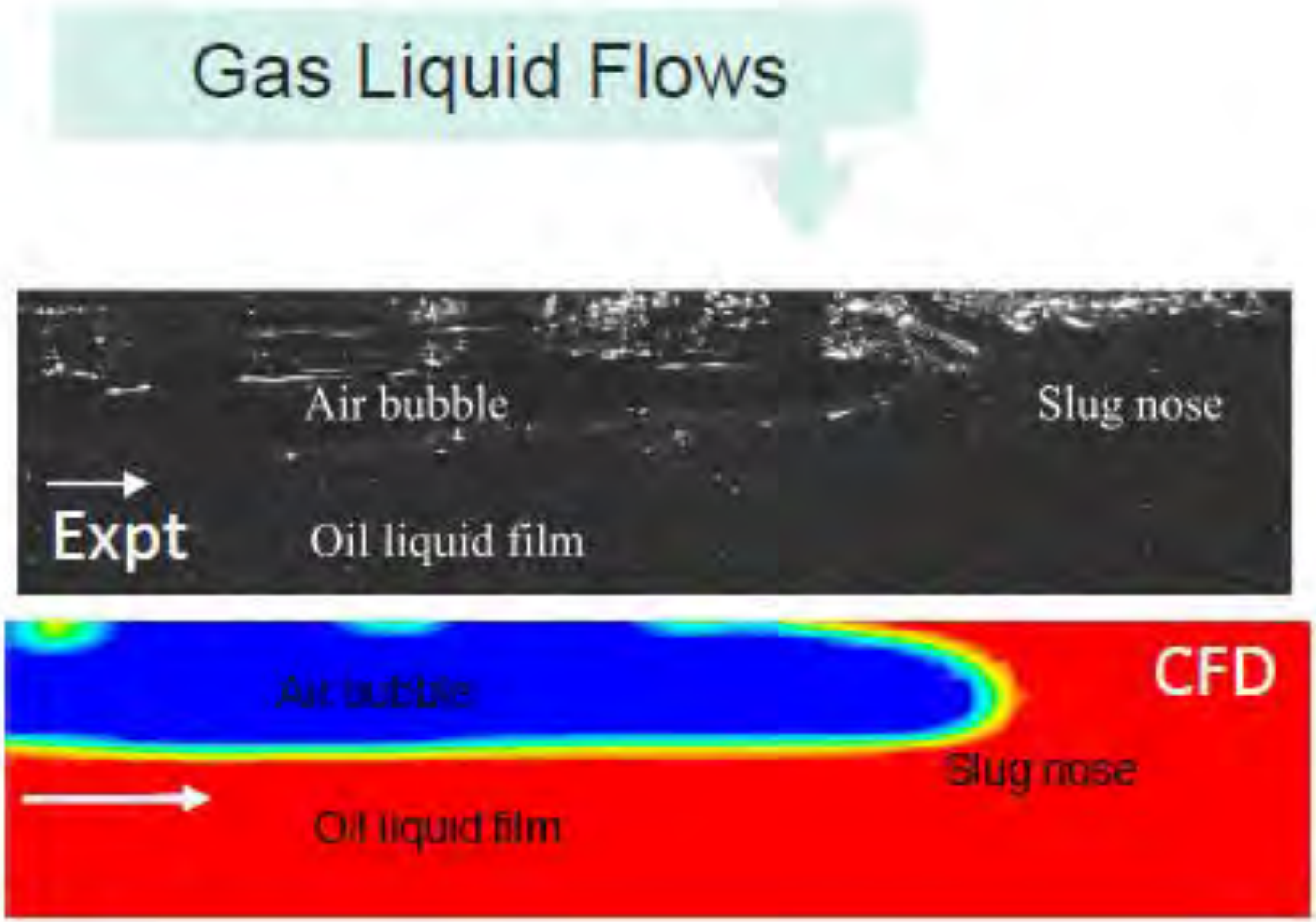
- Purists, working in the early days of (structural) engineering analysis would claim that validation requires the precise analytical solution against which the results of a simulation may be compared
- This is unhelpful for many classes of problem and engineering applications, particularly in an industrial context
- From some perspectives, if we can calculate a precise analytical solution, then a simulation is unnecessary

# Practicalities

- The fundamental requirement is to determine how closely a simulation represents the behaviour it is attempting to capture.
- If we can determine that behaviour in some way, it can be used as a comparison for the simulation results.
- The most obvious solution is to take measurements of what happens in the physical world.

- This in itself can be problematic. For the flow of fluids and heat transfer, the behaviour can be difficult to observe.
- In many cases the introduction of measurement equipment can alter the behaviour of the flow so unless the measurement equipment can remain in place during operation and also be included in any simulations, it may be considered of limited use.
- Qualitative data may be the best option – using imaging techniques

# Multiphase flows

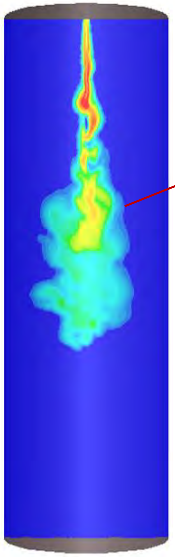


# Pharmaceutical manufacturing

Active Pharmaceutical Ingredient (API) is precipitated out by dissolving supercritical anti-solvent (usually $CO_2$) into the API solution.

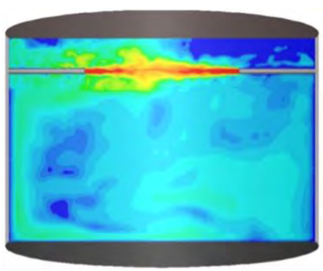
*PSD is a strong function of the jet dispersion characteristics*

- Challenges:
  - Predicting physical properties such as density and viscosity of supercritical fluid
  - Thermodynamic modeling of mixture properties

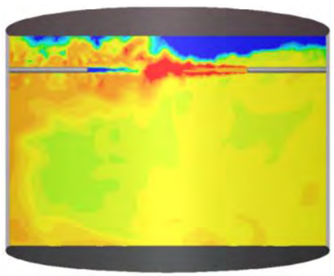


Jet Dispersion characteristics studied using advanced CFD models

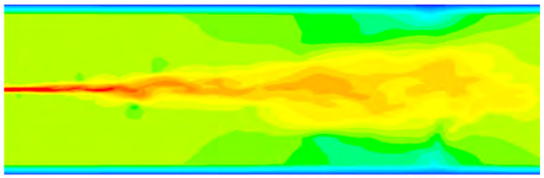
Contours of density



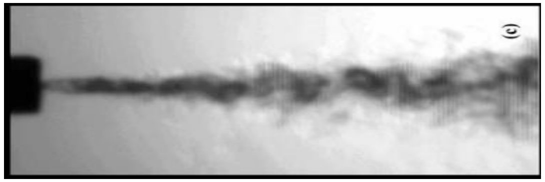
Contours of velocity for impinging jet system



Contours of density for impinging jet system



CFD predictions by Tridiagonal



Experiments of Badens et al. (2005)‡

*Successfully predicted density variation of the API solvent & supercritical $CO_2$*

‡ Source: Badens, E., Boutin, O., Charbit, G., 2005. Laminar jet dispersion and jet atomization in pressurized carbon dioxide. *Journal of Supercritical Fluids* 36, 81-90.

# Validation options

- These challenges have led engineers to use a variety of techniques for validation
- Often to use a number of them are used in combination to provide confidence in the results of simulations.
- If the behaviour of interest is difficult to measure, it may be that other features of the flow can be measured which can provide confidence in the simulation as a whole.
- Alternative simulation tools and approaches may be used and compared.
- Hand calculations can provide insight into expected behaviours and ball park values.
- Where measurements of the industrial application are not possible due to size or safety issues, smaller scale controlled experiments can prove useful.

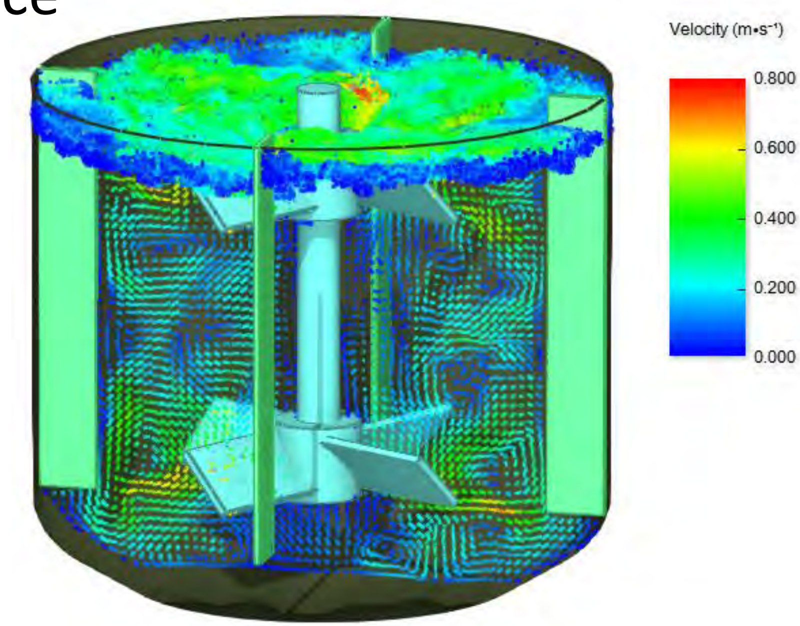
# Examples

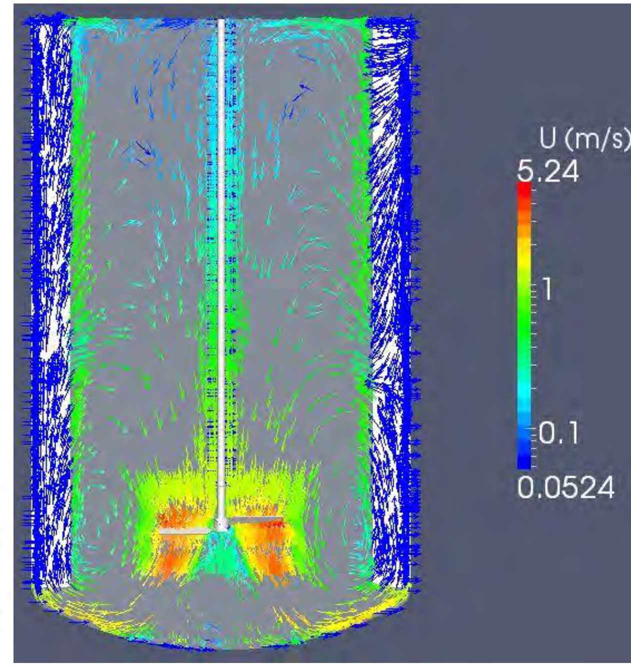
- To provide
  - Ideas
  - Insight
  - Inspiration
  - Confidence
  - Reassurance

# Stirred Tank Reactors

Several challenges

- Moving geometry
- Multiphase
- Turbulent
- Free surface
- Transient



# Problem Definition

- Customer currently uses CFD methodologies to perform quick 2D simulations based on ANSYS-FLUENT
- The team is now interested in developing a tool to perform automated 3D flow analysis in stirred reactors using OpenFOAM
- They would like to benchmark the results obtained using open source tools. The results will be compared with commercial CFD solvers

# Objective

- Objective is to benchmark results obtained using OpenFOAM for stirred tank simulations for three cases as follows

| | Case - 1 | Case - 2 | Case - 3 | Units |
|---|---|---|---|---|
| Tank Diameter | 3000 | 3000 | 6000 | [mm] |
| Total Liquid Height | 5000 | 3000 | 12000 | [mm] |
| Bottom Shape | ASME F&D | Flat | ASME F&D | |
| Lower Type | A200 | R100 | A310 | |
| Upper Type | None | None | A310 | |
| $D_{Lower}$ | 1000 | 1000 | 2000 | [mm] |
| $D_{Upper}$ | N/A | N/A | 2000 | [mm] |
| Impeller Speed | 100 | 125 | 68 | [RPM] |
| OB | 1000 | 1000 | 1500 | [mm] |
| Space | N/A | N/A | 4500 | [mm] |
| Coverage | 4000 | 2000 | 6000 | [mm] |
| Viscosity | 1 | 20 | 10 | [cP] |
| Density | 1000 | 1000 | 1000 | [kg/m$^3$] |

- All three tanks are to have four standard on wall baffles
- Width equal to 10% of tank diameter
- Baffles can run from bottom tangent line (or floor) through the top of the liquid level

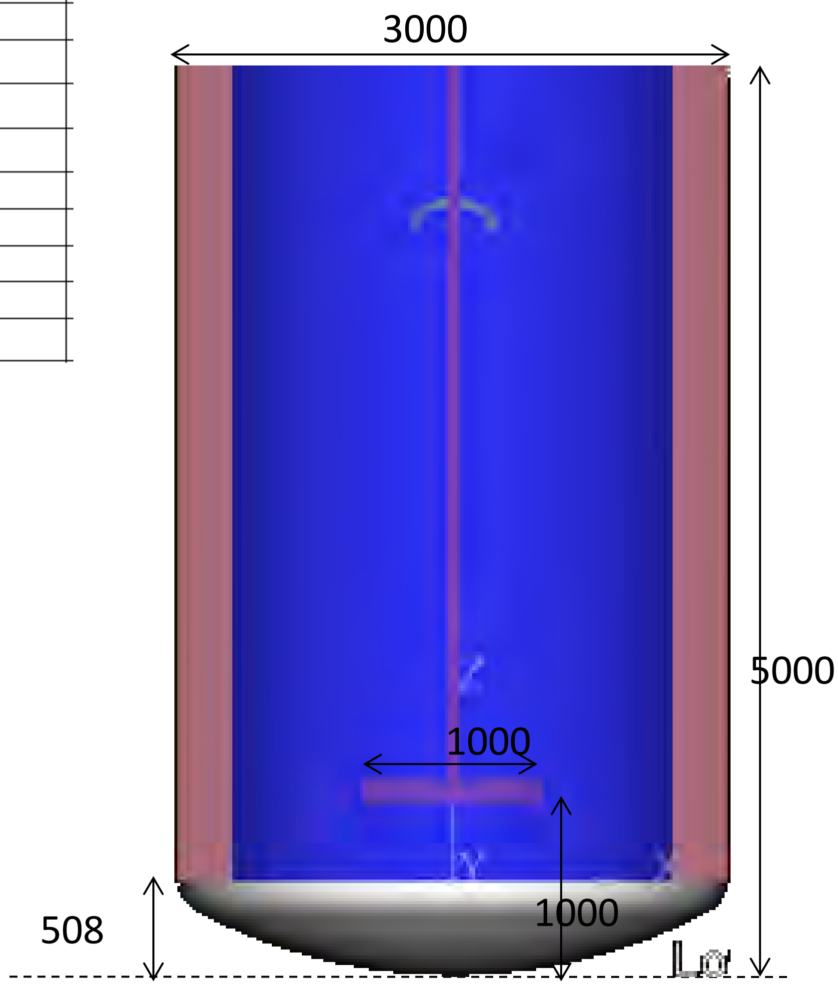
- What results to match.
  - Moving objects
  - Time varying velocity field
  - Averaged data over time is used
  - Power Number and Flow Numbers: Where to record Flow Numbers
- Single phase cases with MRF
- Top surface modelled as slip/symmetry vs Free Surface
  - VOF is time and compute intensive
- Single vs Multiple Impeller sets
  - Their impact on results
  - Transient behaviour

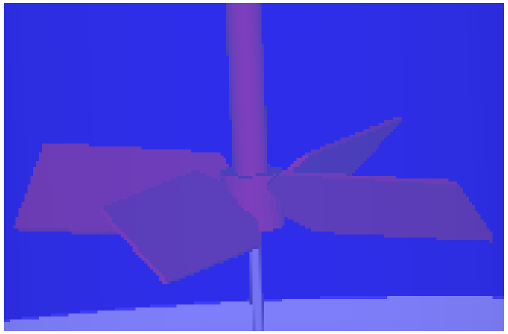
# Solution Approach

- Prepare closed 3D model based on the geometry details provided by the customer
- Generate a good quality mesh (1.5 – 4 M cells) using snappyHexMesh
  - The areas of higher gradient will be refined as appropriate
- Solve for steady-state, single-phase flow using customized Foam solver
- Verify the convergence based on residuals and solution monitors
- Analyze the results in the form of graphical and alphanumeric data for key areas of interest
  - Flow pattern, power consumptions, flow number, power number, etc.

