

On-Demand Webinar

# Multiphysische Probleme in der Prozessindustrie: ein Weg über Simulation

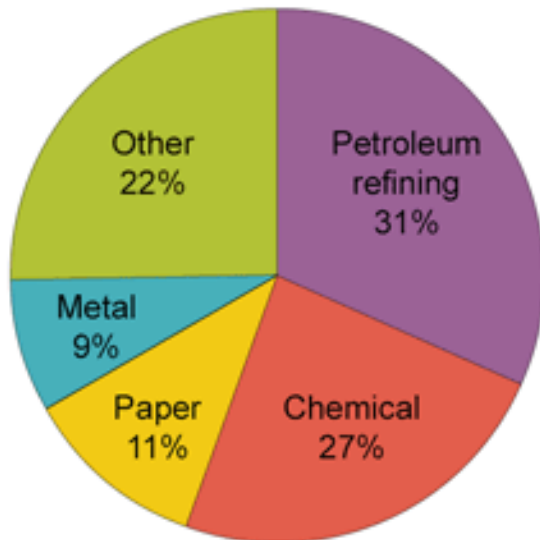
Peter Jeszencsak, Felix Klippel

# What are the Challenges in the Chemical and Process Industry?

## Sustainability

Use of fuel, power and steam

Energy use by type of industry

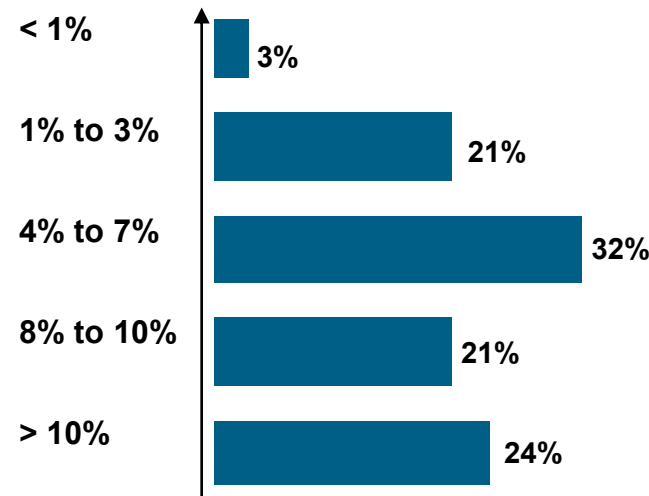


Source: U.S. Energy Information Administration  
Manufacturing Energy consumption Survey 2010

## Resource Efficiency

Increase yield and throughput

Expected impact to bottom line

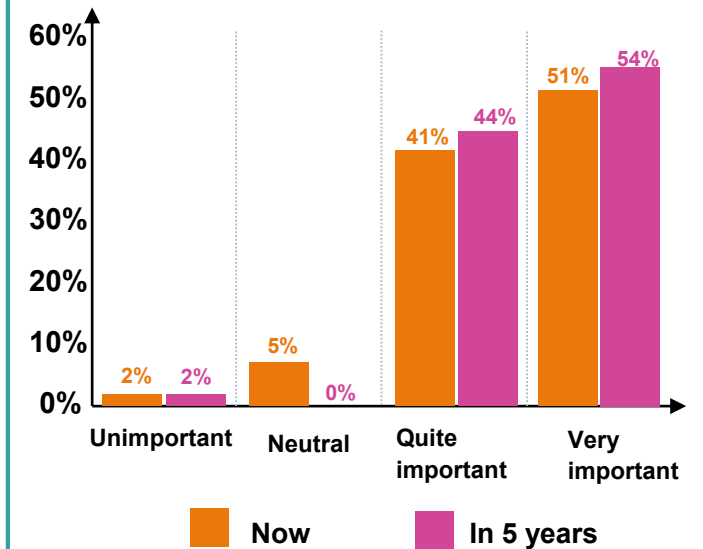


Source: ICIS/Accenture

## Innovation Agility

Reduce time to market

Importance of innovation to success



Source: PwC Global Innovation Survey 2013



# Implications for the Process Industry

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Increase Energy Efficiency

Improve Process Efficiency

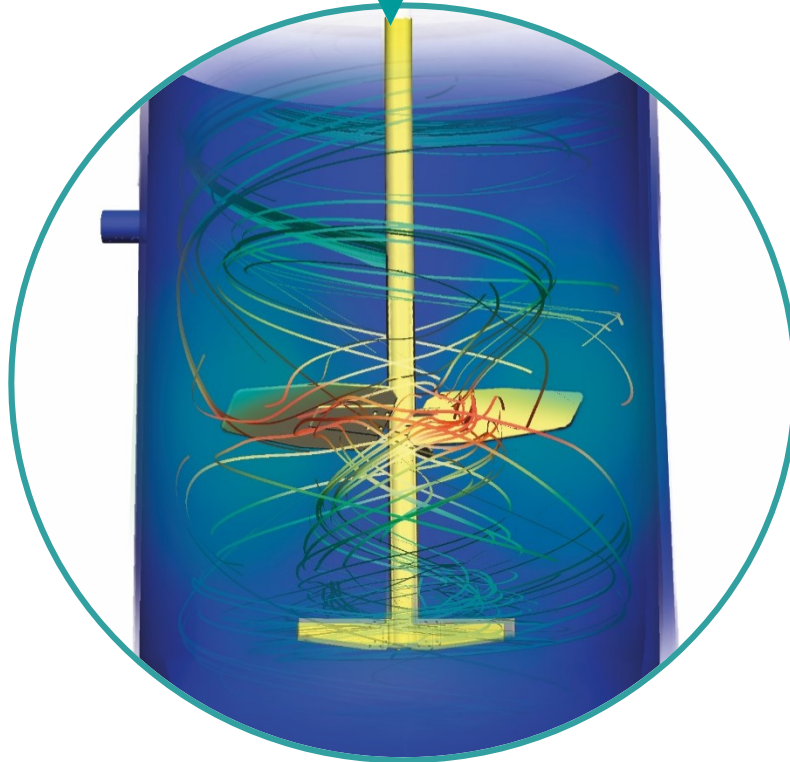
Accelerate Innovation Efficiency

Achieve Operational Excellence

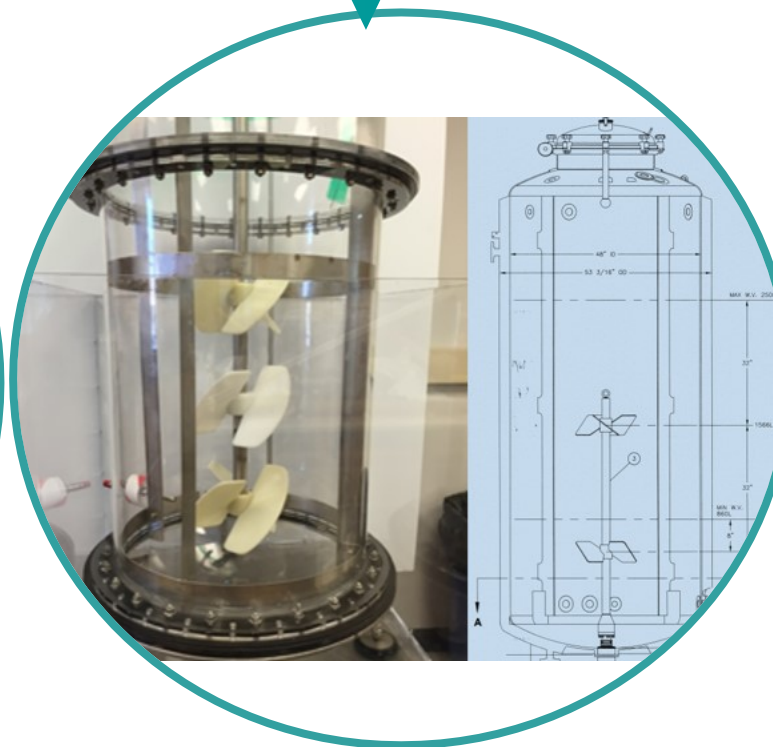
# Digital Transformation with a Holistic Digital Twin

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Ideation  
Performance



Realization  
Scale-Up



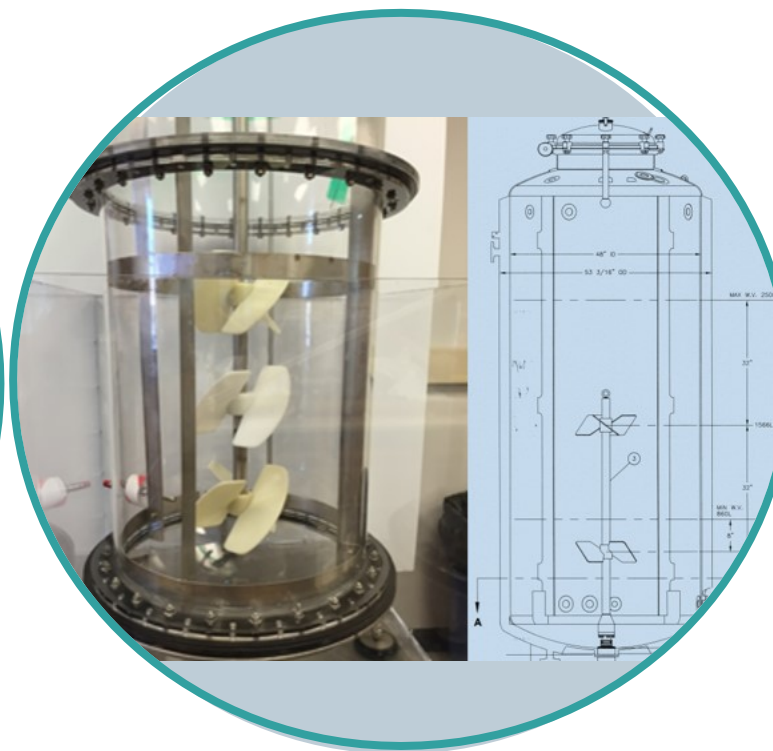
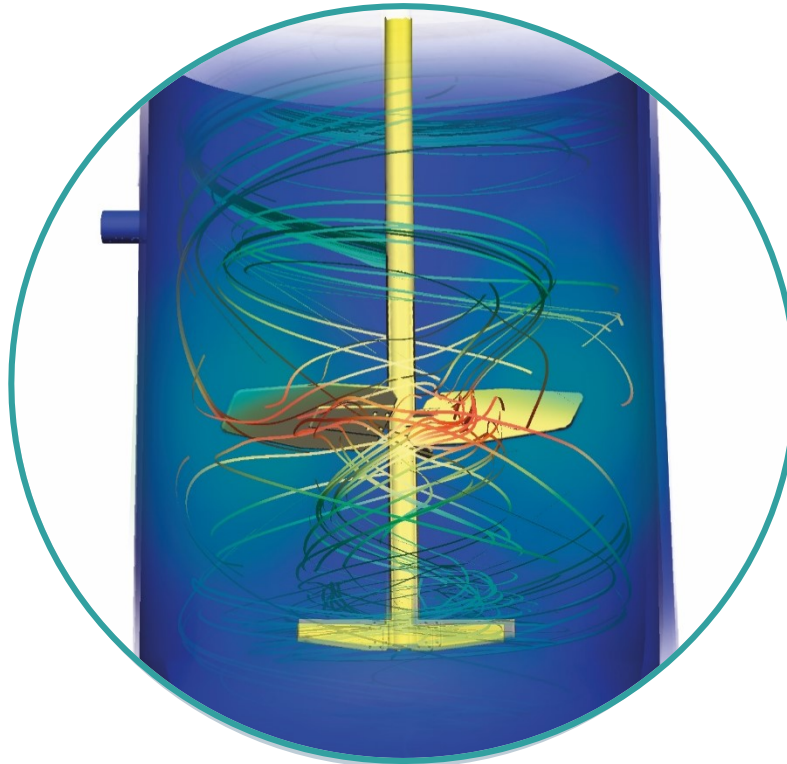
Utilization  
Operation