# Case – 1 : Geometry

| | Case - 1 |
|---|---|
| Tank Diameter | 3000 |
| Total Liquid Height | 5000 |
| Bottom Shape | ASME F&D |
| Lower Type | A200 |
| Upper Type | None |
| $D_{Lower}$ | 1000 |
| $D_{Upper}$ | N/A |
| Impeller Speed | 100 |
| OB | 1000 |
| Space | N/A |
| Coverage | 4000 |
| Viscosity | 1 |
| Density | 1000 |



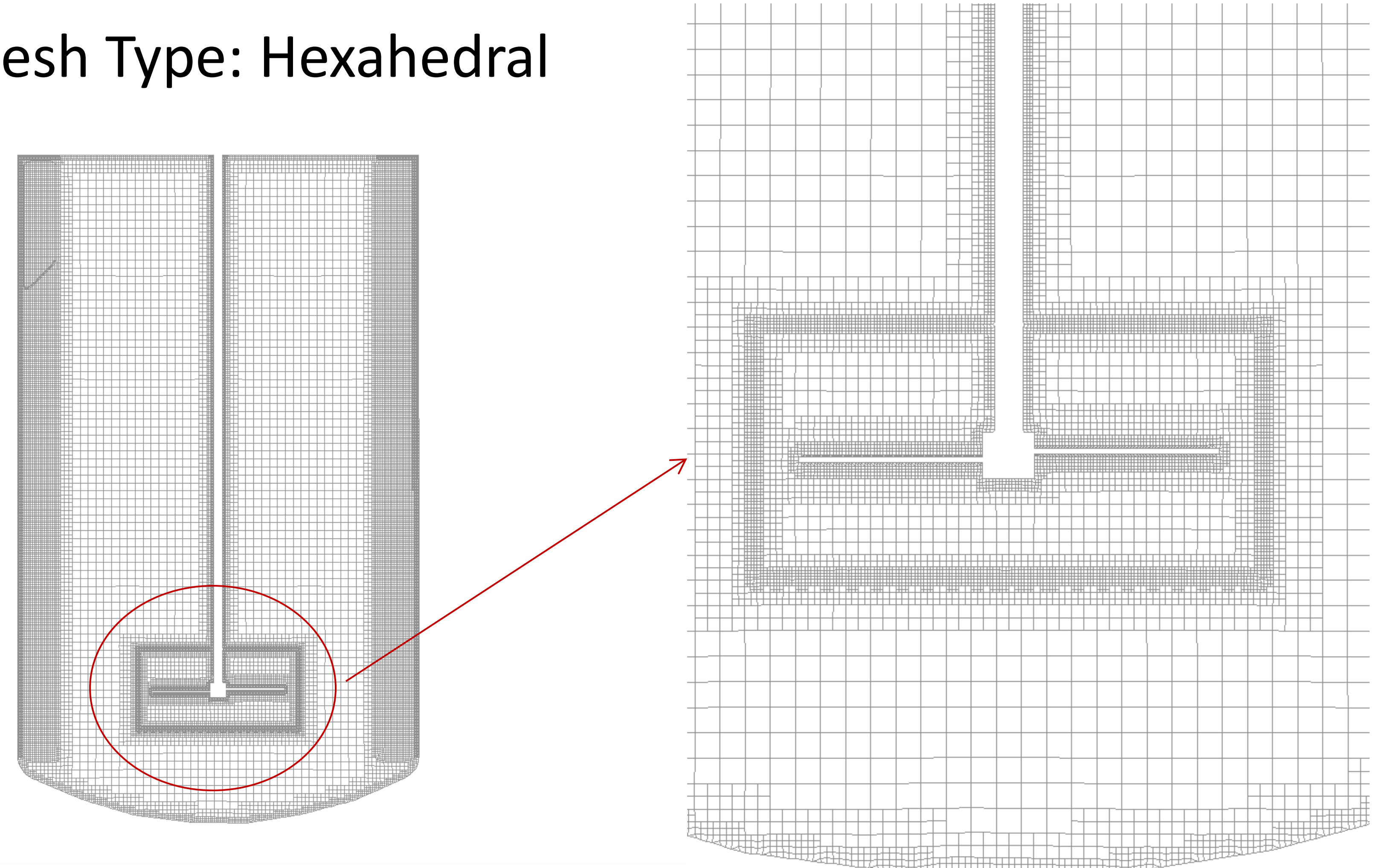



**Impeller – A200**

**All dimensions in 'mm'**

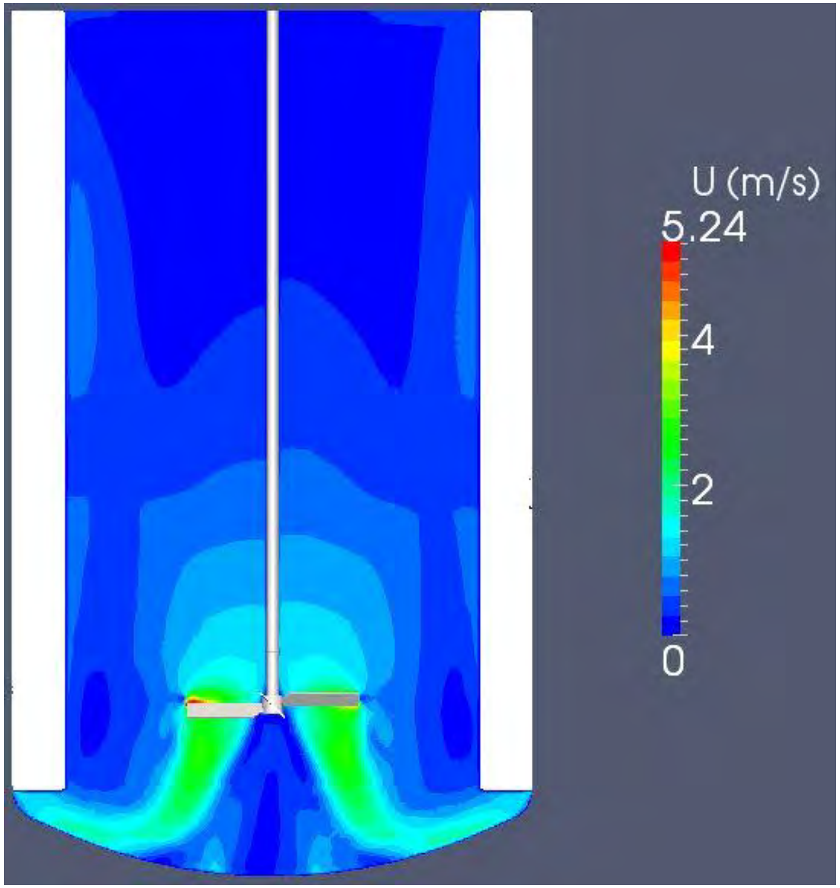
# Case – 1 : Mesh Details

- Mesh size: 2.2 Million
- Mesh Type: Hexahedral

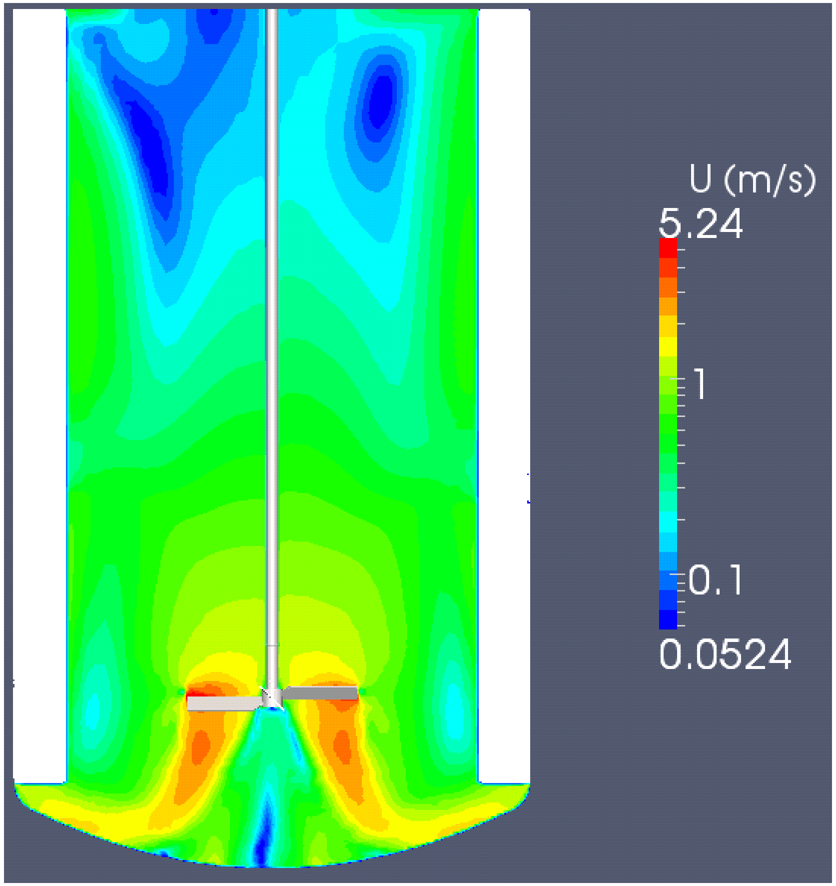


# Case – 1 : Results

- Velocity Contours (m/s)




Linear Scale




Logarithmic Scale

# Case – 1 : Results…

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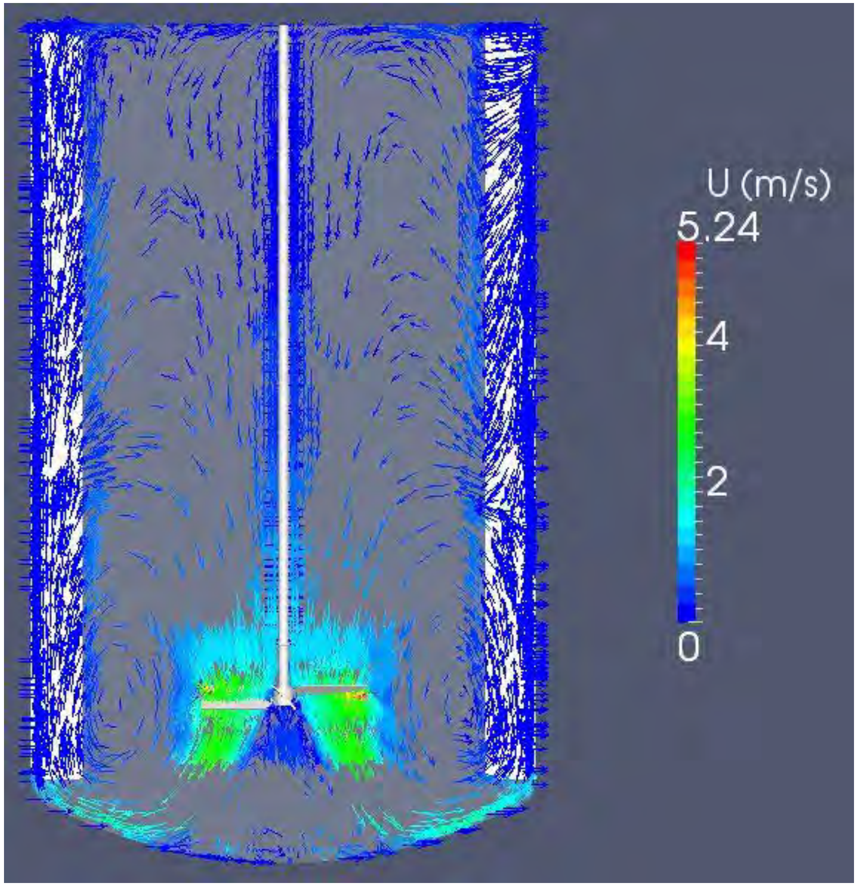
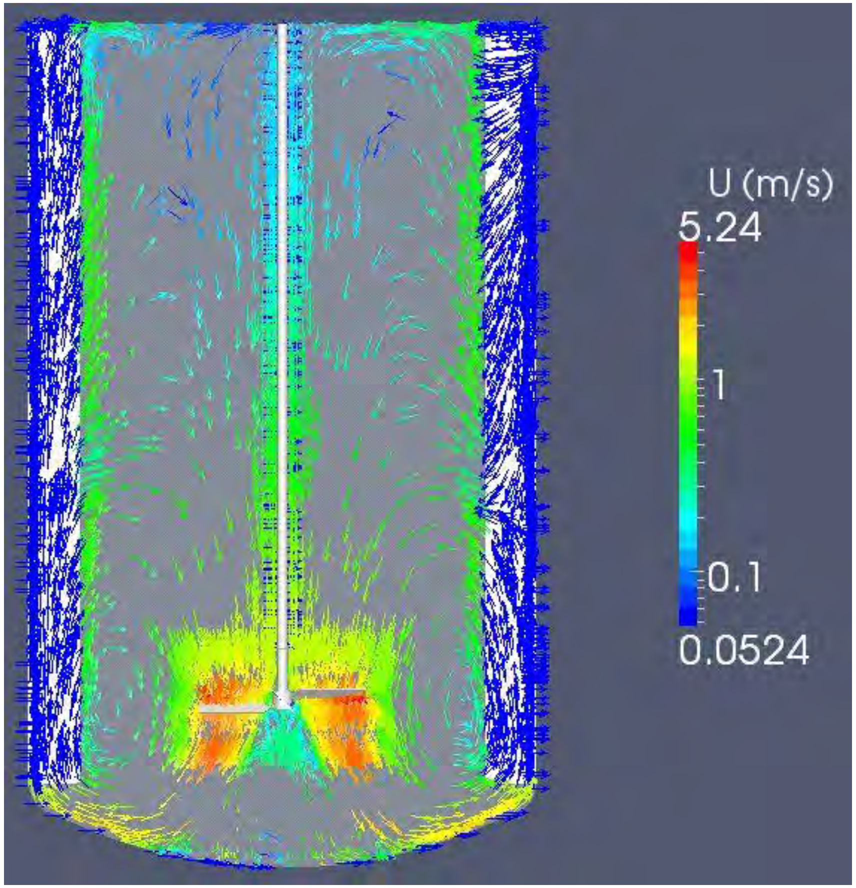
- Velocity Vectors (m/s)



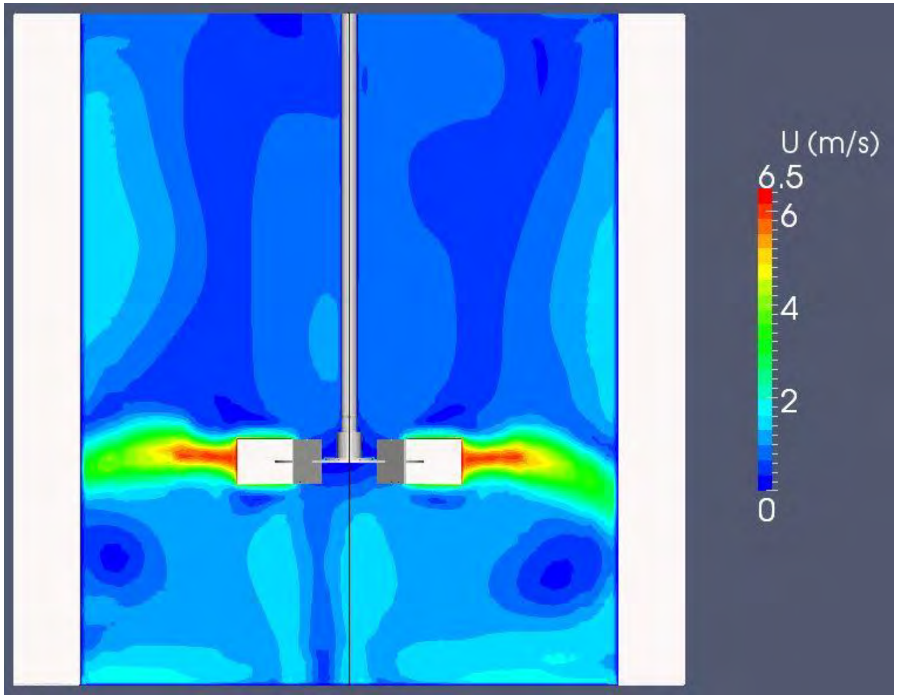




Linear Scale

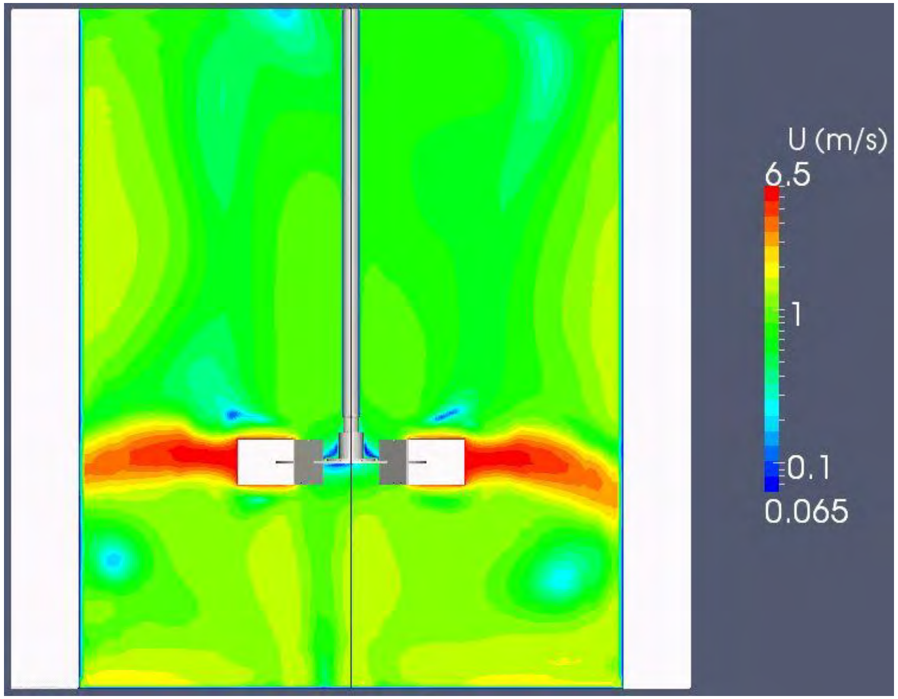
Logarithmic Scale

# Case – 2 : Results

- Velocity contours (m/s)




Linear Scale




Logarithmic Scale

# Case – 2 : Results…

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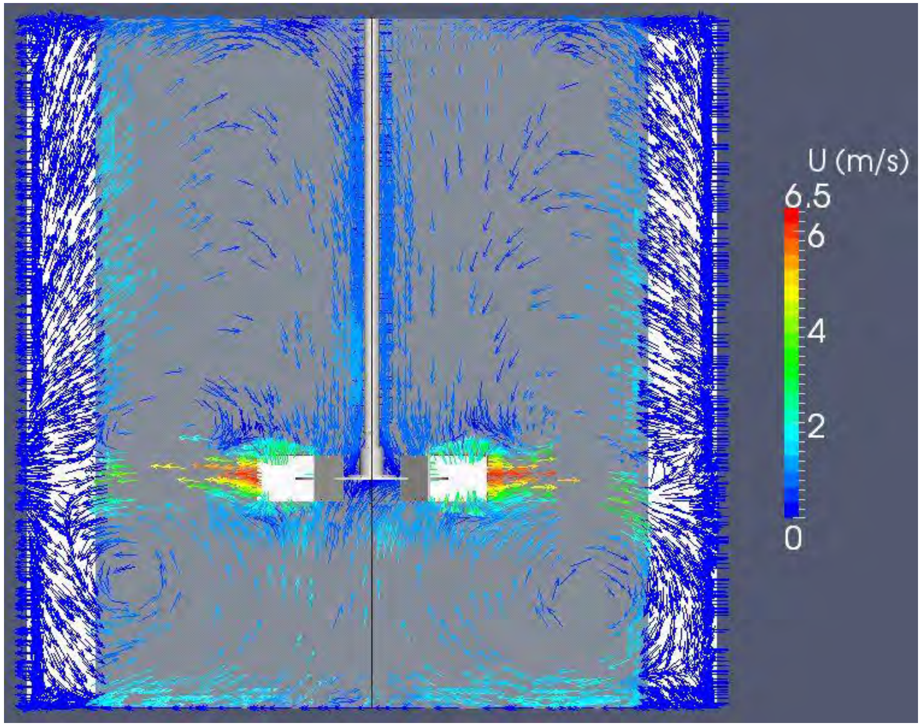
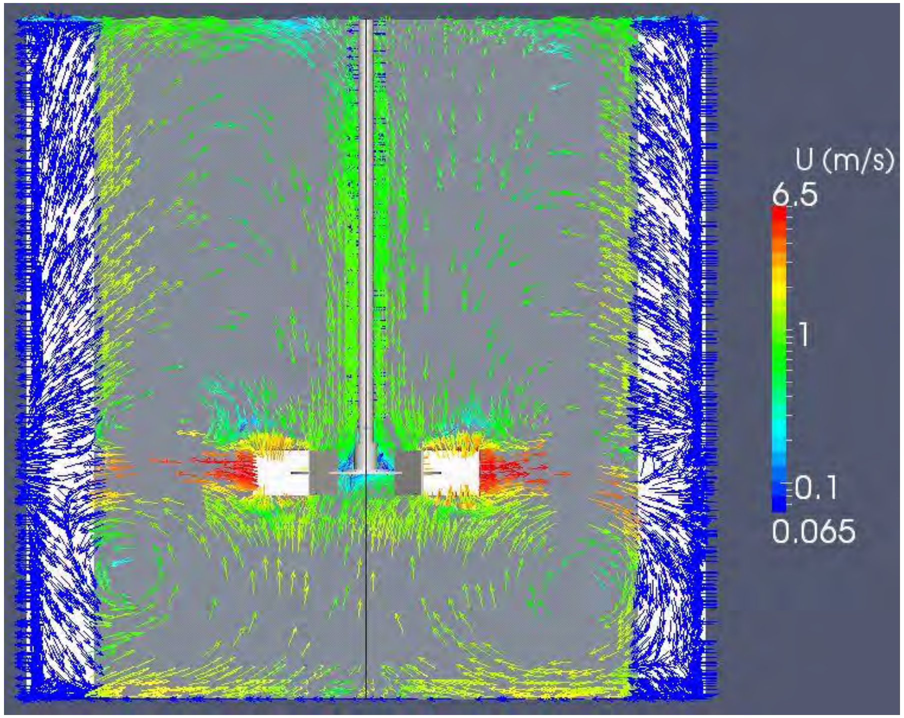
- Velocity Vectors (m/s)



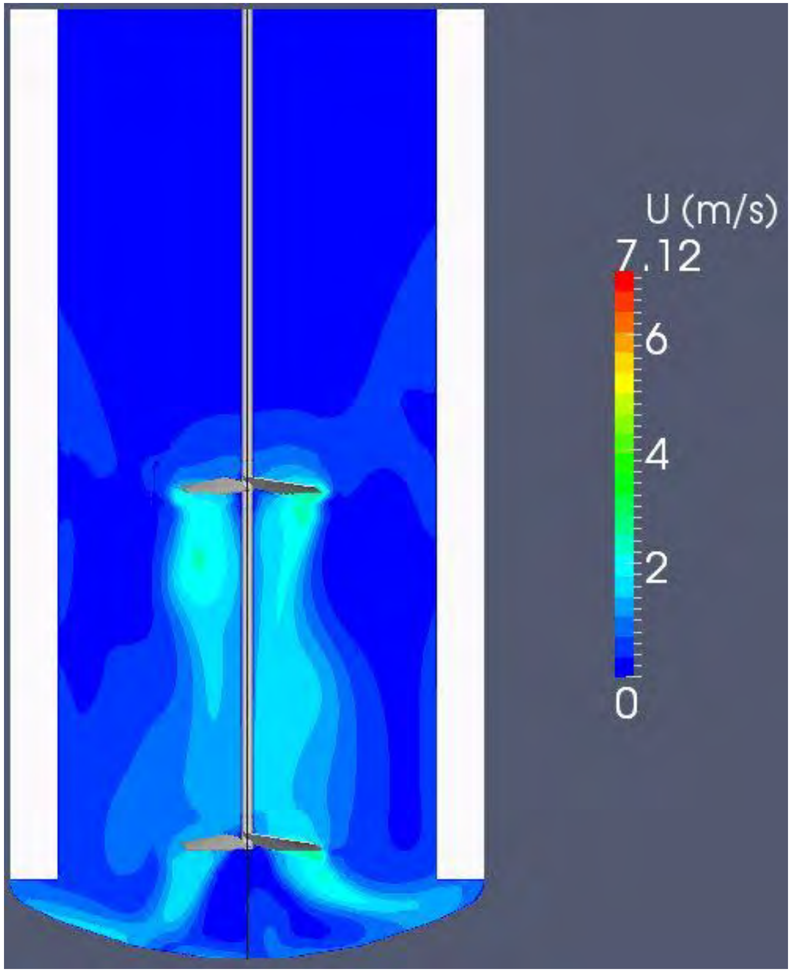




Linear Scale

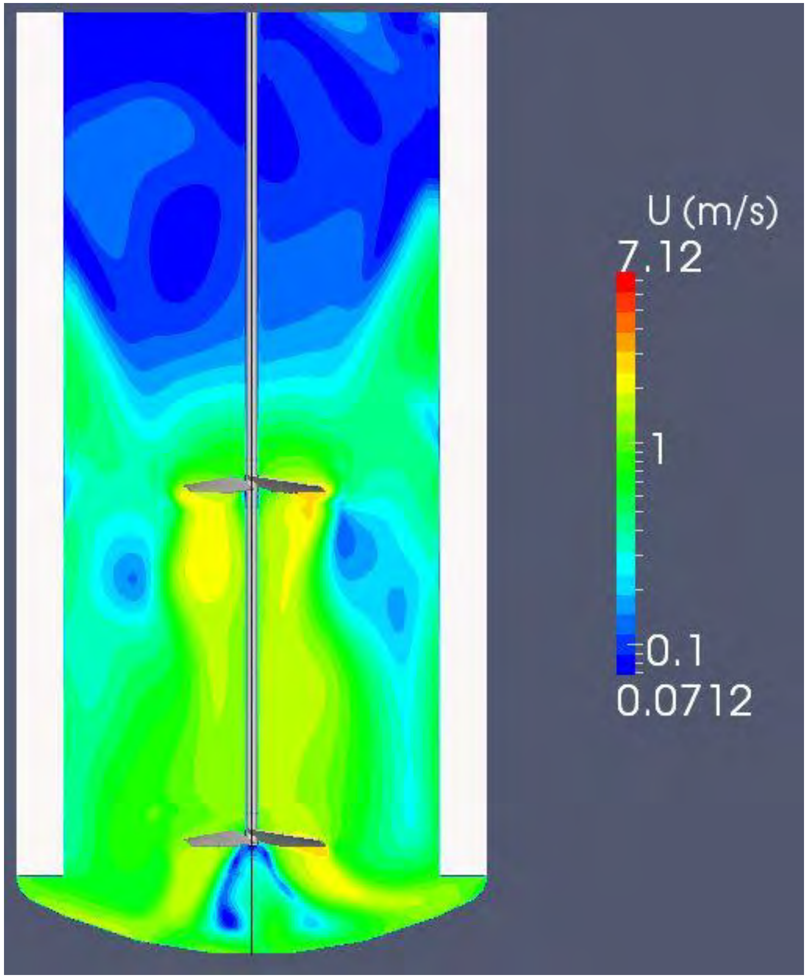
Logarithmic Scale

# Case – 3 : Results

- Velocity contours (m/s)



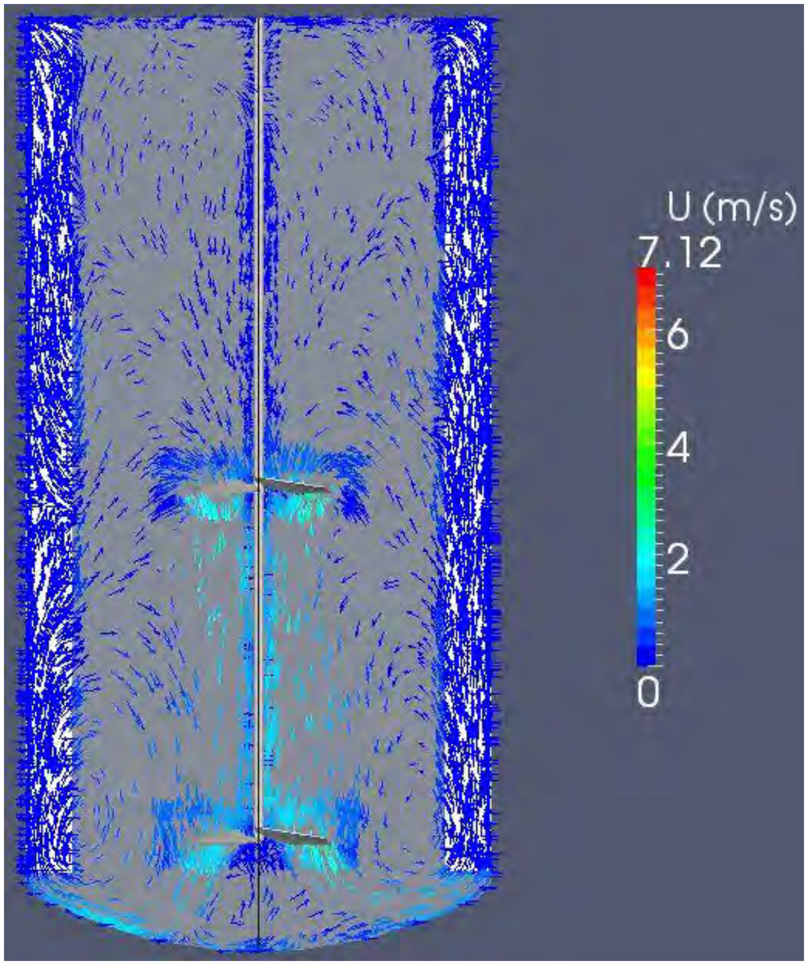

Linear Scale



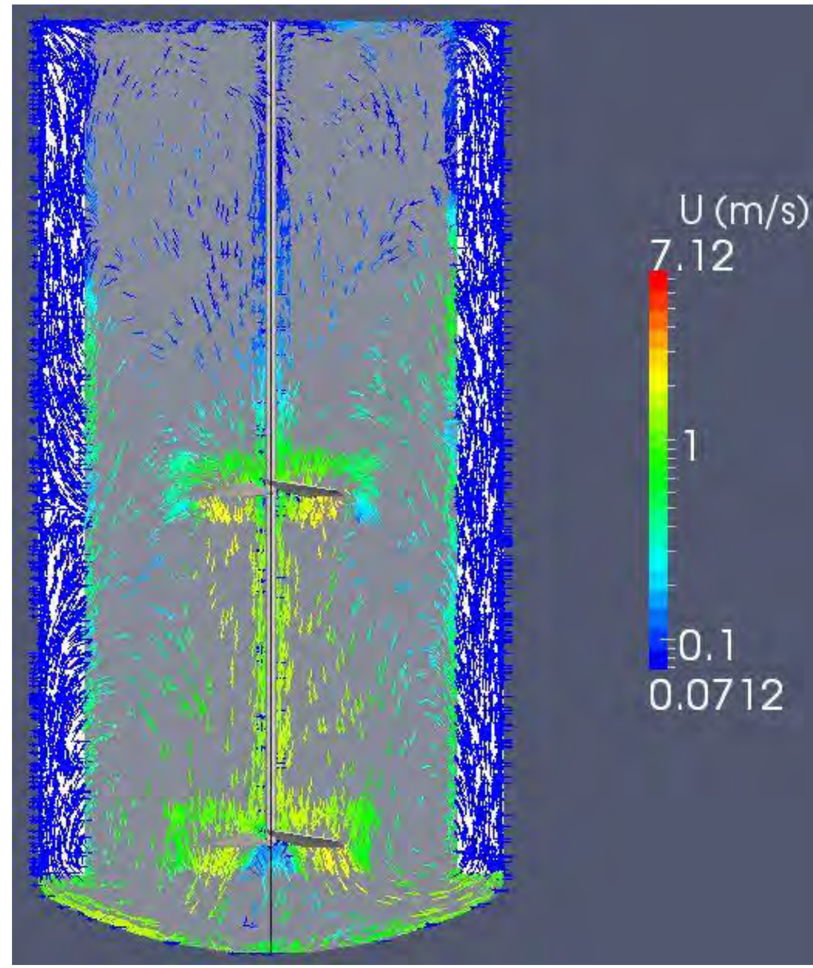

Logarithmic Scale

# Case – 3 : Results…

- Velocity Vectors (m/s)




Linear Scale




Logarithmic Scale

# Results…

- Performance Parameters

| Parameter | Case 1 | Case 2 | Case 3 (bottom) | Case 3 (top) |
|---|---|---|---|---|
| Tip Speed (m/s) | 5.24 | 6.54 | 7.12 | 7.12 |
| Power Number | 1.22 | 5.2 | 0.28 | 0.27 |
| Flow Number | 0.84 | 0.85 | 0.39 | 0.46 |
| Power Cons (kW) | 5.65 | 47.02 | 13.04 | 12.58 |
| P/V (kW/m3) | 0.166 | 2.22 | 0.078 | |

Case-1 and Case-2 matched experimental data *(unable to publish)*

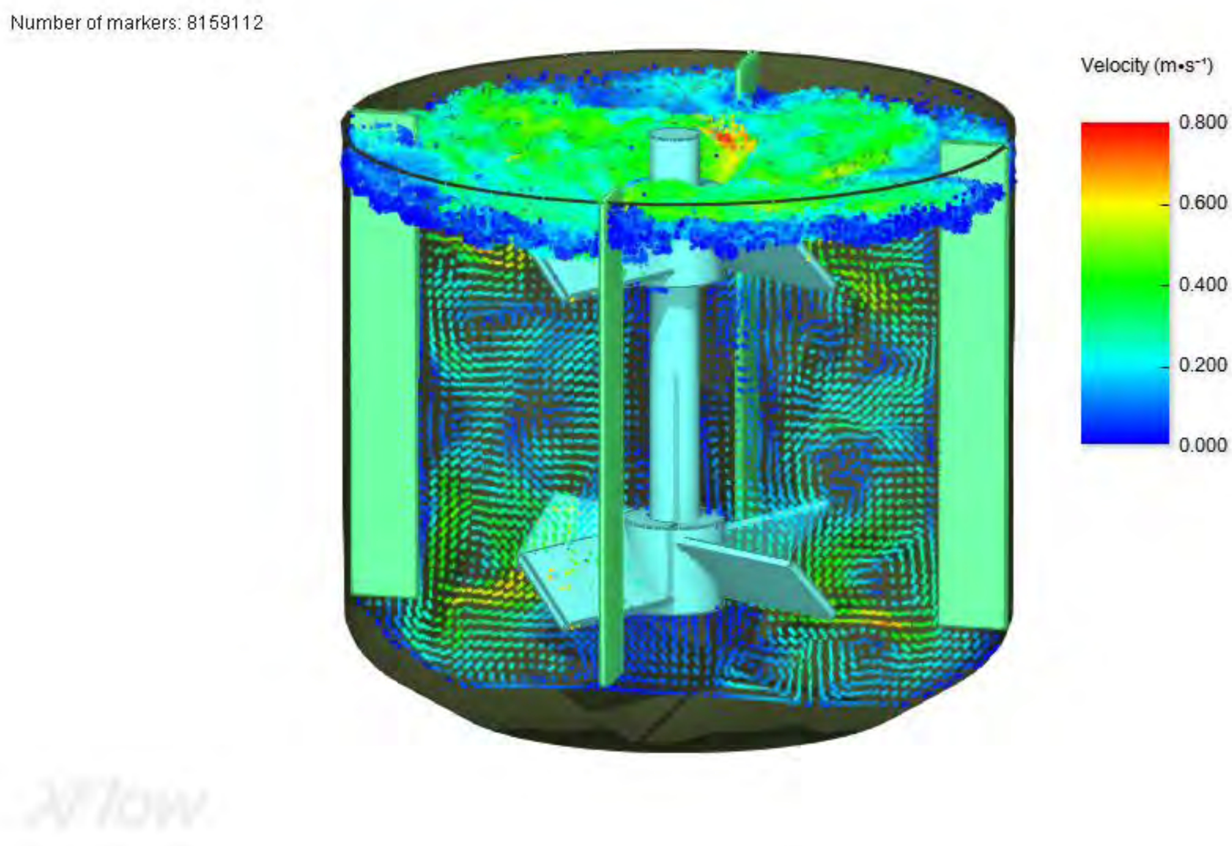
Hence case-3 should also be a good match if the same approach is used (even with a new geometry)

**Need to use best practices plus experience**

# Stirred Tank Reactors

Additional validation can be taken from alternative simulation types and different sets of assumptions, such as this lattice-boltzmann simulation

- Single phase
- Free surface

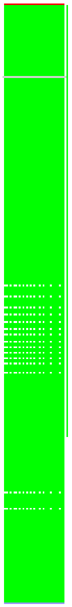


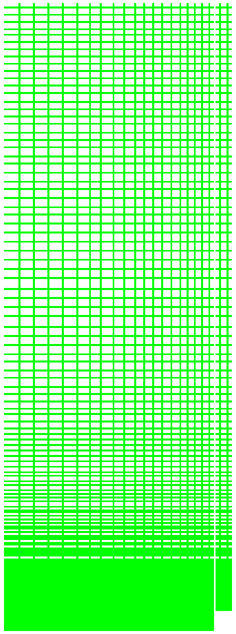
# Boiling Simulations: Objectives

- To implement wall boiling model along with the auxiliary functions as described by Koncar and Krepper (2008)
- To evaluate the model using the example described in Koncar and Krepper (2008)
- Review published information on CFD modeling of wall and bulk boiling
  - "CFD simulation of convective flow boiling of refrigerant in a vertical annulus", Bostjan Koncar, Eckhard Krepper, Nuclear Engineering and Design, 2008

# 2D Axis Symmetric Simulations

- A 2D section along with the metal tube was considered for simulations
- Geometry was meshed with complete Quad cells
- Fine mesh of total cell count
  - 13260 cells generated





# Case setup

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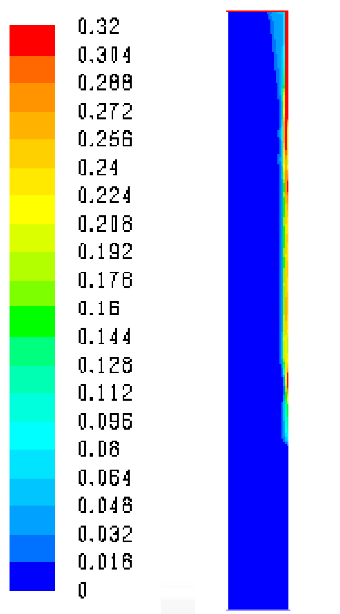
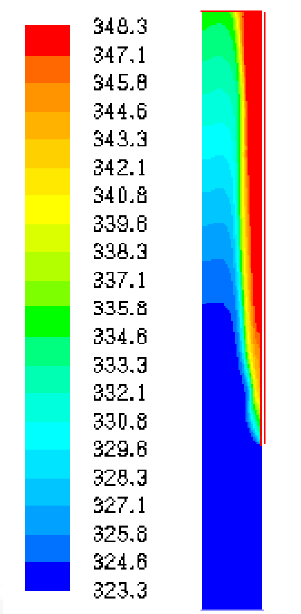
- RNG k-ε turbulence with standard wall functions
- The E-E multiphase model
- Working fluid is R-113
  - Operating pressure 2.69 bar
- Constant bubble diameter of 1.2mm was considered
- Unsteady solver was used
- Inlet boundary conditions
  - Constant velocity and temperature was set
- Outlet boundary conditions
  - Pressure outlet with 0 gauge value

# Results

- Simulations was iterated in unsteady solver to achieve steady state solution
- Quantity of vapor generated increases as we move from bottom to top
- Less bubbles are pushed to the side