# Closing the Loop with the Holistic Digital Twin

Feed back insights to continuously improve product and production



# Redefining Performance Engineering for the Digital Twin

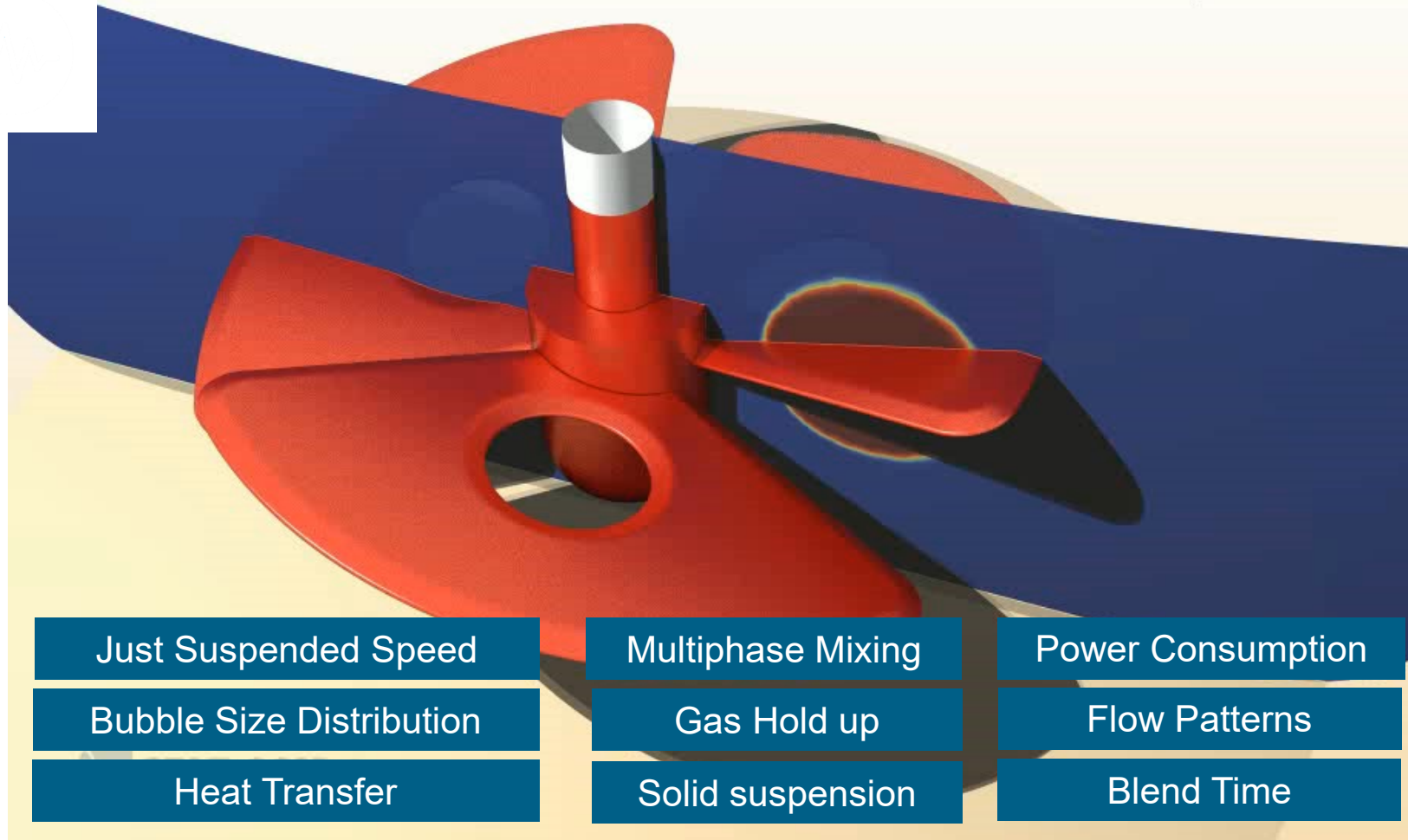


# Simcenter for Mixing Reactor Performance

Covering a wide range of performance indicators

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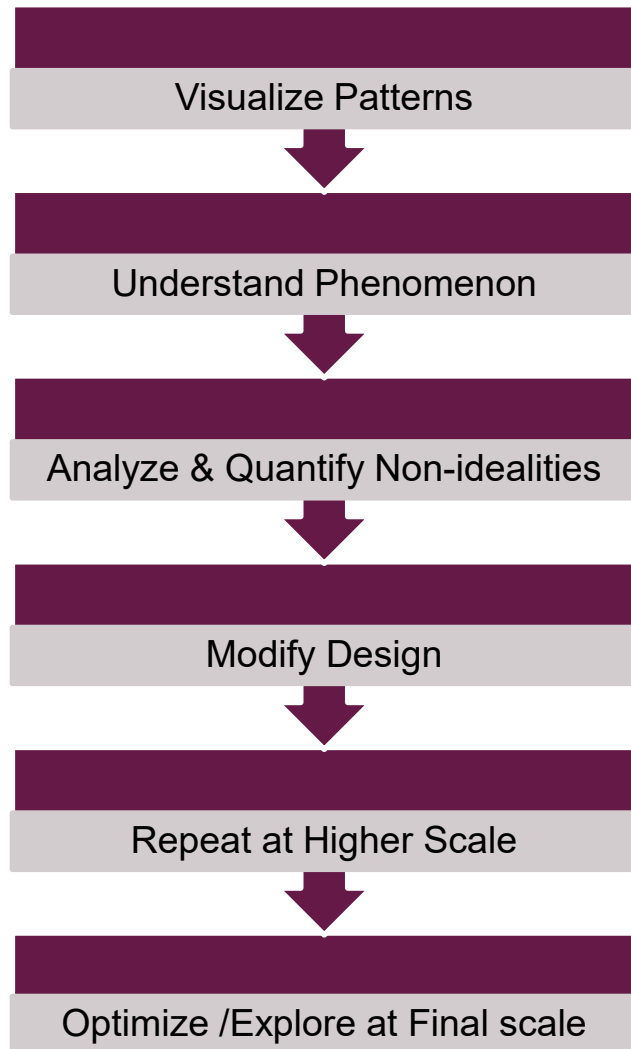
Time Step 362





# Simcenter for Mixing & Reactor Performance

## Scale-up: virtual prototyping for process sufficiency

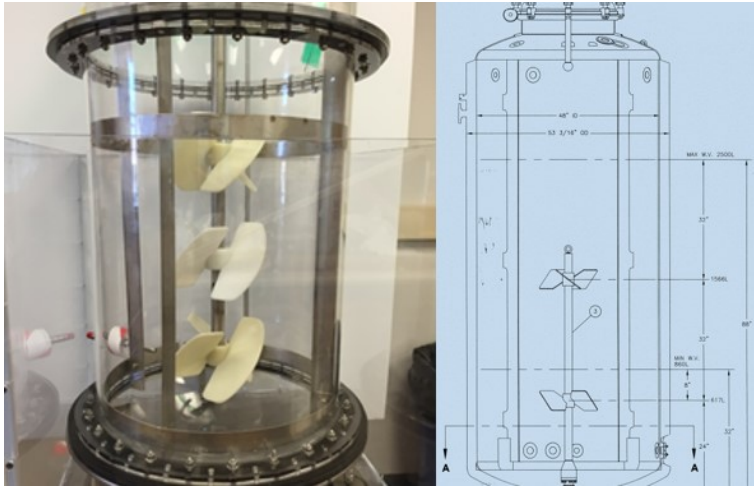


<p><b>Lab or Bench</b> Simulation + Experiment = Validation</p>	<p><b>Pilot Scale</b> Simulation + Experiment = Scale up Rules</p>	<p><b>Plant Scale</b> Only Simulation = Reliability, Confidence, = Value</p>



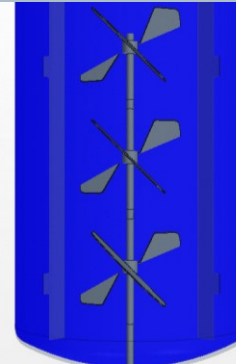
# ABEC Inc.

## Improving scale-up time and productivity



- Achieved 54% reduction in blend time in the scaled-up reactor
- Saved \$1 MM in product by getting full scale behavior right first time
- Reduced scale-up time by gaining insight of flow & mixing behavior

### Using simulation to understand mixing behavior



Baseline design to understand mixing behavior & validate against lab data



Explore effect of impeller type and number of impellers on a shaft on blend time

- Use simulation early in the scale-up process to understand hydrodynamic behavior of various design parameters and process needs

**“Simulation and the improved process understanding that it provides can have a large impact on the performance of the process, reducing time to scale-up and minimizing wasted product samples”**

Paul Kubera, Vice President, Process Technology

# Simcenter for Mixing Reactor Performance

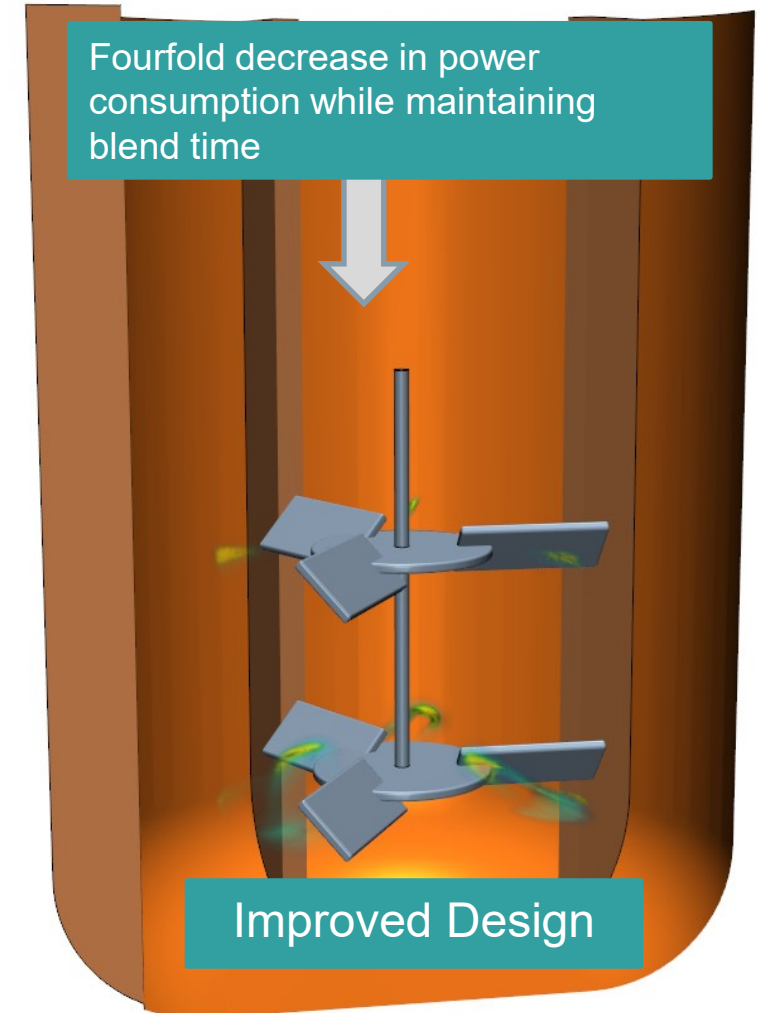
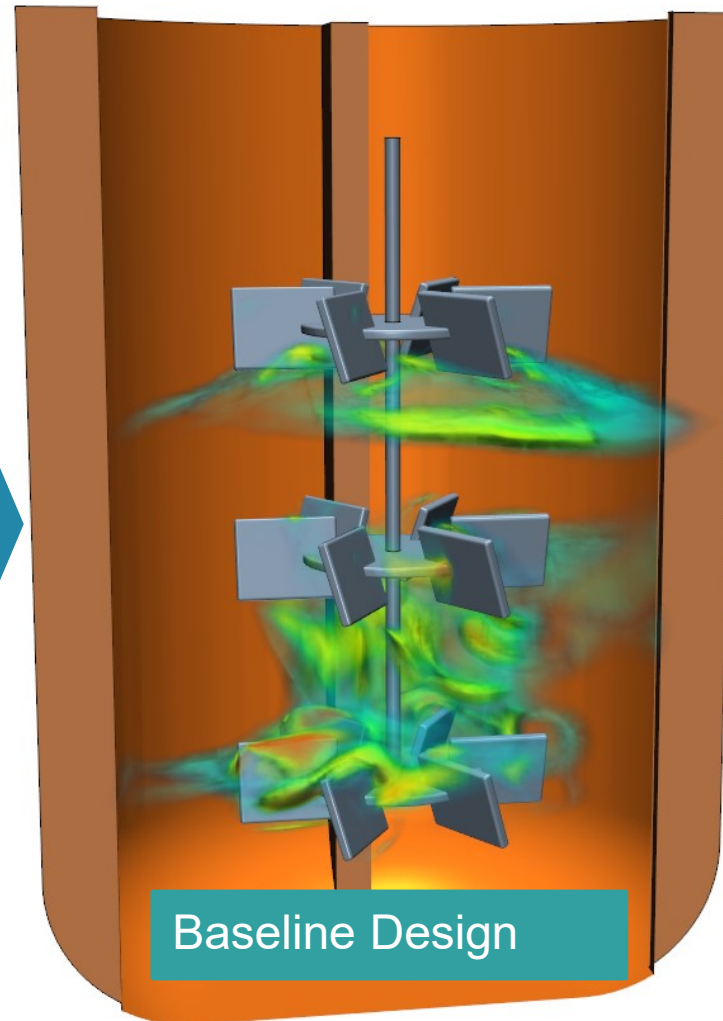
Optimizer processes: explore design and operating conditions

- Evaluate effect of design change

- Evaluate effect of operating condition change

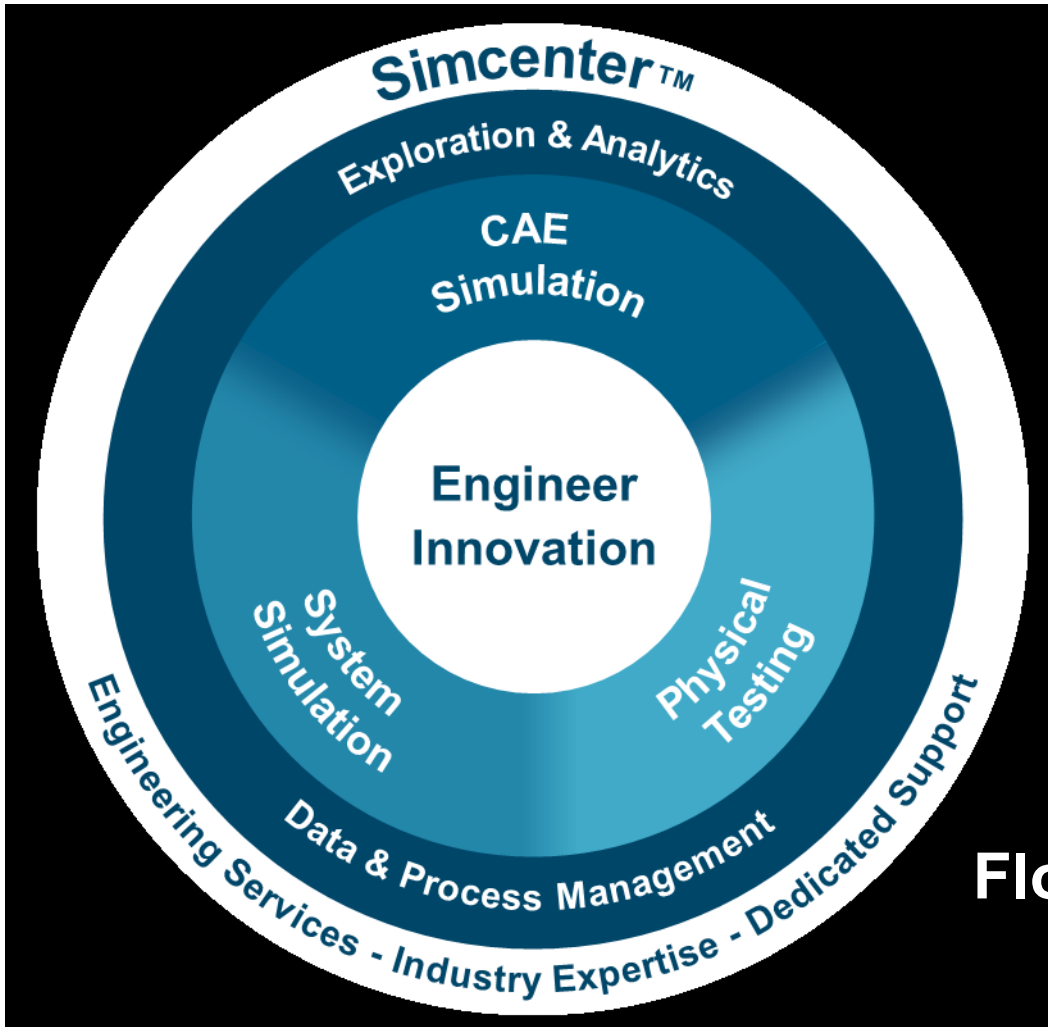
- Understand correlation of multiple variables

- Balance counteracting parameters



# Simcenter Portfolio

Engineer innovation for chemical processing applications



## Mixing and Stirred Reactors

Turbulence, blend time, mean age & RTD, heat transfer



## Multiphase Reactors

Gas & solid distribution, mass transfer, catalytic reactors



## High Temperature Processes

Thermal efficiency, heat transfer, pollution in combustion



## Particulate Processes

Fluidize beds, particle mixing, particle heat transfer



## Flow Distribution & Separation Processes

Cyclones, filtration, distillation columns





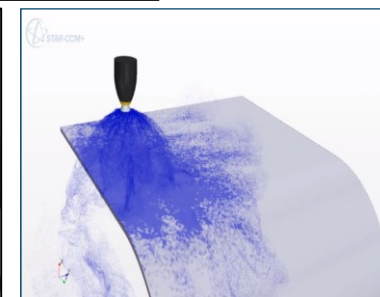
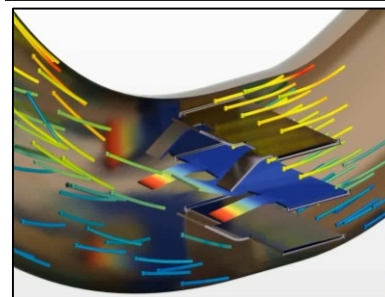
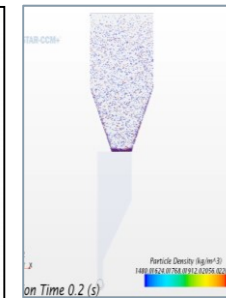
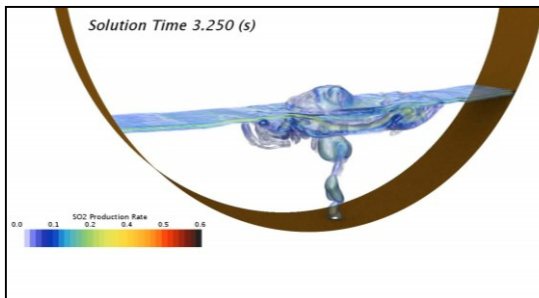
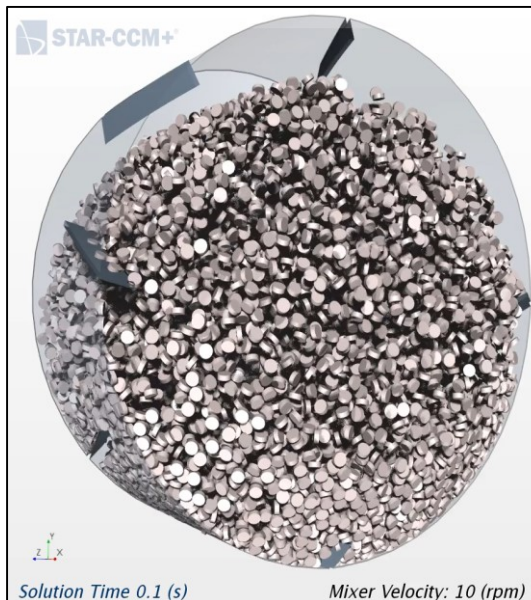
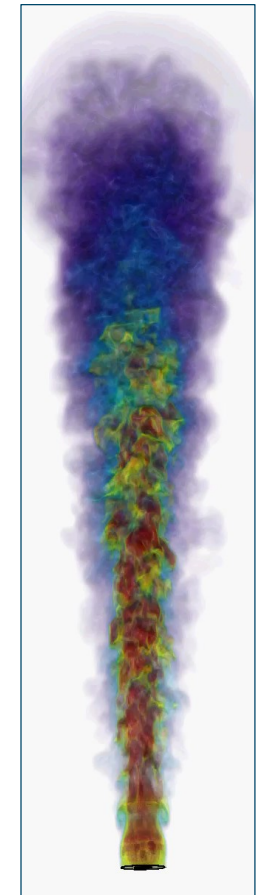
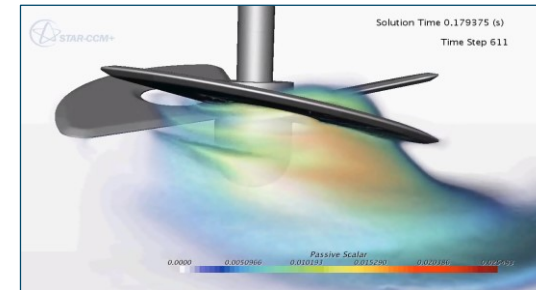
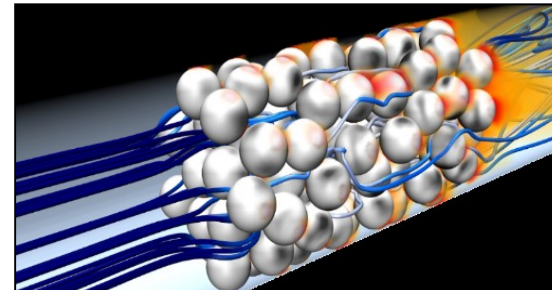
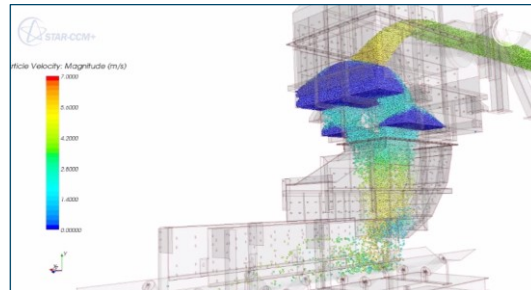
# Simcenter STAR-CCM+