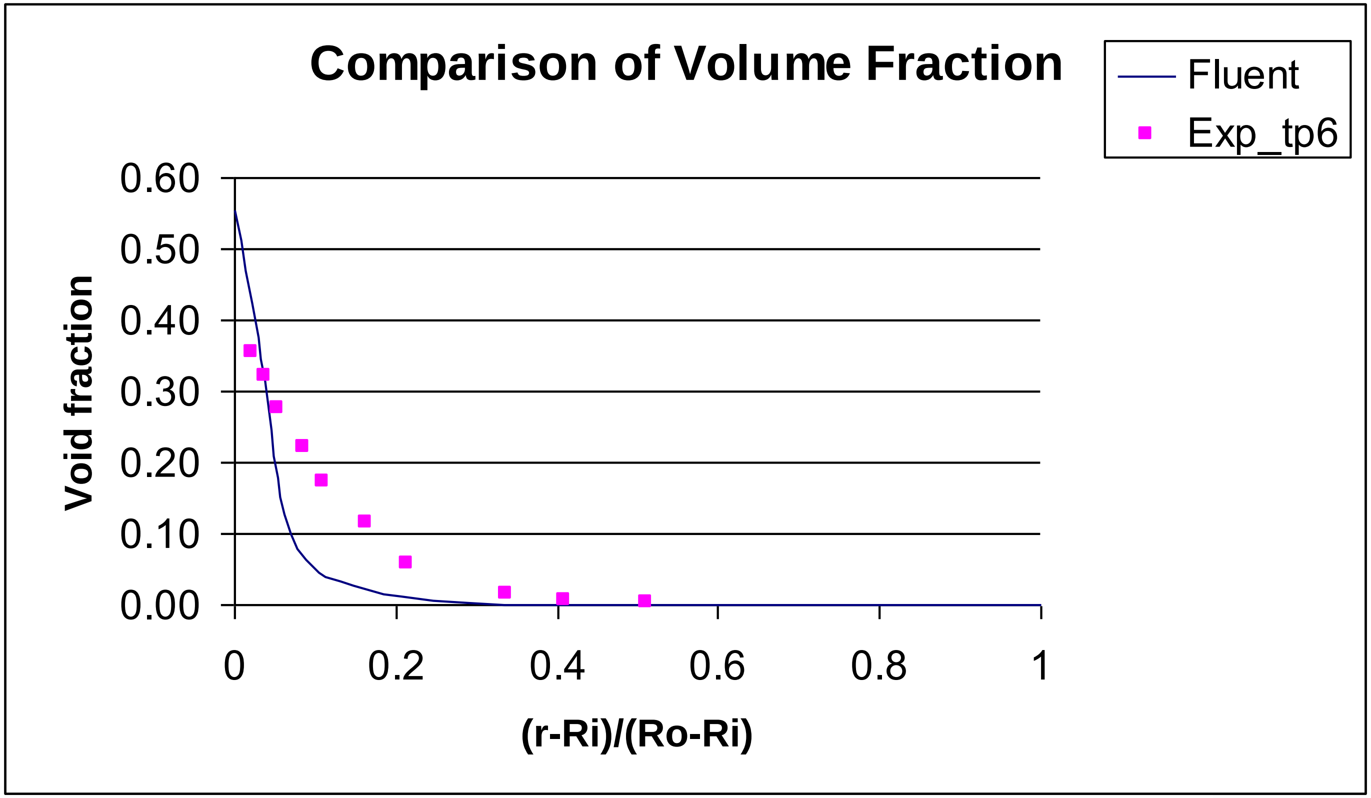



# Results..

- To compare the results presented by Koncar and Krepper radial profiles at the specified axial location were considered. Following results were compared:
  - Volume fraction of vapor
  - Liquid velocity
  - Gas velocity
  - Liquid temperature

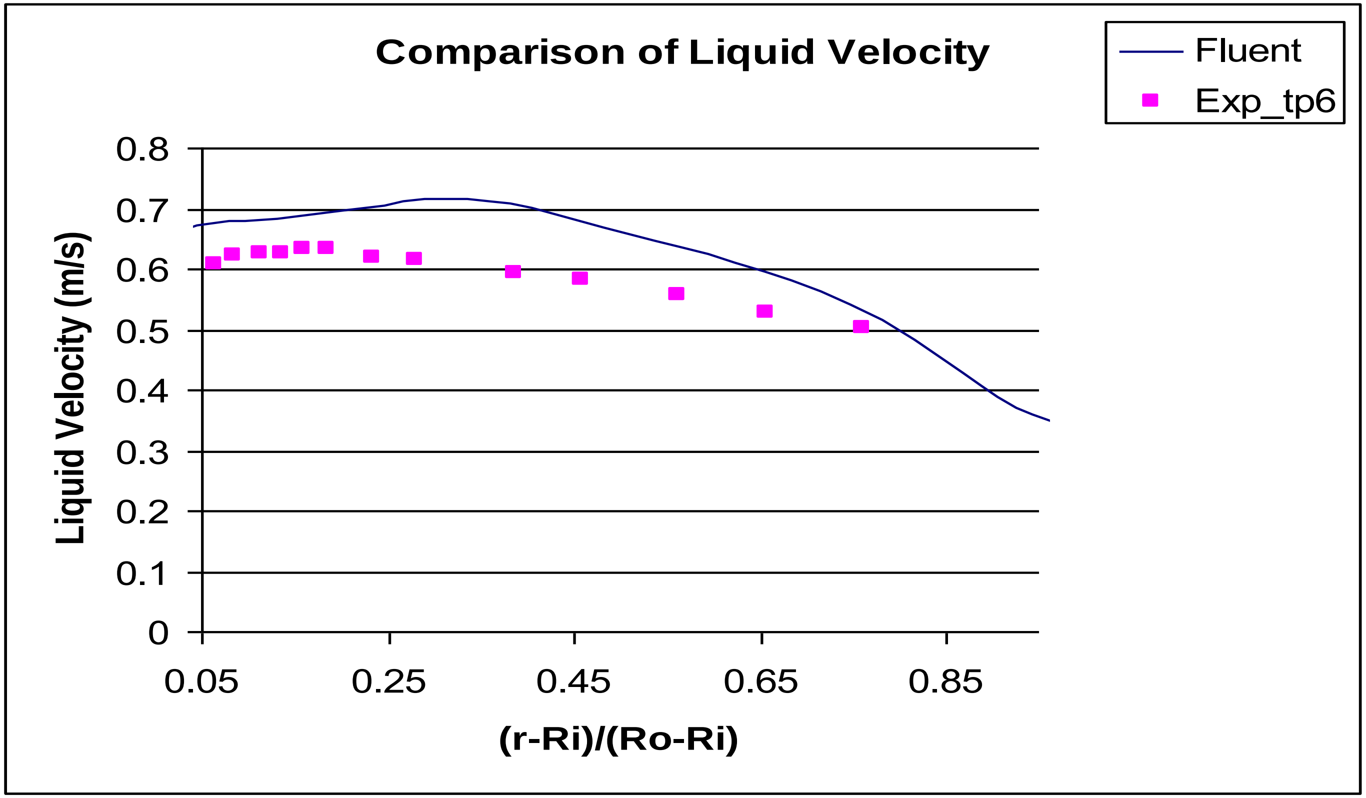
# Comparison of Void Fraction

- The trend is captured well
- Void fraction in the bulk is under predicted and near the wall is over predicted



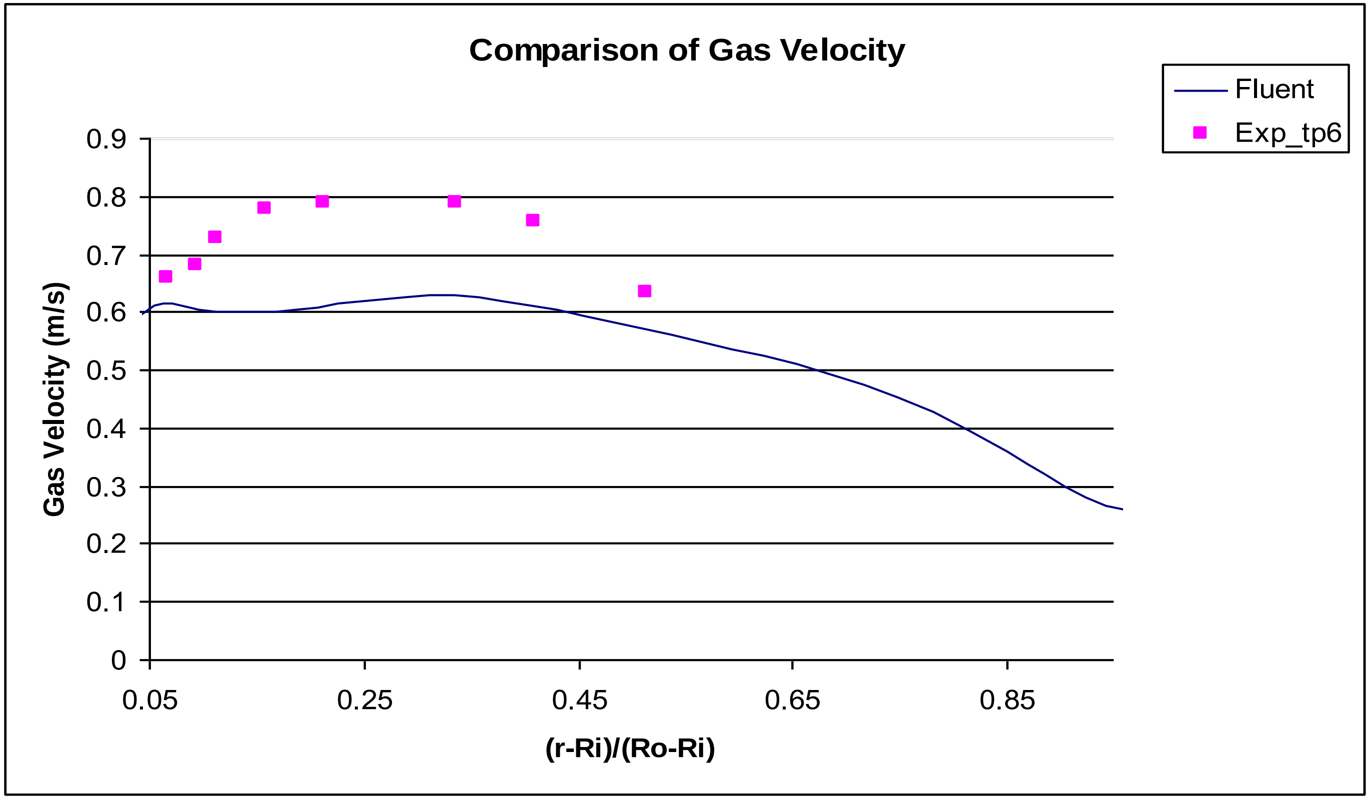
# Comparison of Liquid velocity

- Trend is captured well
- However liquid velocity is slightly over predicted



# Comparison of Gas Velocity

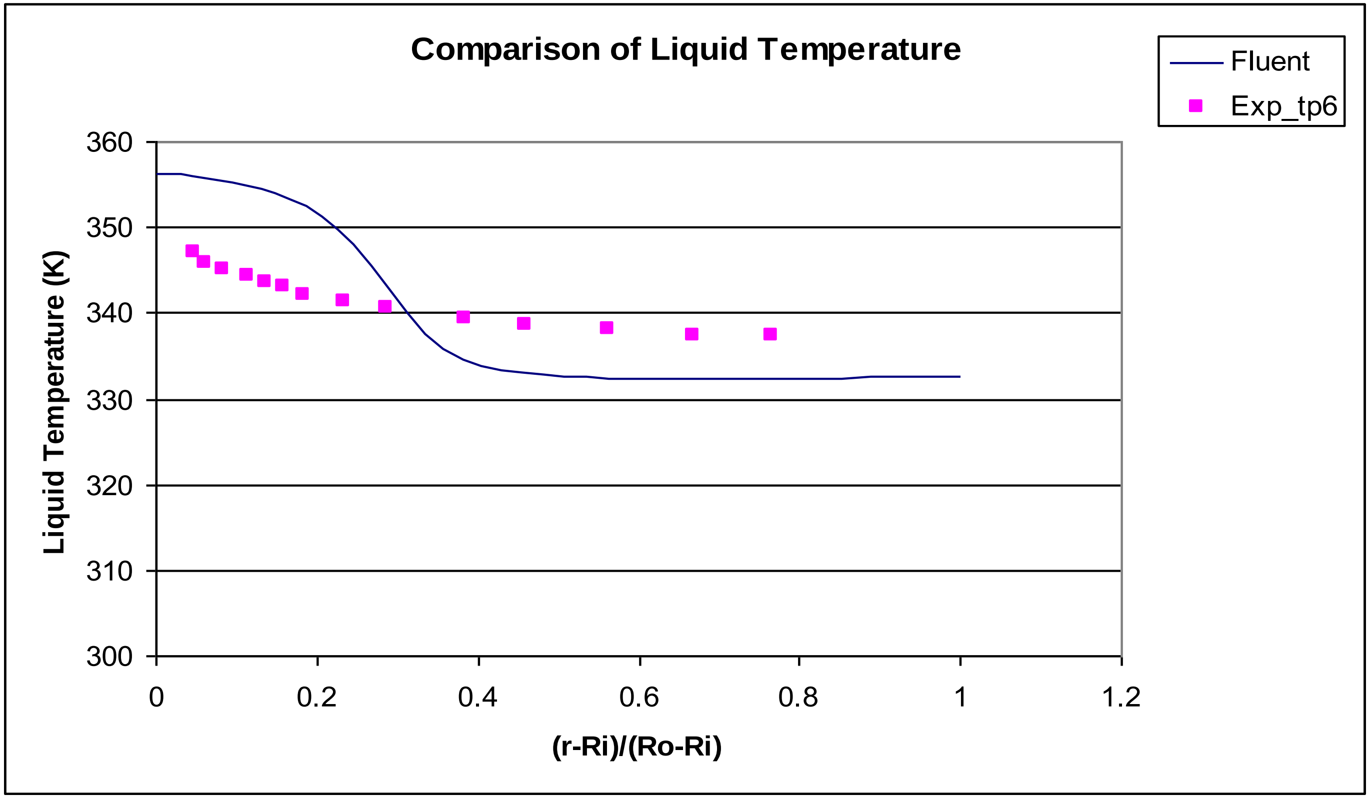
- Gas velocity is under predicted



# Comparison of Liquid Temperature



- Near wall temperature is over-predicted (and bulk region temperatures are under-predicted)



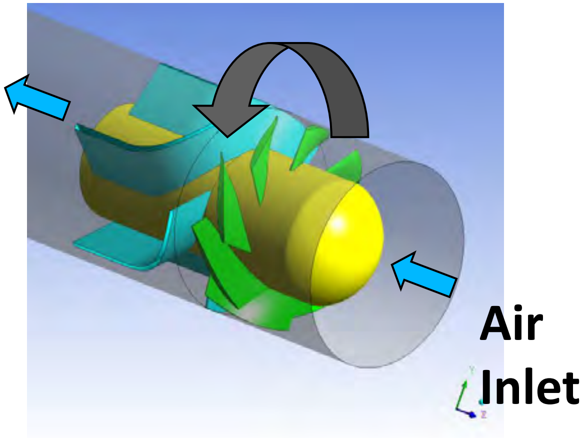
# Comments

- Note that in these cases, the comparison with experimental results is considered good
- These are difficult conditions for measurements
- They are advanced simulations
- This level of correlation is considered good for advanced CFD

- Different degrees of correlation are considered good for different analysis types
  - i.e. single phase CFD vs linear FEA vs phase change CFD vs crack propagation etc etc

## Problem Description

- Axial fan operating at high rpm, delivers air to free atmosphere
- Objective of Simulation
  - Study flow through the fan
  - Validate noise generated due to turbulence & rotor-stator interaction
  - Improve fan design to reduce noise




- Operating Conditions:
  - Speed: 10000 rpm
  - Head: 6” of water
  - Flow Rate: 1250 CFM

# Experimental Noise Determination

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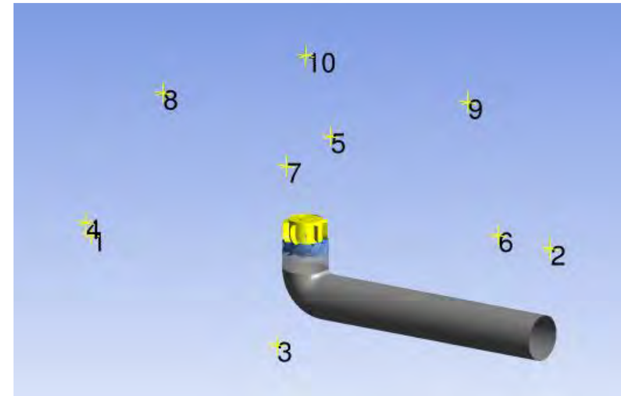
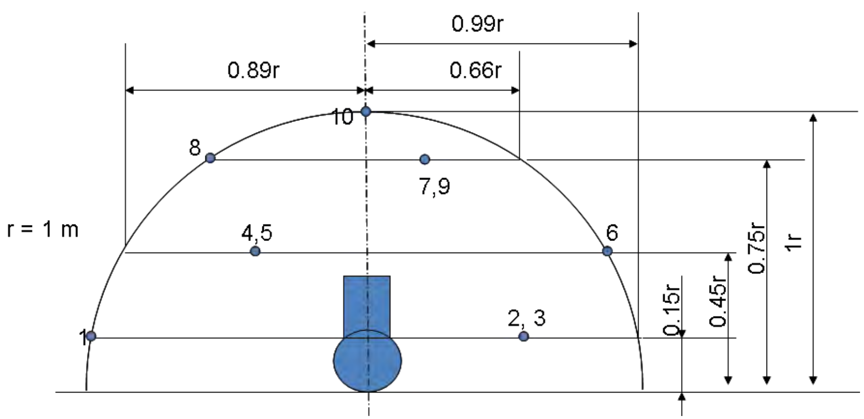
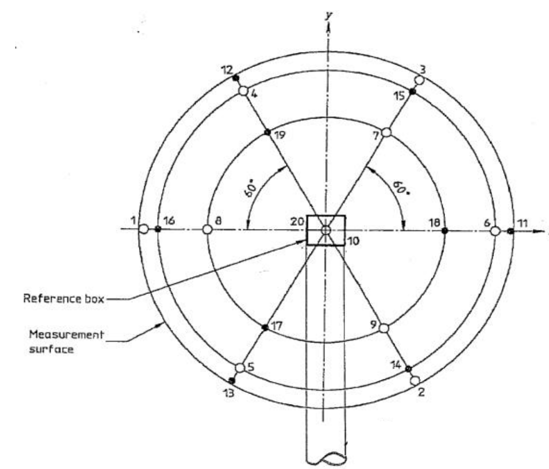
- ISO 3744
- Measurement locations on Hemisphere
- Measurements on hard reflecting floor
- Corrections for Background Noise