## An integrated multiphysics solution for process efficiency

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### Realism with multiphysics

- Fluid dynamics
- Multiphase flows
- Reacting flows
- Solid mechanics
- Particle flows
- Rheology
- Electrochemistry
- Electromagnetics
- Aero-acoustics
- Fluid-structure interaction
- Conjugate heat transfer



# Key Requirements

## Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

Powerful Data Analysis

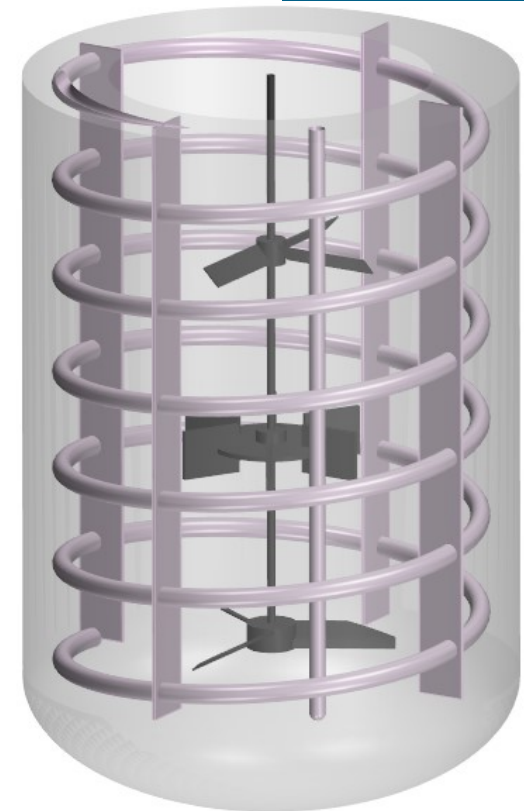
Workflow Automation

Intelligent Design Exploration

- Ability to import CAD from a variety of sources, including directly from external CAD packages
- Tools to create, modify or repair complex geometry



STAR-CCM+



# Key Requirements

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

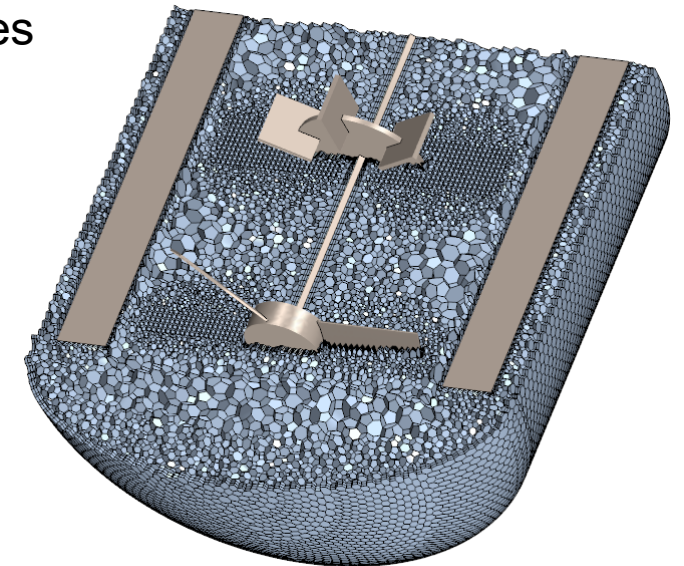
Powerful Data Analysis

Workflow Automation

Intelligent Design Exploration

STAR-CCM+

- Robust meshing to capture complex geometry features
- Detailed resolution of both fluid and solid regions for heat transfer simulation at walls and around impeller
- Robust prism layer mesh resolves turbulent boundary layer
- Specialized thin mesher for meshing thin solids involved in heat transfer calculations
- Easy control of local mesh refinement





# Key Requirements

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

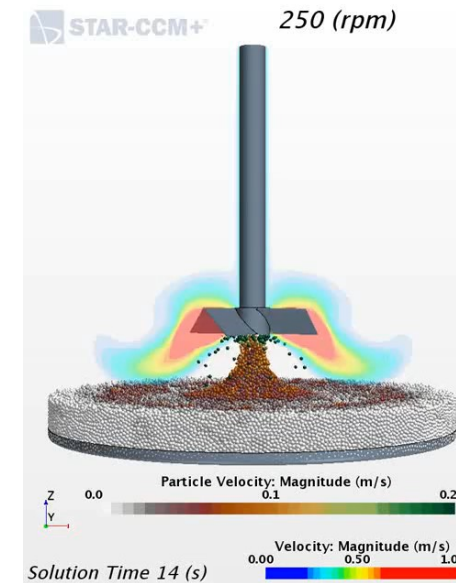
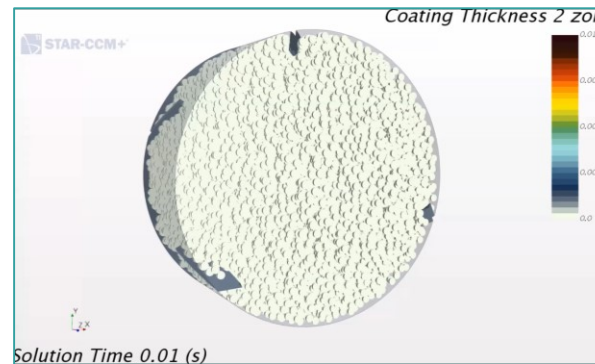
Powerful Data Analysis

Workflow Automation

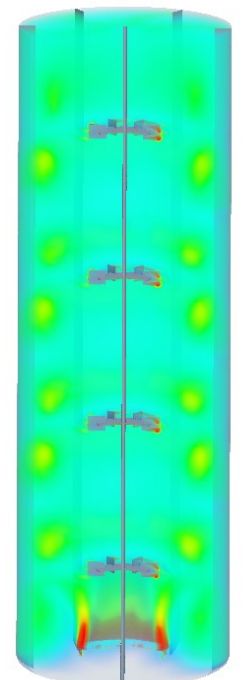
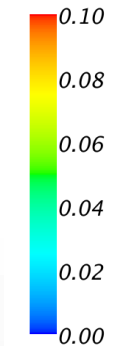
Intelligent Design Exploration