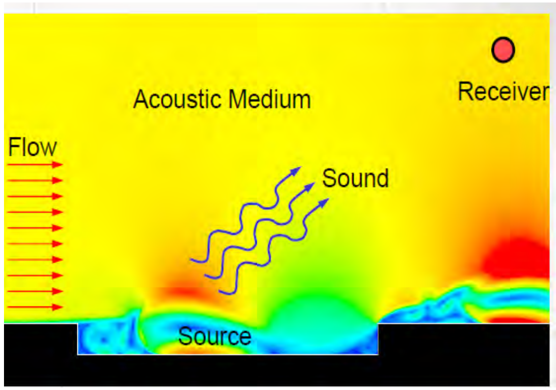


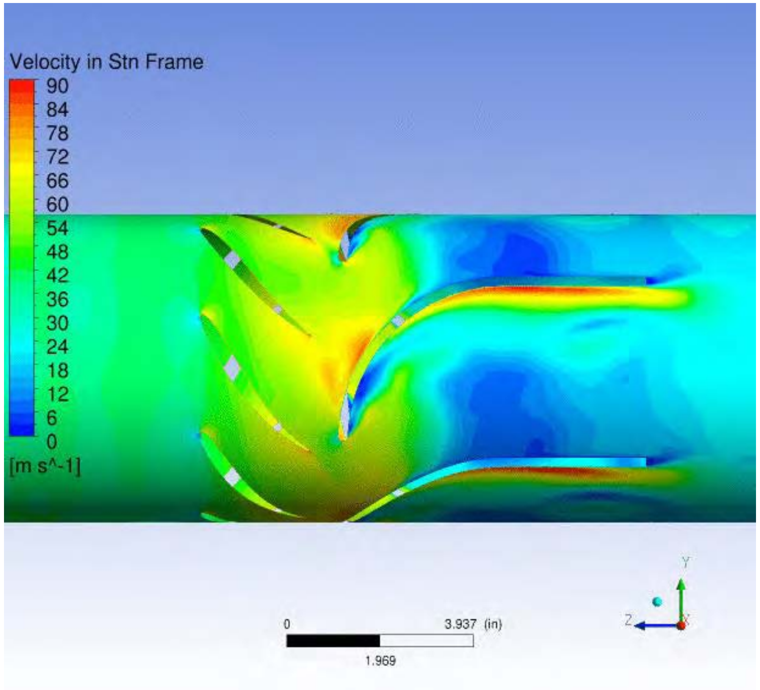



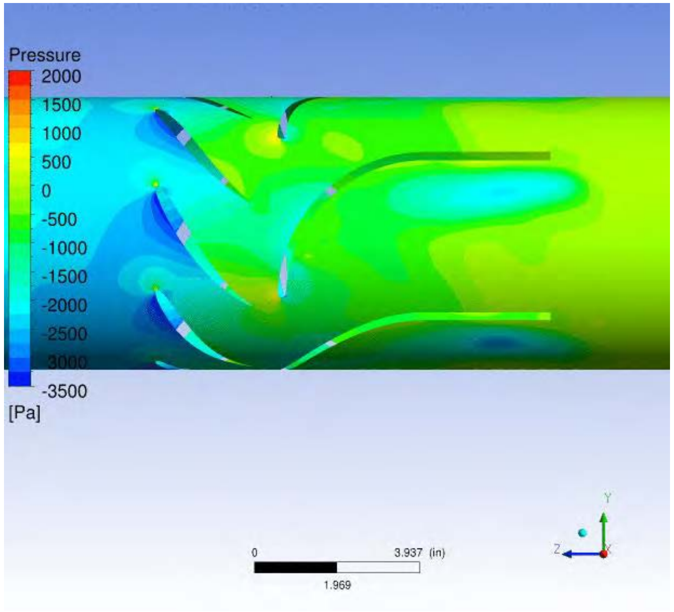
# Simulation Details

| | |
|---|---|
| Solver | ANSYS-Fluent 12.1 |
| Inlet | Mass Flow Inlet |
| Outlet | Pressure Outlet |
| Wall-Treatment | Standard wall Function |
| Steady state | |
| Rotating Frame Model | Moving Reference Frame |
| Acoustic Model | Broadband Model |
| Transient Set-up | |
| Rotating Frame Model | Sliding Mesh Model |
| Acoustic Model | Ffowcs – William & Hawkings |

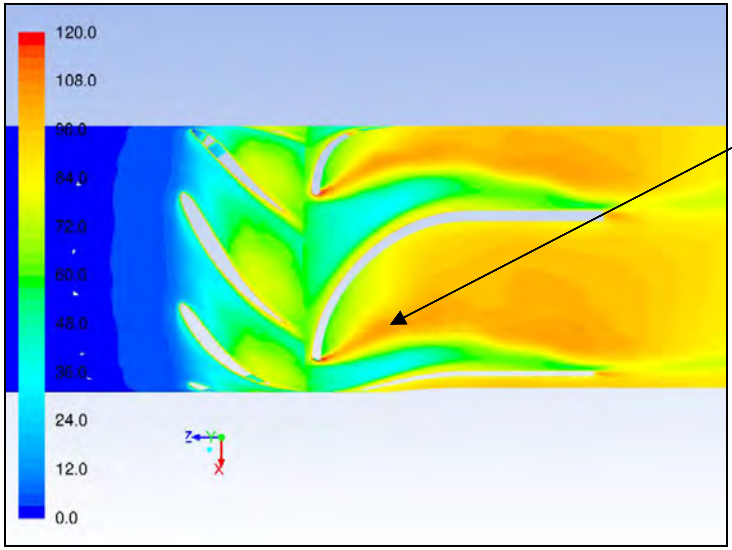


# Rotor-Stator Interaction

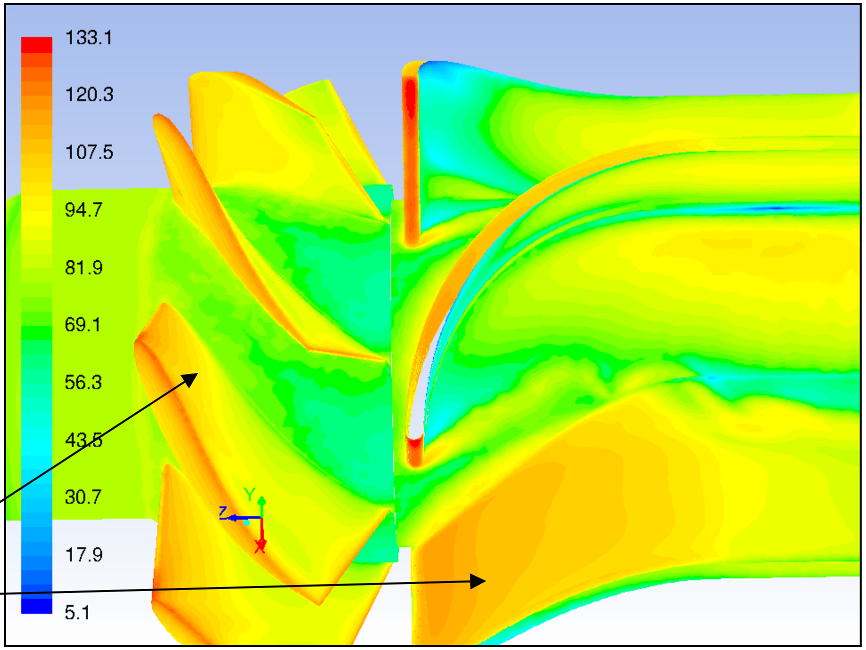


# Broadband Noise

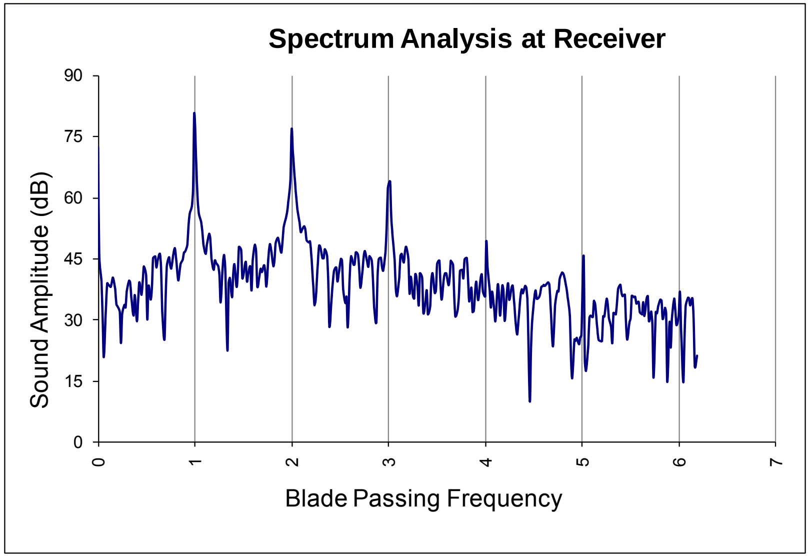


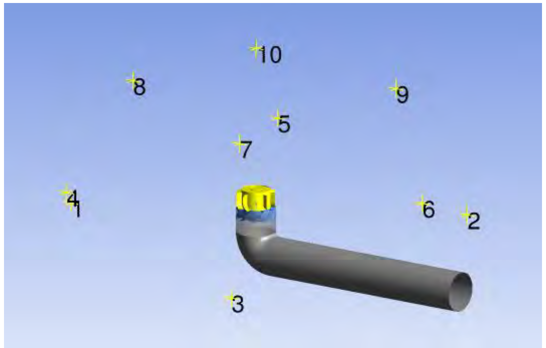

Noise Due to Separation

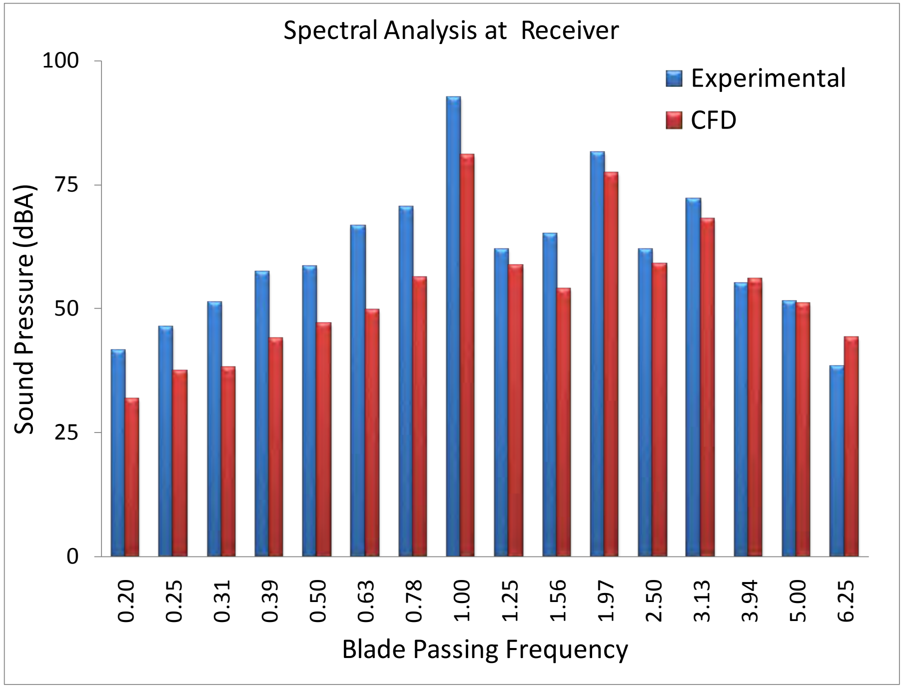



Noise Due to Shear

# Spectral Analysis



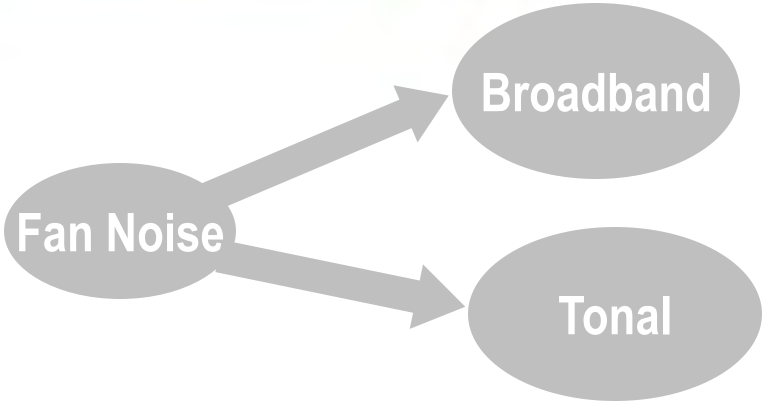



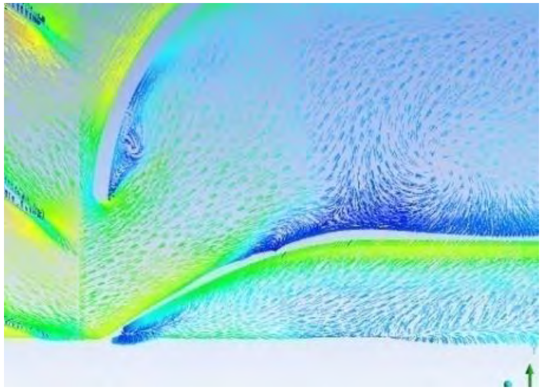




Similar form to results is sufficient for comparative studies to identify improvements

# Design Changes

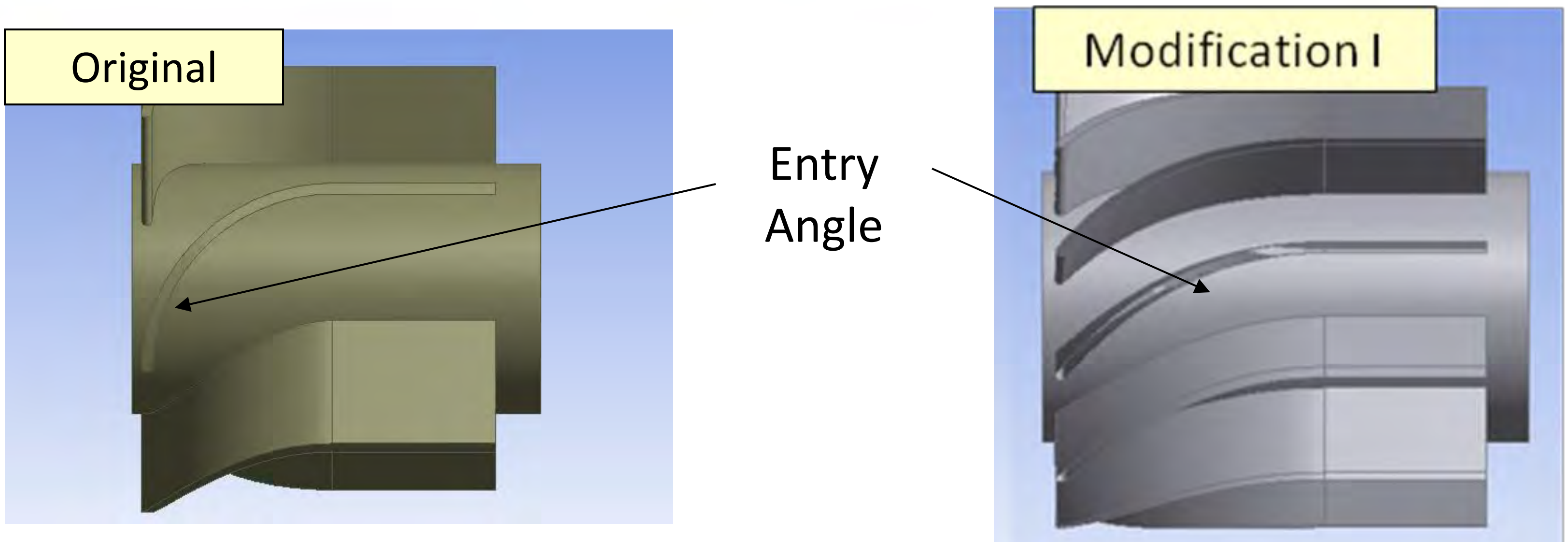
- Design Modification I
  - Number of stator blades
  - Blade Entry Angle
- Design Modification II
  - Rake Angle
  - Sudden Steps Removed
- Design Modification III
  - Airfoil Shaped Stator
  - Gap between rotor-stator



# Design Modification: I






- Number of blades increased from 5 to 13
- Entry angle changed to reduce separation
- Entry angle changes from hub to shroud to allow radial variation of the entry angle

# Design Modification I

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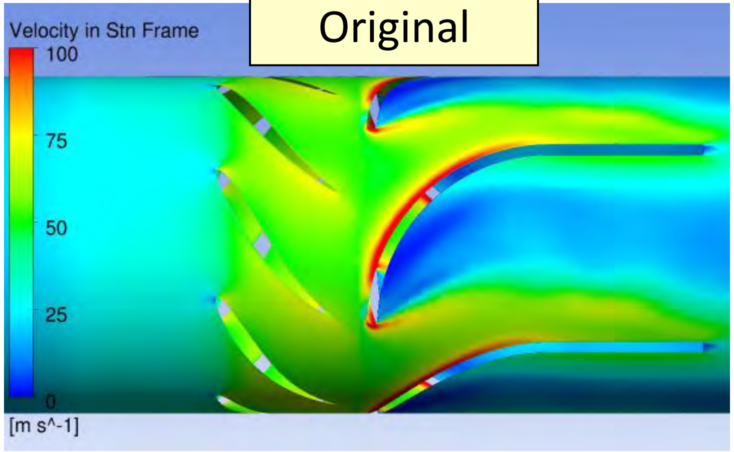
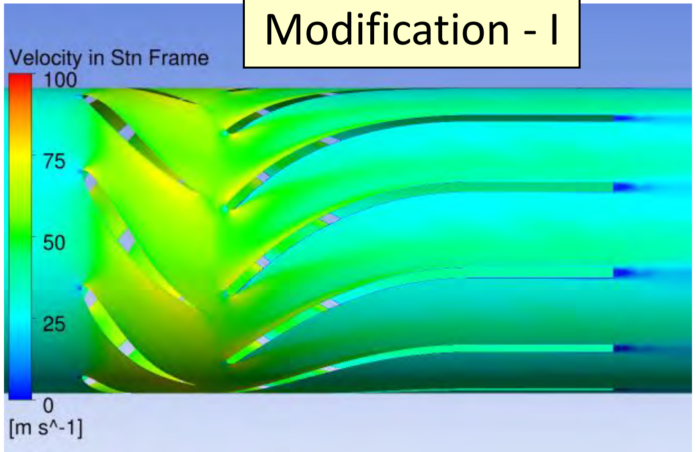
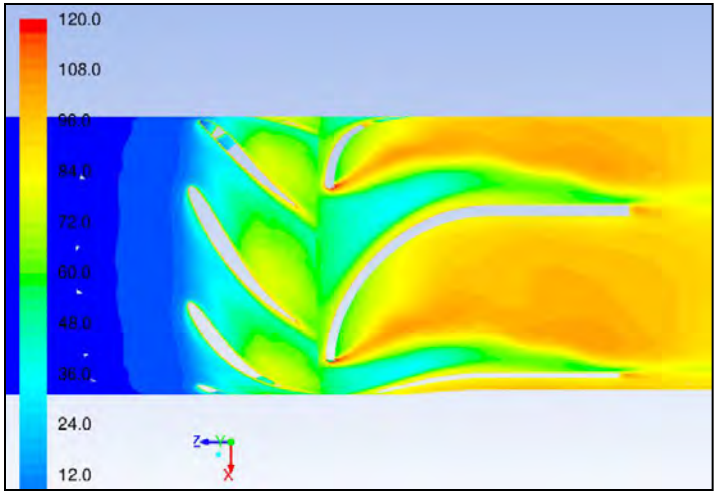
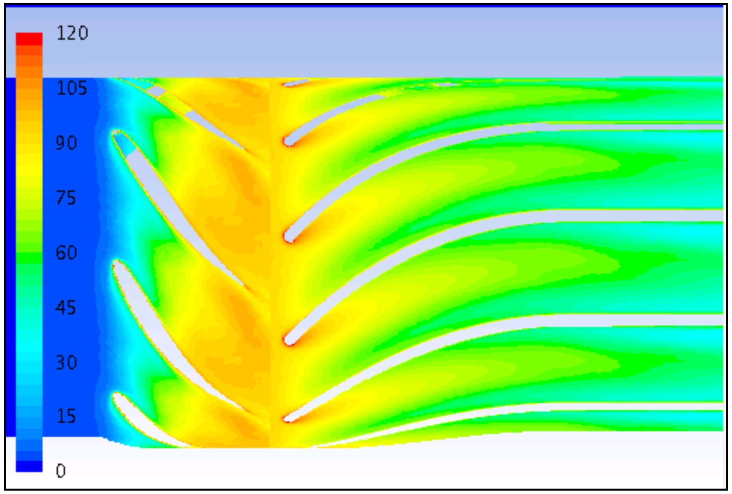
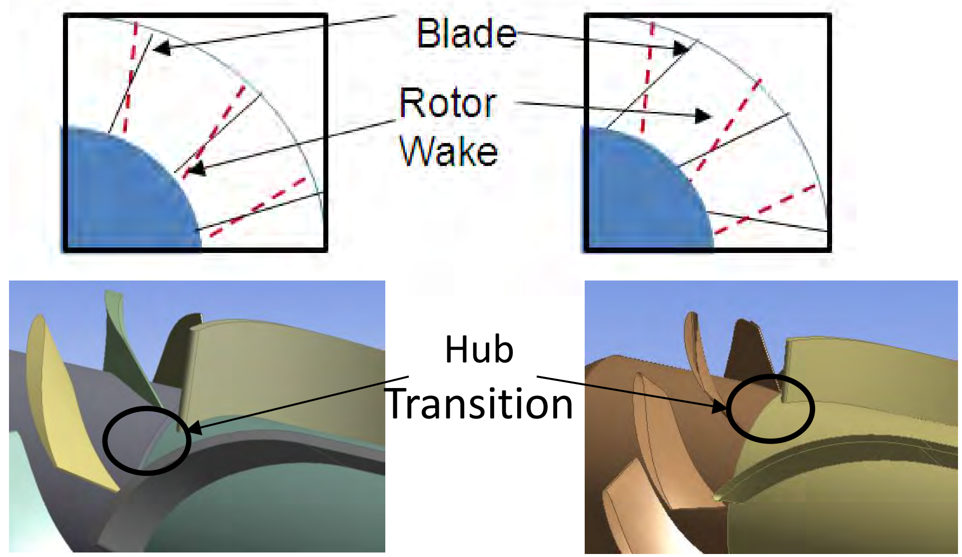
| | Original | Modification - I |
|---|---|---|
| Velocity |  |  |
| Broadband Noise |  |  |

# Design Modification II

- Rake angle of the stator blade changed
  - Helps to reduce impact load and hence tonal noise from the fan
- Any steps causing flow separation removed
  - Helps to reduce broadband noise



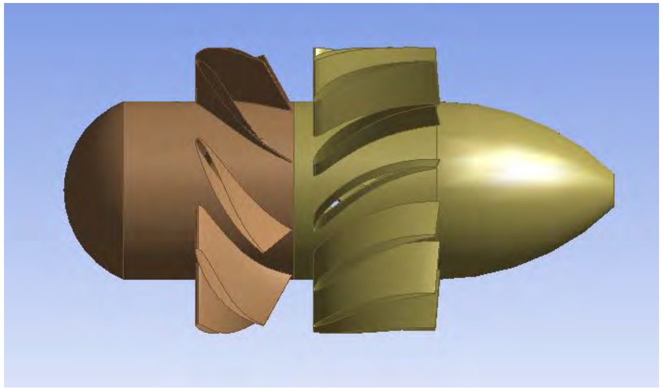




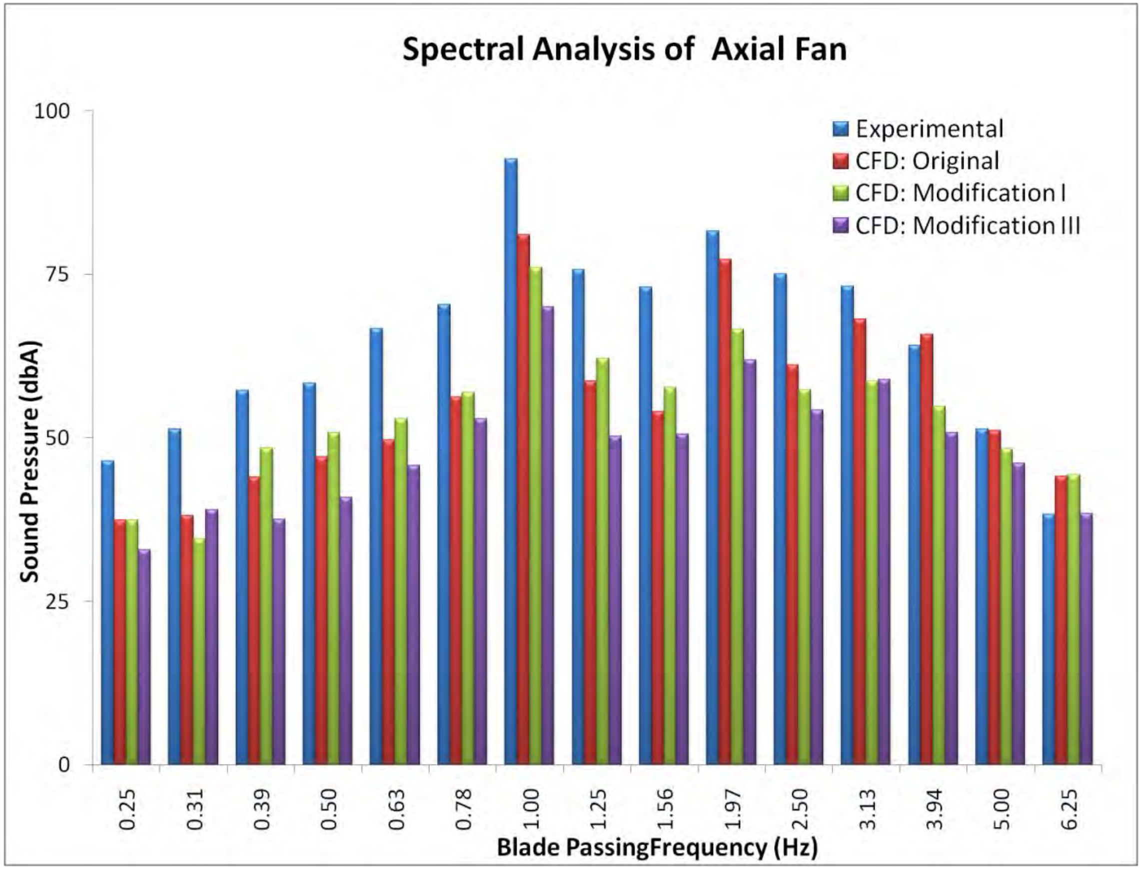

50

# Design Modification: II & III

- Airfoil Shaped Stator
  - Helps to reduce separation and gain pressure in stator
  - Less chances of separation away from design point
- Gap between rotor-stator
  - Increases flow mixing in rotor wake region
  - Reduced tonal noise, however some loss in pressure



# Spectrum Analysis




| Design | Overall Sound Power Level |
|---|---|
| Original (expt) | 98 dB |
| Original (CFD) | 93 dB |
| Mod I (CFD) | 86 dB |
| Mod III (CFD) | 80 dB |
| Mod III (Expt) | 88 dB |

# Summary

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- Fan noise prediction using Computational Aero Acoustic methods close to experimental results
- Tonal Noise reduction achieved using
  - Correct number of rotor-stator blade count
  - Gap between rotor-stator
  - Rake angle of the stator blade
- Broadband noise reduction achieved using
  - Correct blade angles
  - Removing steps & sudden expansions
- Significant noise reduction was achieved with improved efficiency
- **Although some deviation compared to expt, CFD useful to reduce fan noise with minimum cost**

# Application – helicopter engine protection

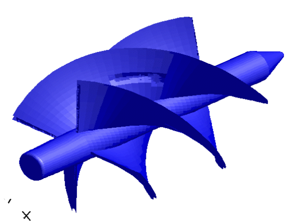


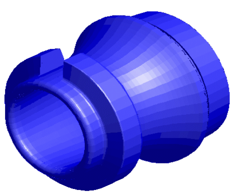
The ingress of particulate matter, dust, sand etc. into a helicopter engine accelerates wear and decreases life.

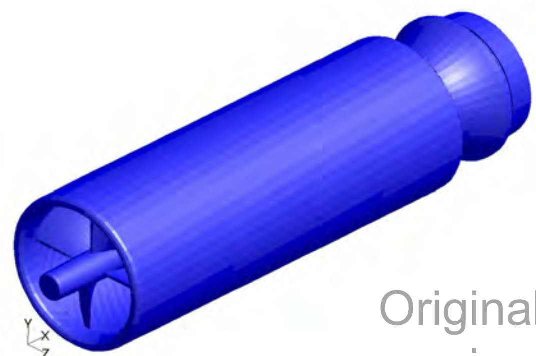
Engine Air Particle Separator (EAPS) installations are used to minimise this.

Panels of static vortex tubes are used upstream from the engine intake plenum.

Tubes are designed to operate at maximum separation efficiency for specific flowrates.







Originally presented at NAFEMS seminar, Industrial Turbulent Flows: CFD simulation and Validation 2003

# Purpose of Simulations

- To predict the effect of the EAPS on the pressure drop to the compressor entry plane.
- To predict the effect of the EAPS on the flow distortion at the compressor entry plane.
- To predict the flow variation across the panels.
- To compare alternative configurations and the effects of design variations.
- To assess the differences between hover and forward flight conditions.

# Why Use CFD?

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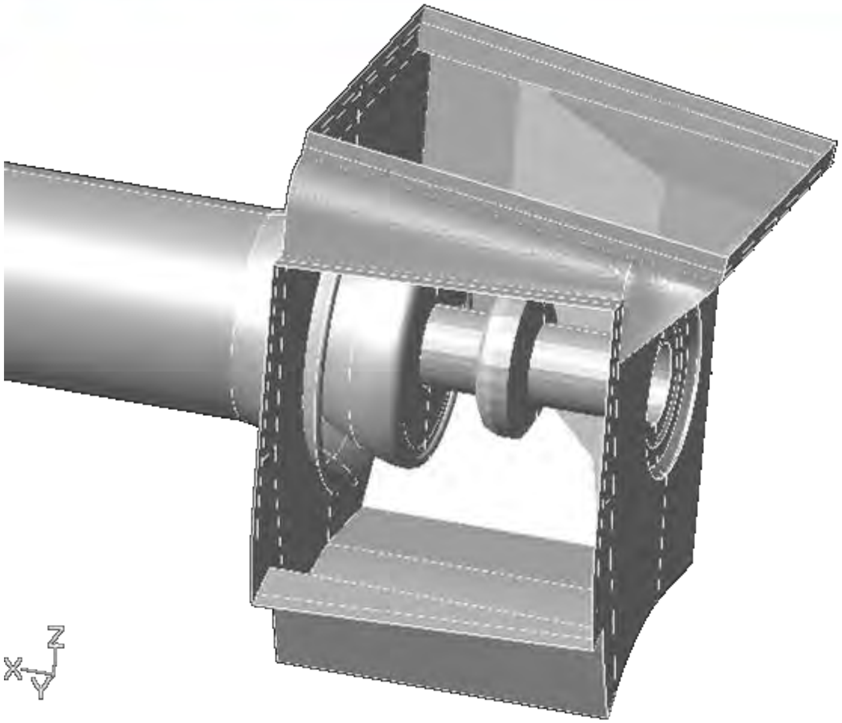
- CFD is used in the design process to limit risk and obtain customer approval for a design without the costs of making and testing a unit.
- Some testing is extremely expensive to carry out, especially for forward flight cases. Although flight certification generally requires flight tests to be carried out, the risk is reduced if any problems can be identified earlier.
- Flow distortion and distribution are difficult to measure, especially over panels.
- Numerous design variations can be assessed cheaply, early in the design process.

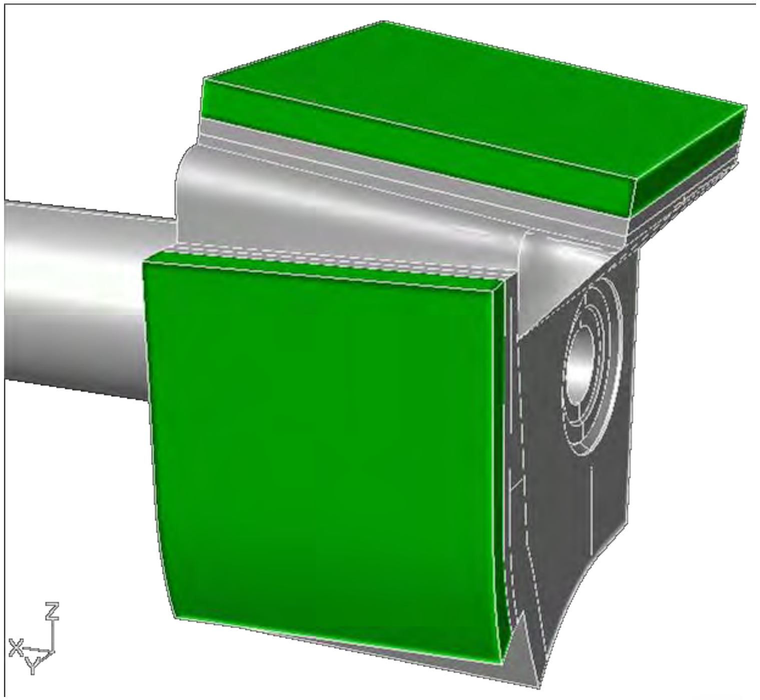
# Validation Opportunities

- It is advisable to validate every CFD simulation, however, often this is not easy in practice.
- Validation may be carried out in several stages.
- Where possible, several parameters should be used for validation (pressure, velocity, temperature etc.).
- Detailed records of previously validated simulations can help design new simulations and give an indication of their likely accuracy.
- Accuracy of both CFD simulations and experimental data should be determined.

# Validation Stages

- Initially a simulated flow can be compared to similar flows or hand calculations. These rarely provide accurate values, but may be enough to give some confidence.
- Once CFD has been used to provide confidence in a specific design, a prototype can be made and tested.
- These test results can be used to back-validate the CFD. The CFD can be repeated if necessary. The lessons learnt from this process should lead to improved future simulations of this type.
- These back-validation cases can be used for subsequent projects to provide confidence in the accuracy of similar CFD simulations.


Z
X
Y


Z
X
Y

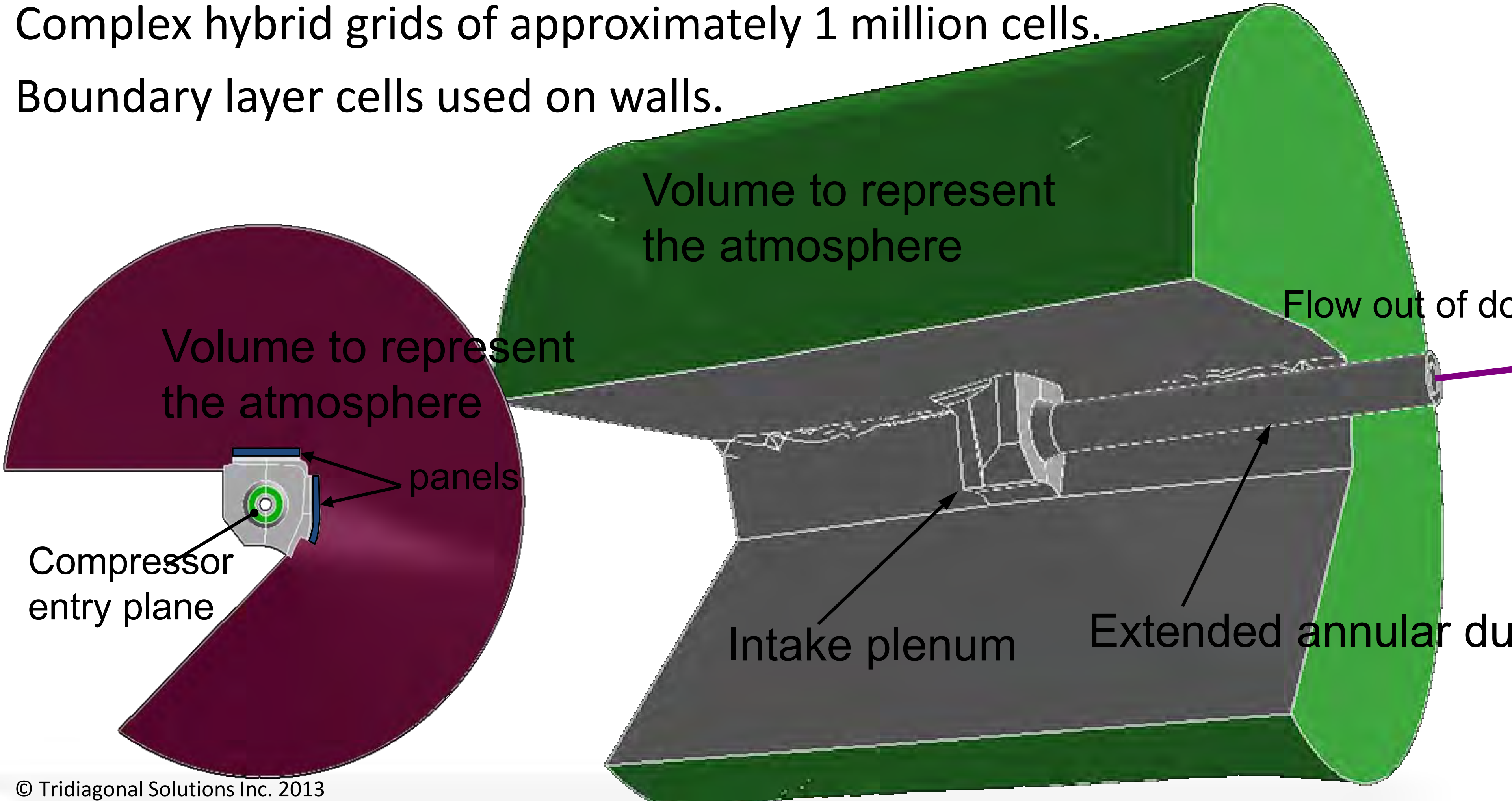
# Computational Domain

Atmospheric volume upstream.