- Ability to model liquids, gases and solids dispersed in liquids
- Heat and mass transfer between phases
- Accurate prediction of conversion and yield
- DEM Method included

**STAR-CCM+**



Volume Fraction of Air



# Key Requirements

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

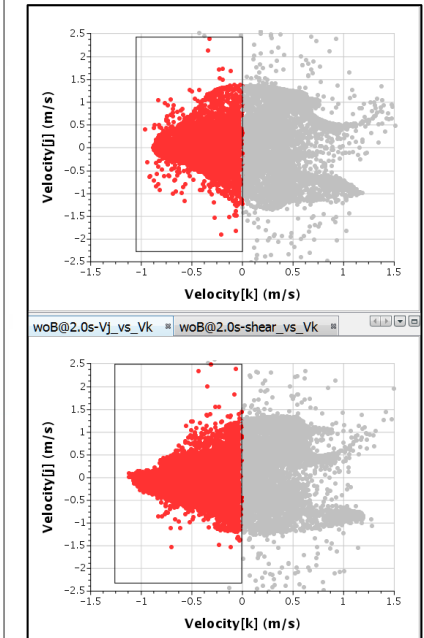
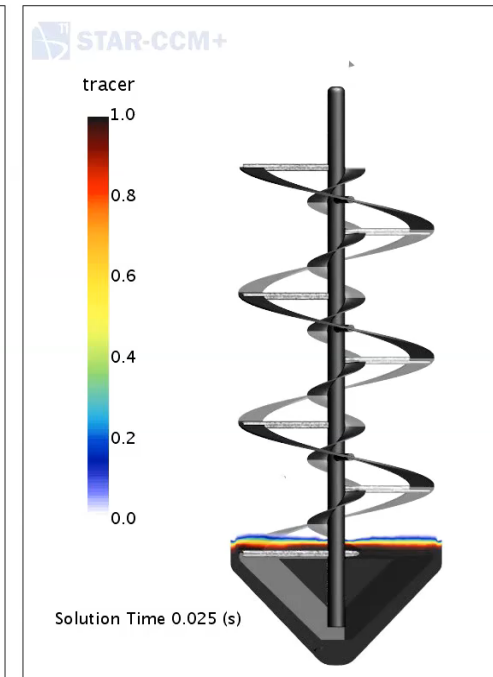
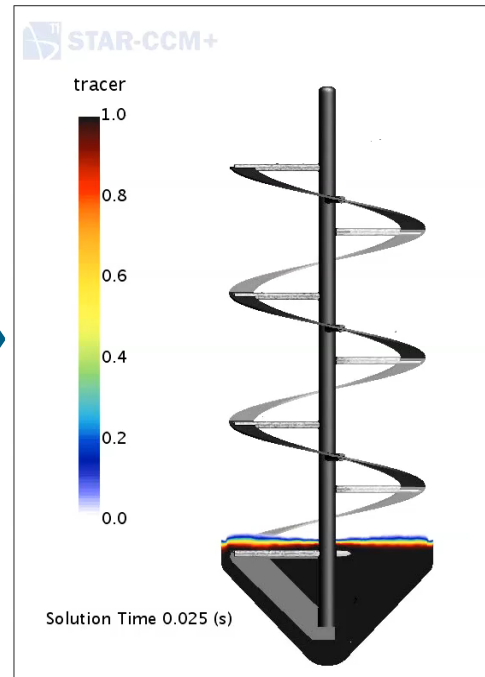
Powerful Data Analysis

Workflow Automation

Intelligent Design Exploration

**STAR-CCM+**

- Powerful post processing and visualization
- Tools to understand complex interdependencies



# Key Requirements

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

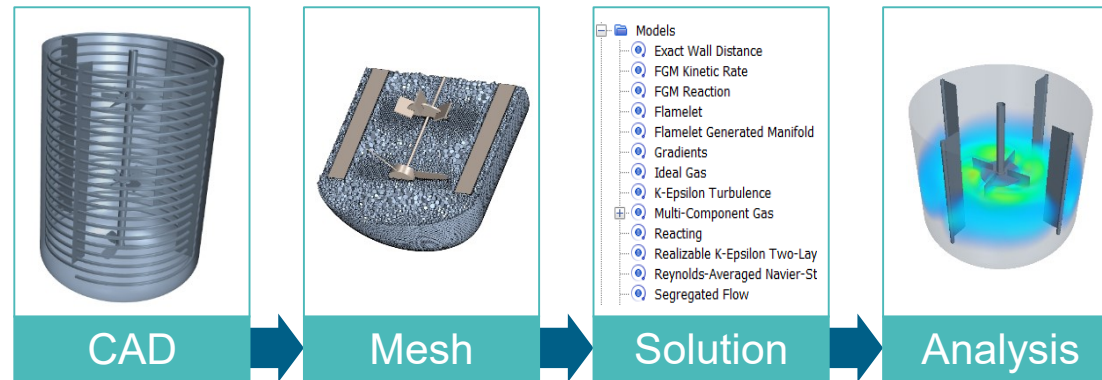
Powerful Data Analysis

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STAR-CCM+

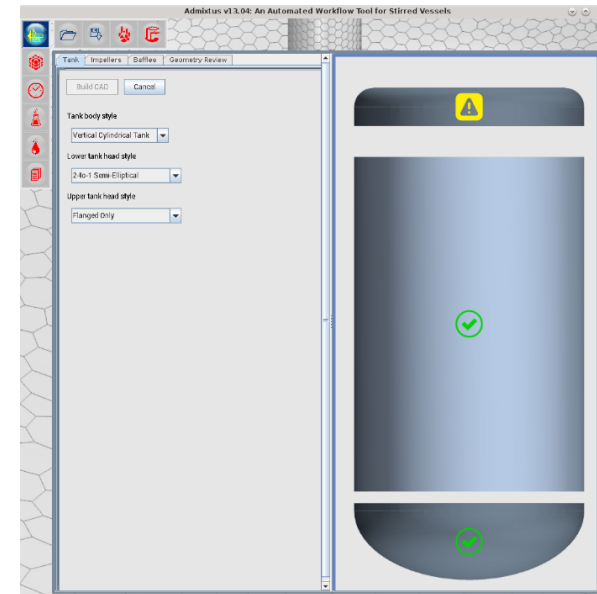
- Convenient user interface for different stages of engineering analysis
- Ability to extend the workflow seamlessly for design exploration studies
- Features for efficient and extensible simulation framework like filters and tagging to facilitate automation and enhance usability



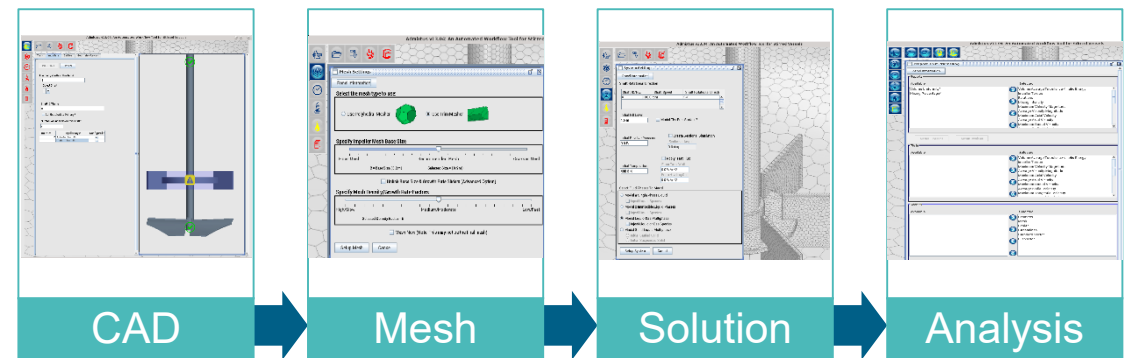


# Workflow Automation with Admixtus

- **Admixtus**, an add-on for STAR-CCM+, is a dedicated tool for design and simulation of mixing vessels
- Setup fully parametrized mixing vessel simulation quickly
  - CAD including vessel, impellers, baffles and internals, selectable from internal libraries
  - Mesh settings based on best practices
  - Physics setup
  - Post-processing including scenes, reports, plots and summaries in Excel-format
- Customizable
- Excellent basis for design space or operating condition exploration