Annular duct ~18∅H downstream.

Complex hybrid grids of approximately 1 million cells.

Boundary layer cells used on walls.



# Assumptions

- Flow is assumed to be time invariant on the macro-scale, k-$\varepsilon$ turbulence model used.
- Flow distortion due to rotors and compressor omitted as per test rig.
- Detailed flow in tubes not simulated. Panels simulated as proved simple porous media momentum sink.
- Scavenge flow included implicitly in porous media parameters.
- All walls hydrodynamically smooth.

# Results

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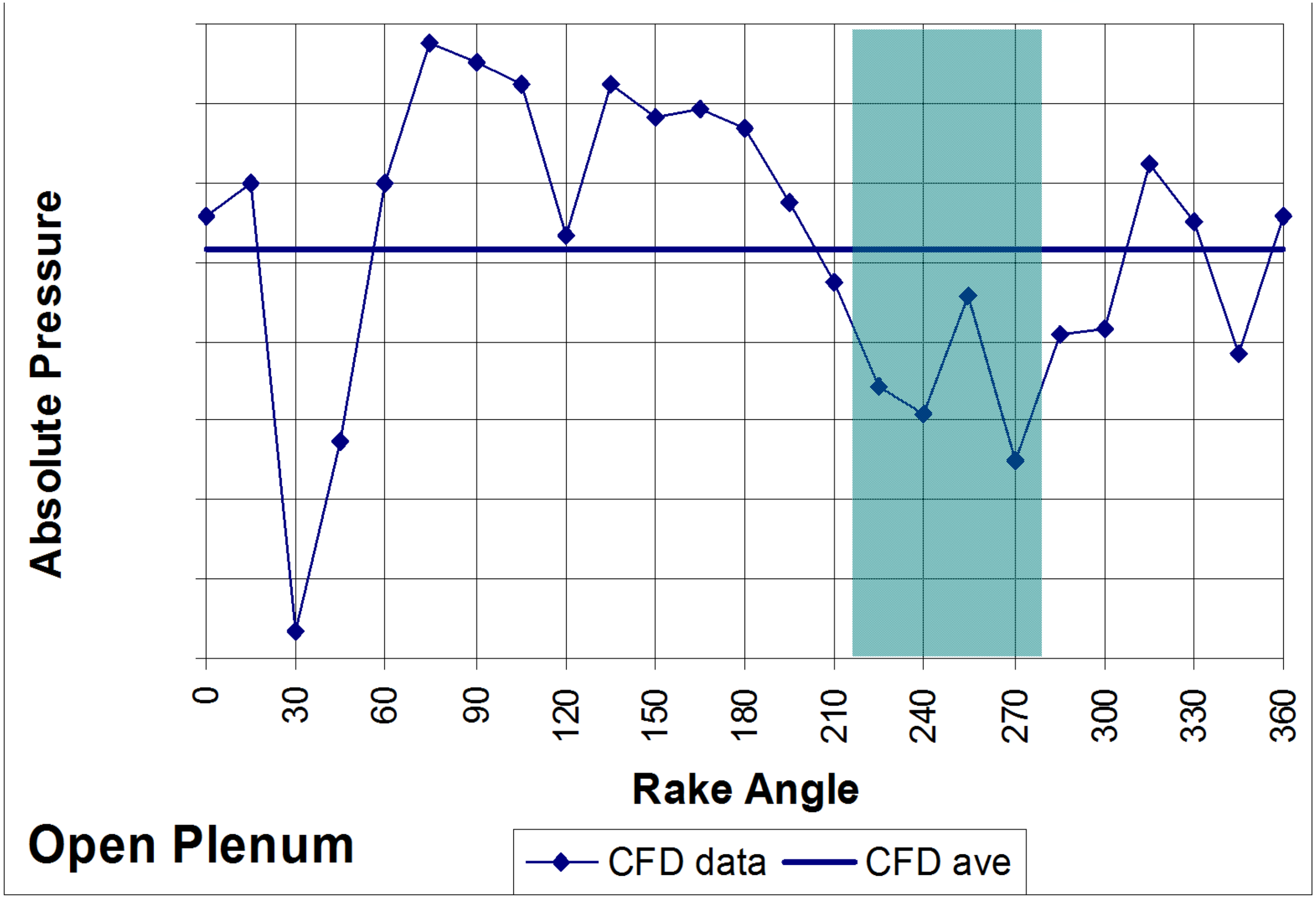
- Pressure drops from atmospheric pressure down to the compressor entry plane.
- Flowrates through panels; calculated by dividing each panel into 16 sections and using mass flow rate, area and number of tubes.
- Flow distortion at compressor entry plane.

# Averaged Pressure Values for each Rake



# Flow distribution through side panel

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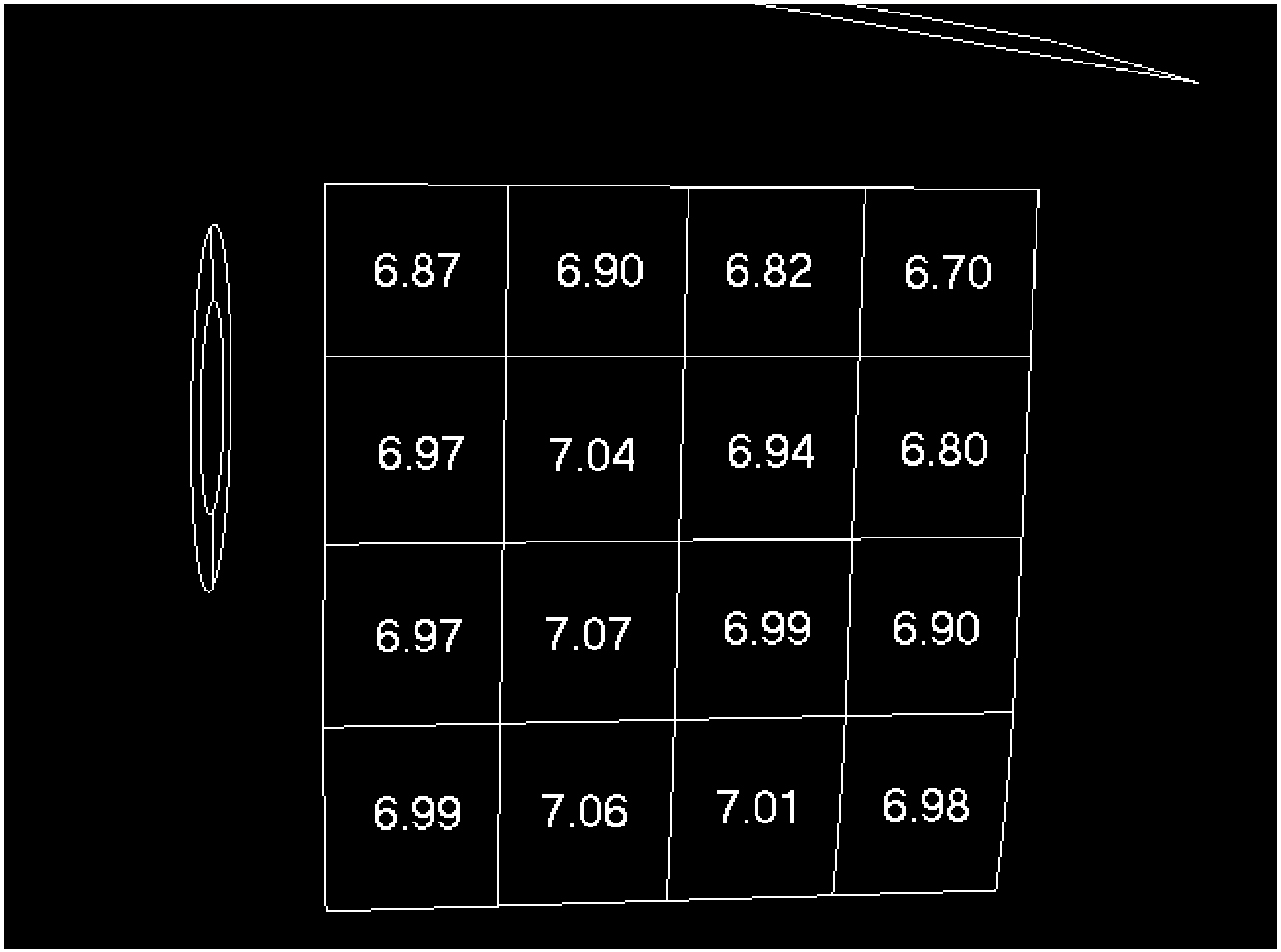


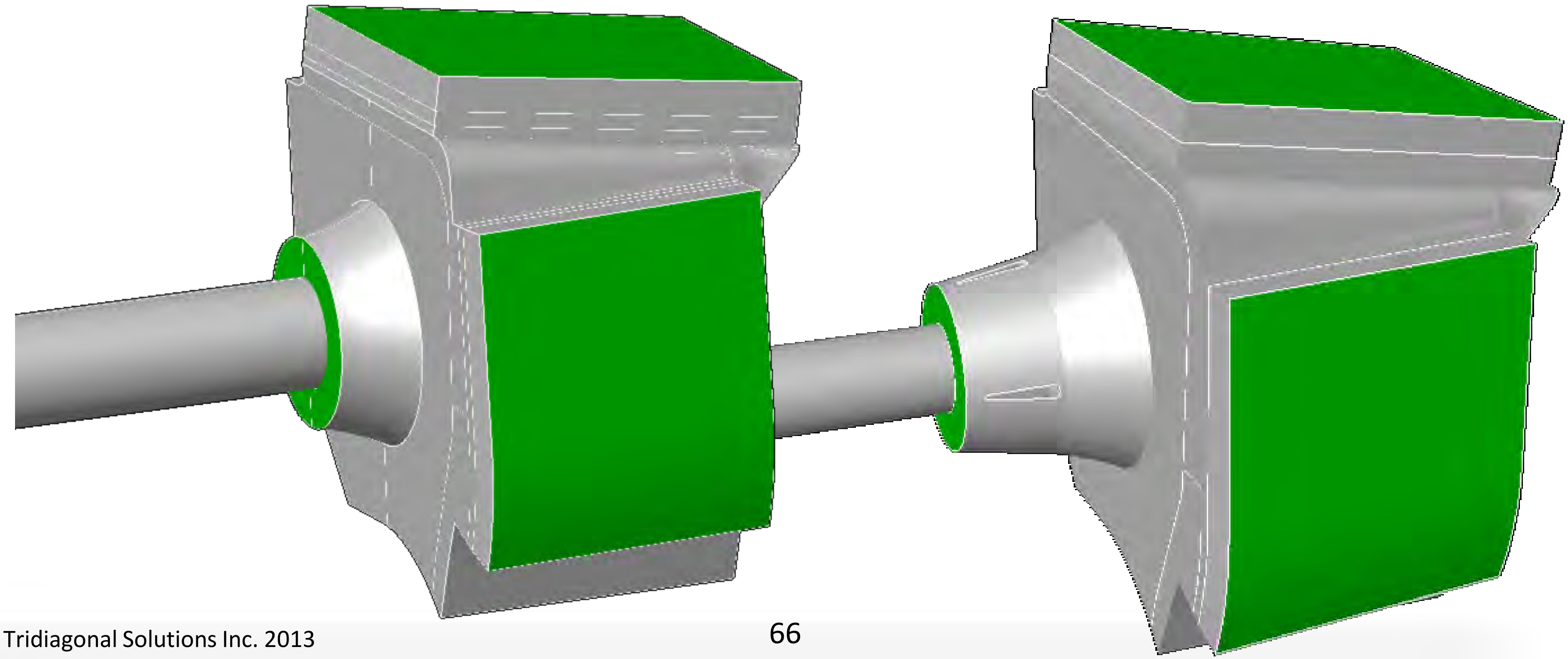
# Comparison with Test Data

- There are two principle differences between the simulated unit and the tested unit:
  - location of engine entry plane
  - location of pressure rakes
- These differences didn't become apparent until the plenum was delivered from the customer for testing.

# Differences between engine entry plane location

The compressor entry plane used in the CFD simulations is the plane at the exit of the originally supplied geometry.

It is approximately 15cm upstream and 34% larger than the compressor entry plane in the test unit.



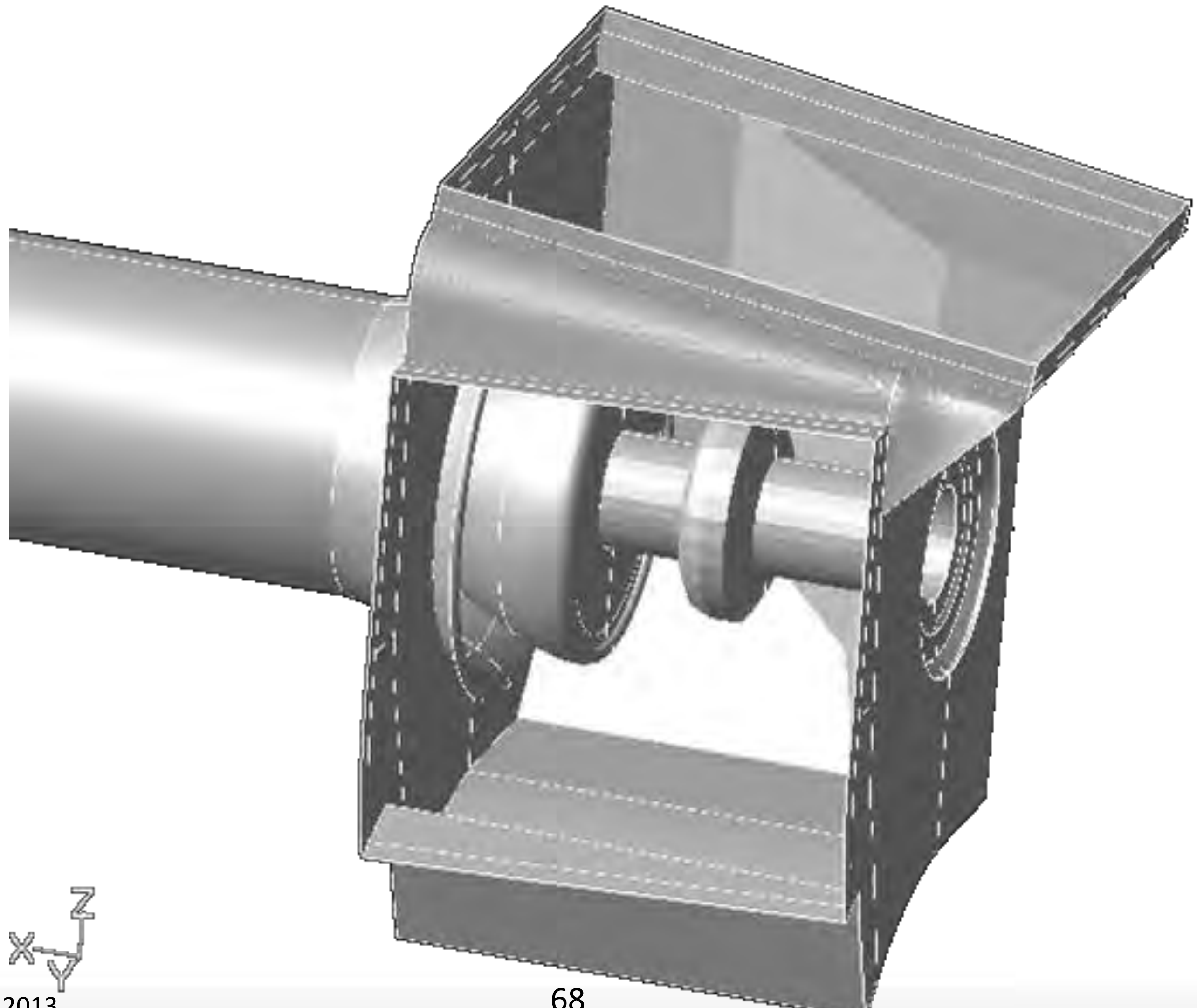
# Differences in pressure rake locations

The rake angles used in the CFD simulations start at TDC. For testing, the rakes were offset by 71/2 degrees.