Admixtus



# Key Requirements

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

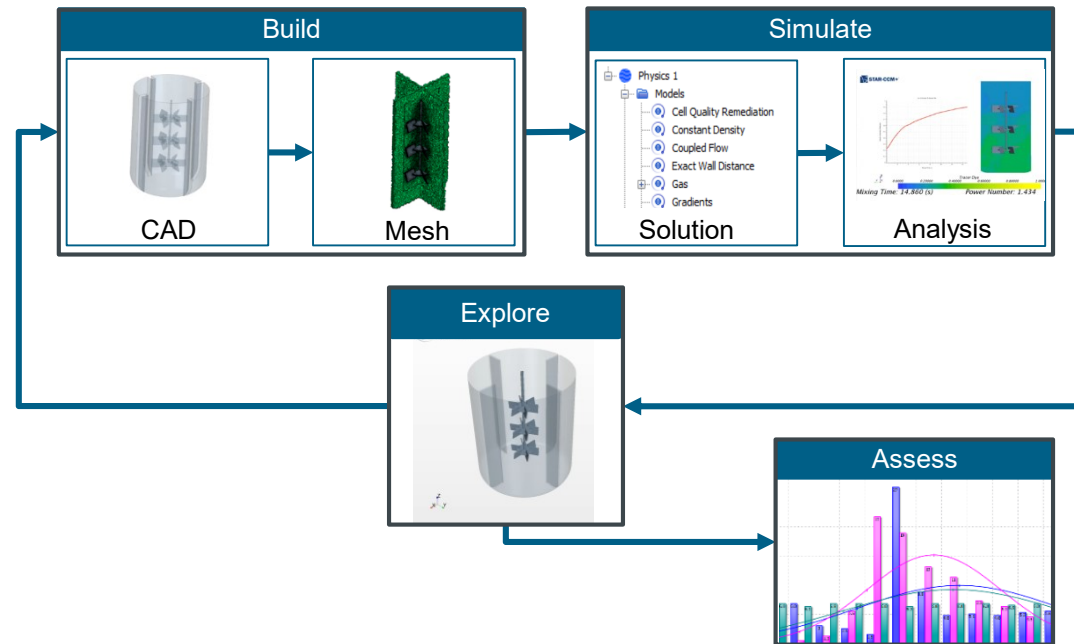
Powerful Data Analysis

Workflow Automation

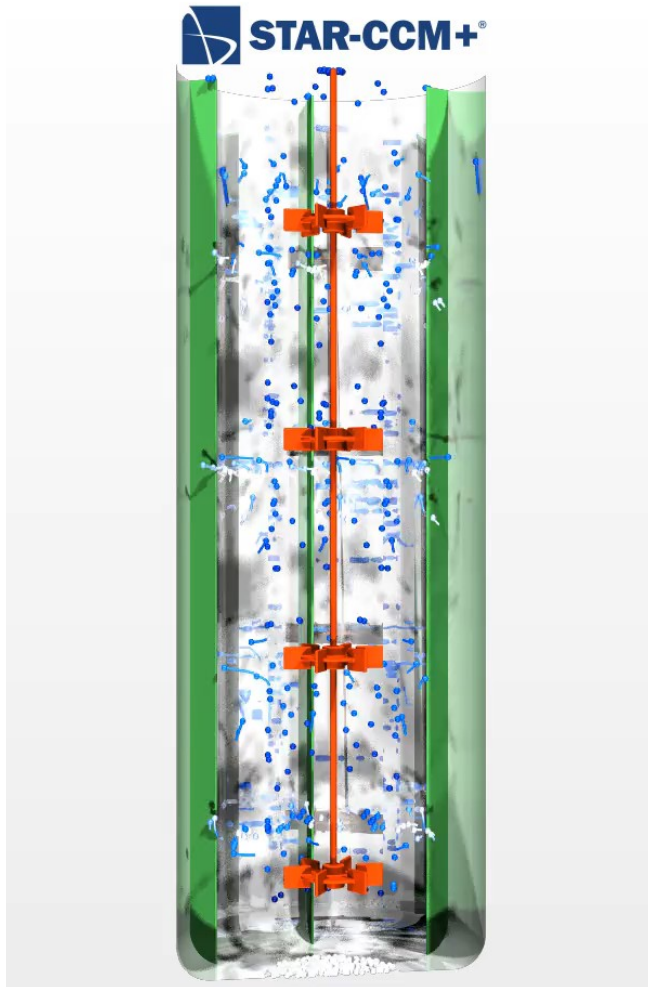
Intelligent Design Exploration

STAR-CCM+

- Intelligent search and design space exploration to improve mixing vessel performance



# Modeling Requirements



Numerical optimization requires that all relevant physics is modeled appropriately.

Fermentation reactors are highly complex systems:

- Fluid dynamics in multiphase, flow field, gas holdup
  - Non-Newtonian rheology
- Mass transfer (interfacial area)
  - Size distribution
  - Coalescence & break-up
- Micro-organism/reaction modeling
  - Time-scales are vastly different



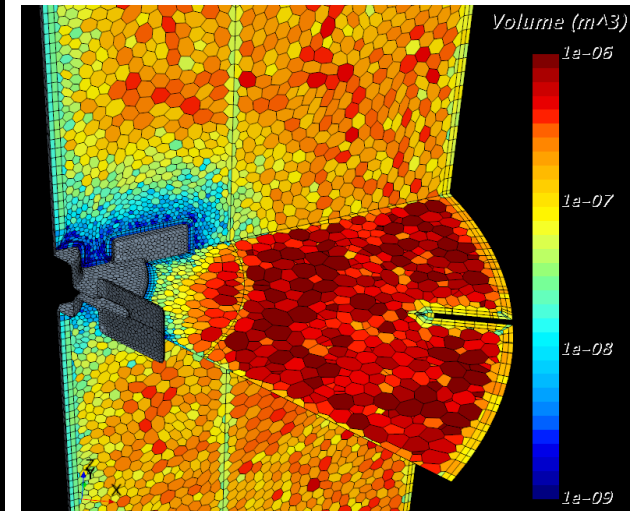
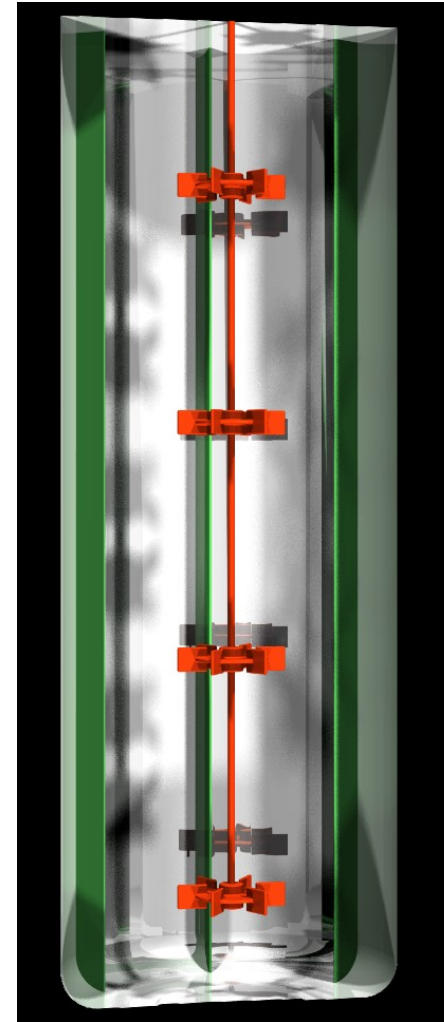
# Modeling