The offset was to move the rakes away from the four engine entry vanes.

| | Open plenum ΔP | EAPS ΔP |
|---|---|---|
| CFD | 5.0 | 14.5 |
| Corrected CFD | 6.0 | 15.5 |
| Test | 3.0 | 15.0 |
| Difference | 3.0 | 0.5 |

# Open plenum (without Centrisep panels)



| | CFD | Corrected CFD | Test |
|---|---|---|---|
| Open plenum Dc60 | -0.037 | -0.020 | -0.015 |
| Open plenum max Dc60 location | 247.5 | 255 | 270 |
| EAPS Dc60 | -0.030 | -0.017 | -0.020 |
| EAPS max Dc60 location | 232.5 | 240 | 255 |

# Open Plenum Comparison with Test Data

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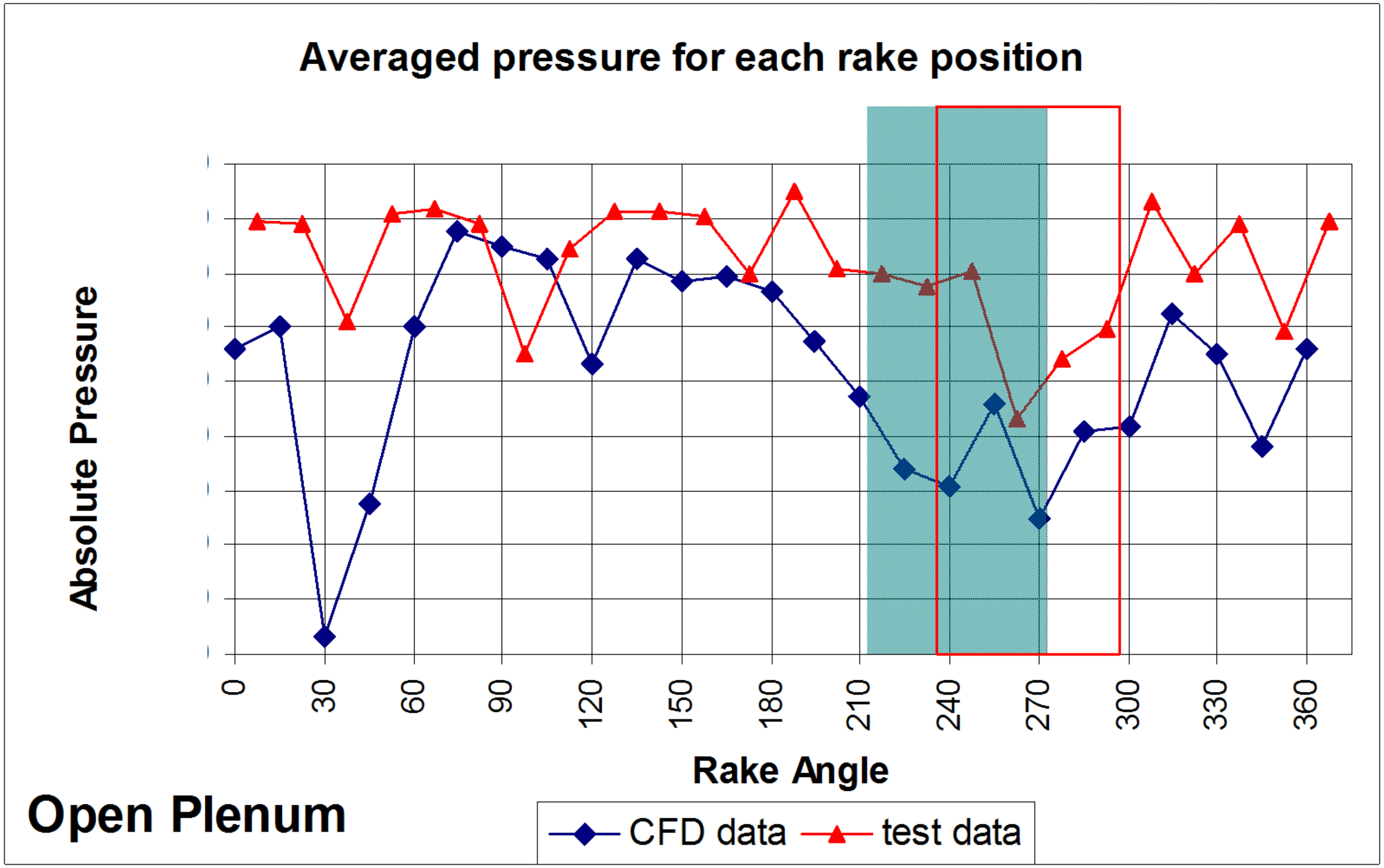

# EAPS Comparison with Test Data

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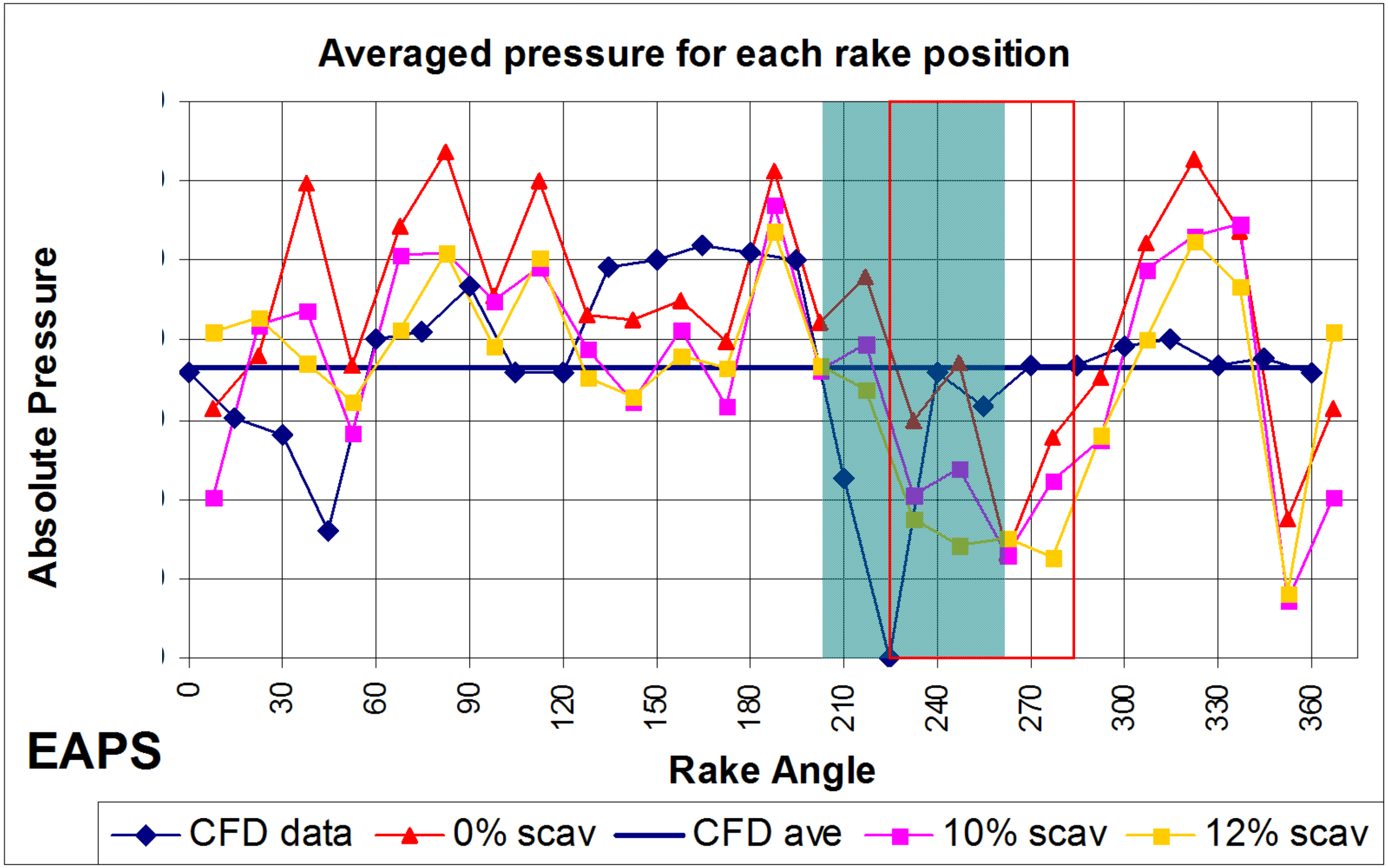
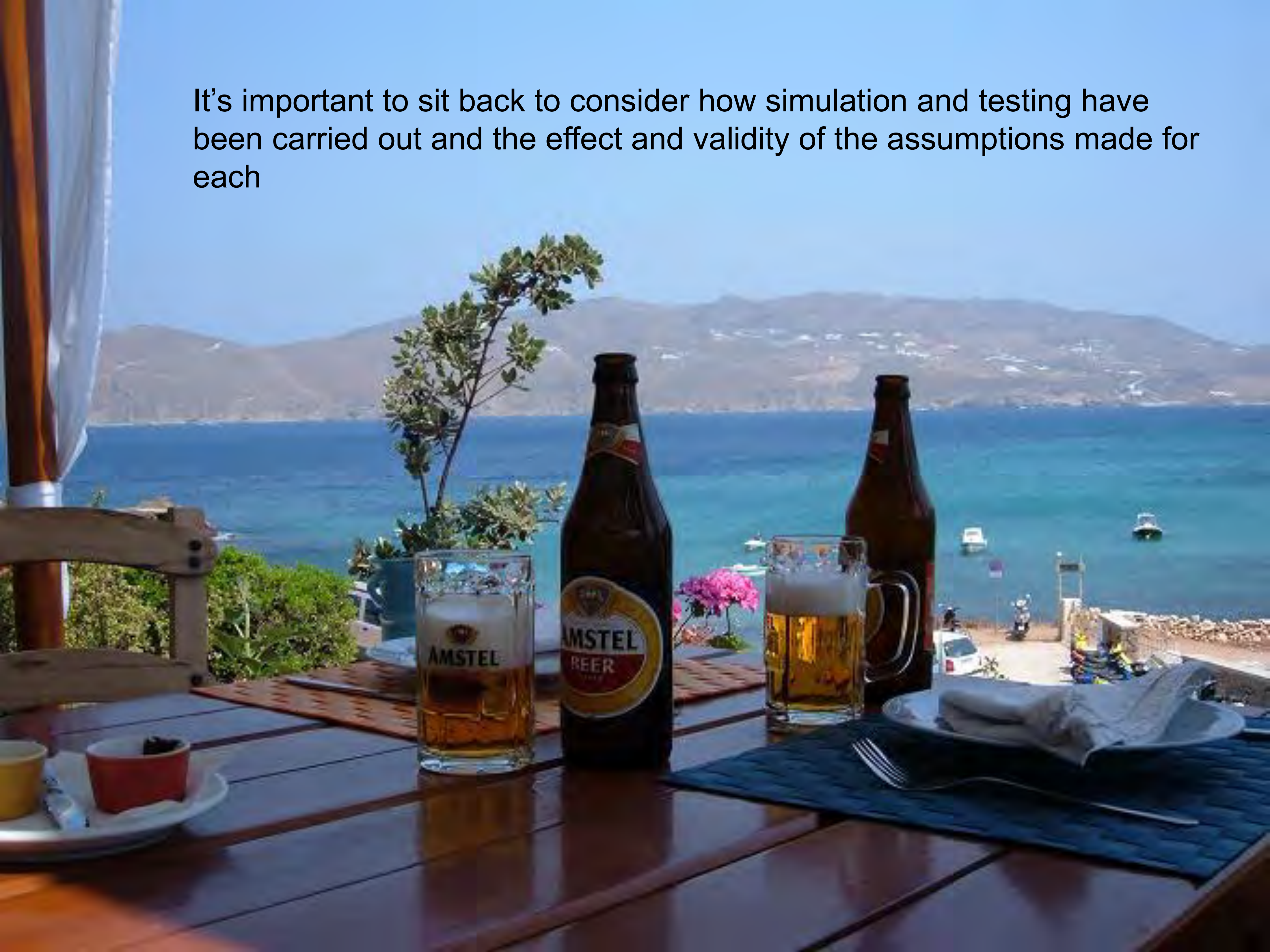


# Points to Remember

- Check how a unit will be subsequently tested including test rig design, measurement methods and locations etc.
- Understand what assumptions are acceptable and will be made for testing (neglect of external effects – compressor, rotor, etc.).
- Double check assumptions in CAD model.
- Allow longer for geometry import of compound CAD (generated from multiple CAD systems by several people).

It’s important to sit back to consider how simulation and testing have been carried out and the effect and validity of the assumptions made for each



# Experimental Fluid Dynamics

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The difficulties that exist for validating CFD simulations has led us to develop in-house test facilities and to work closely with customers throughout all stages of projects

**Airflow distribution Measurements**

Experiments conducted to determine the percent open areas at various stages of piping system to meet process flow requirements

**Gas voidage Measurement - GL flows**

- Local gas-holdup/ bubble frequency/ bubble velocity/ bubble size distribution
- Customized software for signal processing with User manual
- Mixing time measurements (conductivity meter)

# Experimental Fluid Modeling

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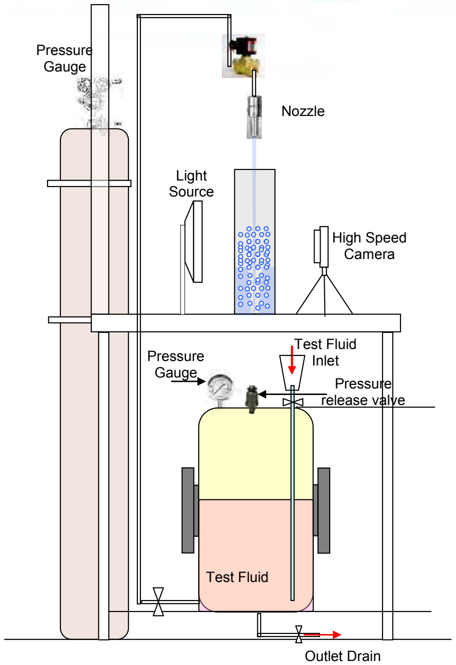
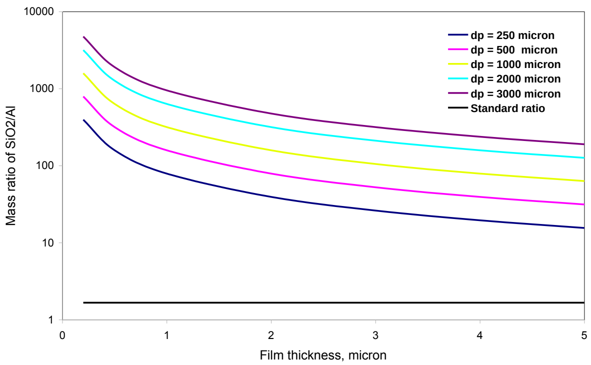
## Aeration & Foaming

- Fabricated experimental rig to simulate bottle filling setup
- Characterize impact of various hydrodynamic parameters (flow rate, nozzle, jet length etc.) and bottle characteristics (size, shape, surface properties) on aeration and foaming.




## Rotary Kiln Modeling

Experiment conducted to develop better understanding of mixing of Silica and molten Aluminum in rotary kiln & the effects of partial size, rotational speed & solid to liquid ratio on the mixing were characterized.

# EFD Lab

- Our Own Facility
- High Pressure Air Compressor
- Water Pump
- Electricity up to 40 hp

# Facts

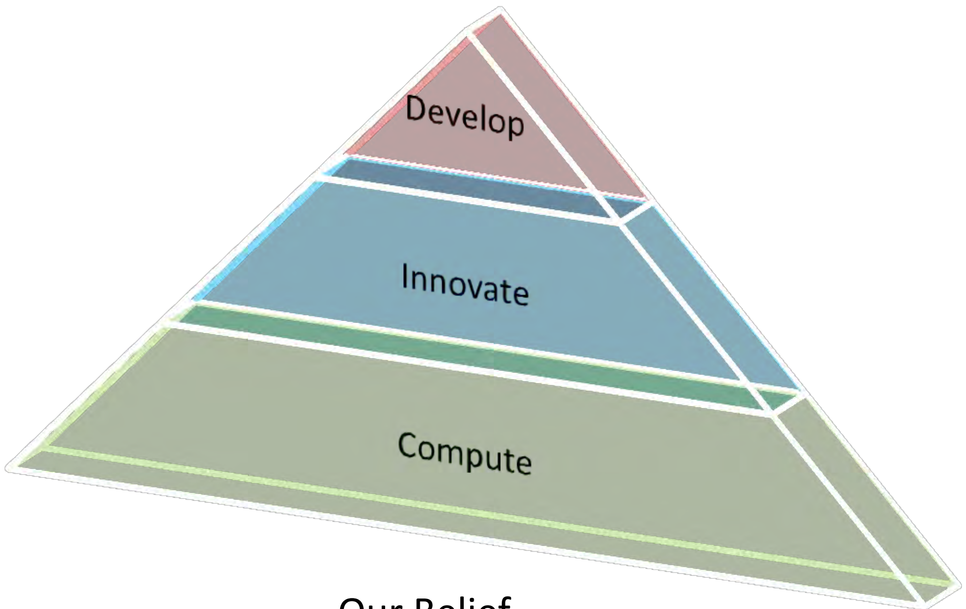
**End to End CFD and Experimental FD Solutions (EFD)**
Our services encompass the complete product and manufacturing process development life cycle from model building, CFD simulation, EFD validation and pilot scale manufacturing

**Domain Expertise**
Chemicals and Process, Oil and Gas, Consumer Goods, HVAC, Power Generation, Automotive

**Team**
30 professionals with PhD and Masters degrees and domain expertise

**Delivery Process**
Global Delivery process comprising of onsite, off site and offshore delivery teams

- Founded in July 2006 by professionals from Fluent and National Chemical Laboratory, Pune
- Offices in USA and India
- "Customer Focused" – Long Term Customer Relationships built on being a trusted Partner




Our Belief

# Solutions Portfolio

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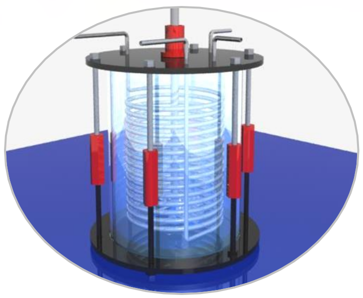
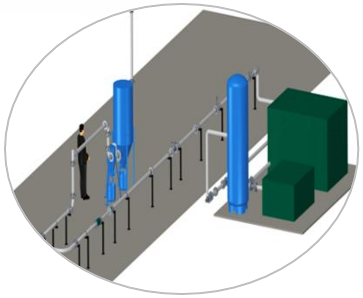
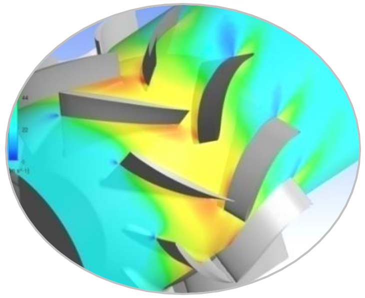
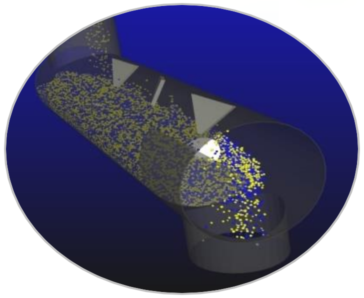
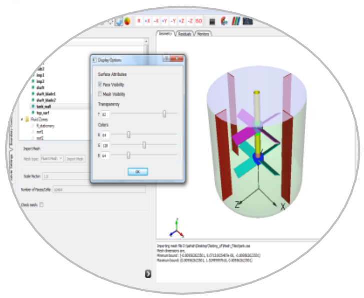

## Process Engineering

- Process Scale Up & Trouble Shooting
- Pilot Experiments
- Pilot Plant Design & Manufacturing

## Experimental Fluid Dynamics

- Build custom experimental setup
- High speed photography
- Pressure & velocity measurement
- Volume fraction measurement

## CFD Modeling & Simulations

- Baseline CFD Model Building
- Simulations using CFD software
- Reports, Animations, etc
- On demand resource placement

## Discrete Element Modeling (DEM)

- Granular Dynamics Consulting
- DEM Simulations
- EDEM - CFD Coupled Simulations

## OpenFOAM Applications

- Customized Solver Development
- GUI and Vertical Application Development
- Training, Support & Implementation