## Optimization goals

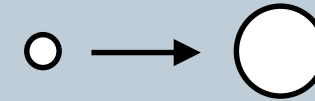
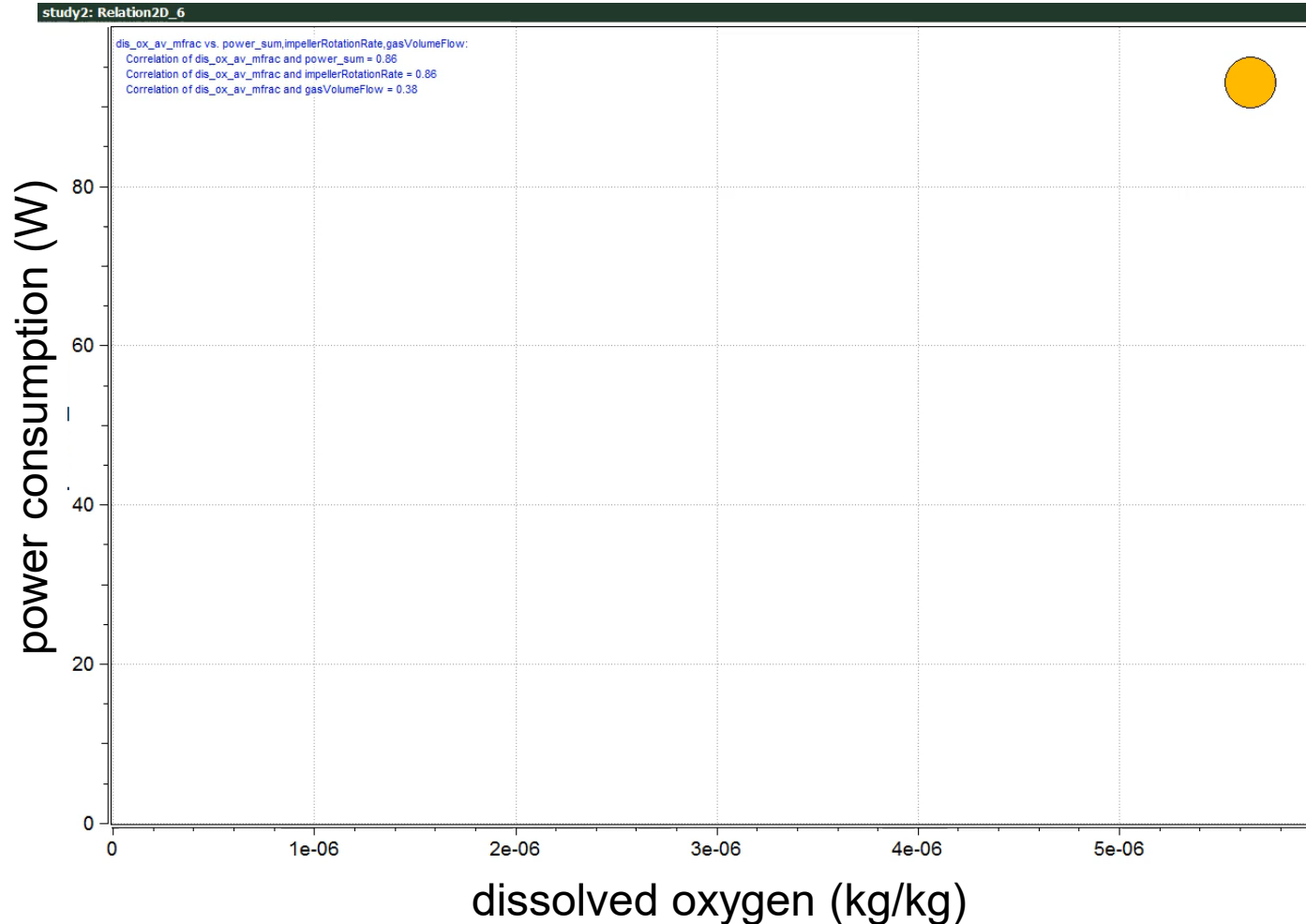
- Minimize total power consumption
  - Compressor:  $P = \dot{V} dp$
  - Impeller:  $P = M \omega$
- Maximize volume-averaged dissolved oxygen
- Variables:  $\dot{V} = 20\text{-}200$  lpm;  $n = 150\text{-}450$  rpm
- Ensure local stress is below  $\tau = 15$  1/s

## Modeling

- Multi-component EMP, steady-state
- gas: nitrogen + oxygen
- Liquid: water + dissolved oxygen
- k- $\epsilon$  turbulence modeling
- Tomiyama drag force & Richardson-Zaki correction
- Oxygen mass transfer
- S-Gamma population balance



# Operating Condition Exploration



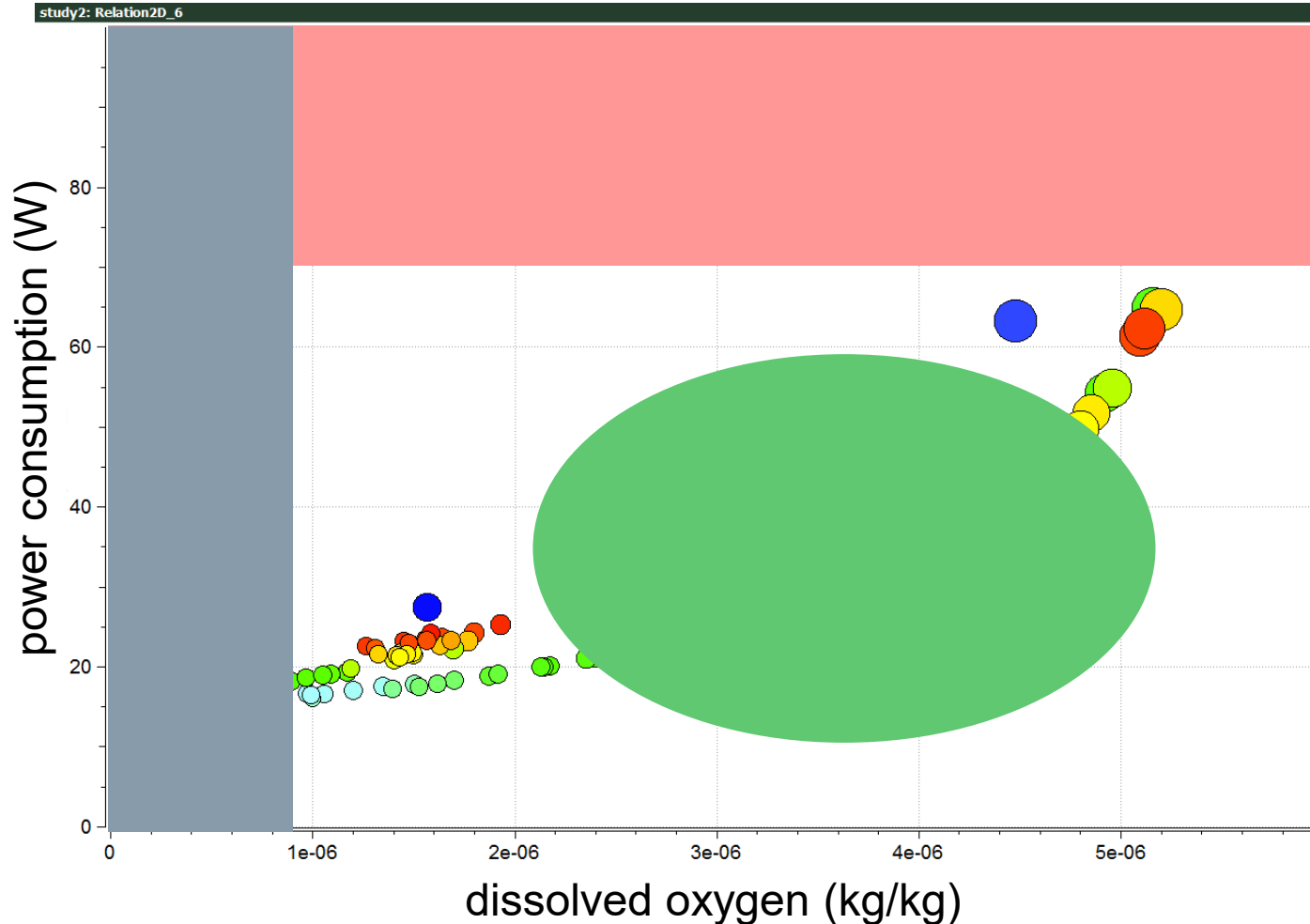
Size: impeller rotation rate ↑



Color: sparger volume flow

- 164 operating conditions (10-30 min / simulation @16 CPUs)
- Pareto front consists of good operation conditions
- Trade-off between power consumption and mass transfer

# Operating Condition Optimization

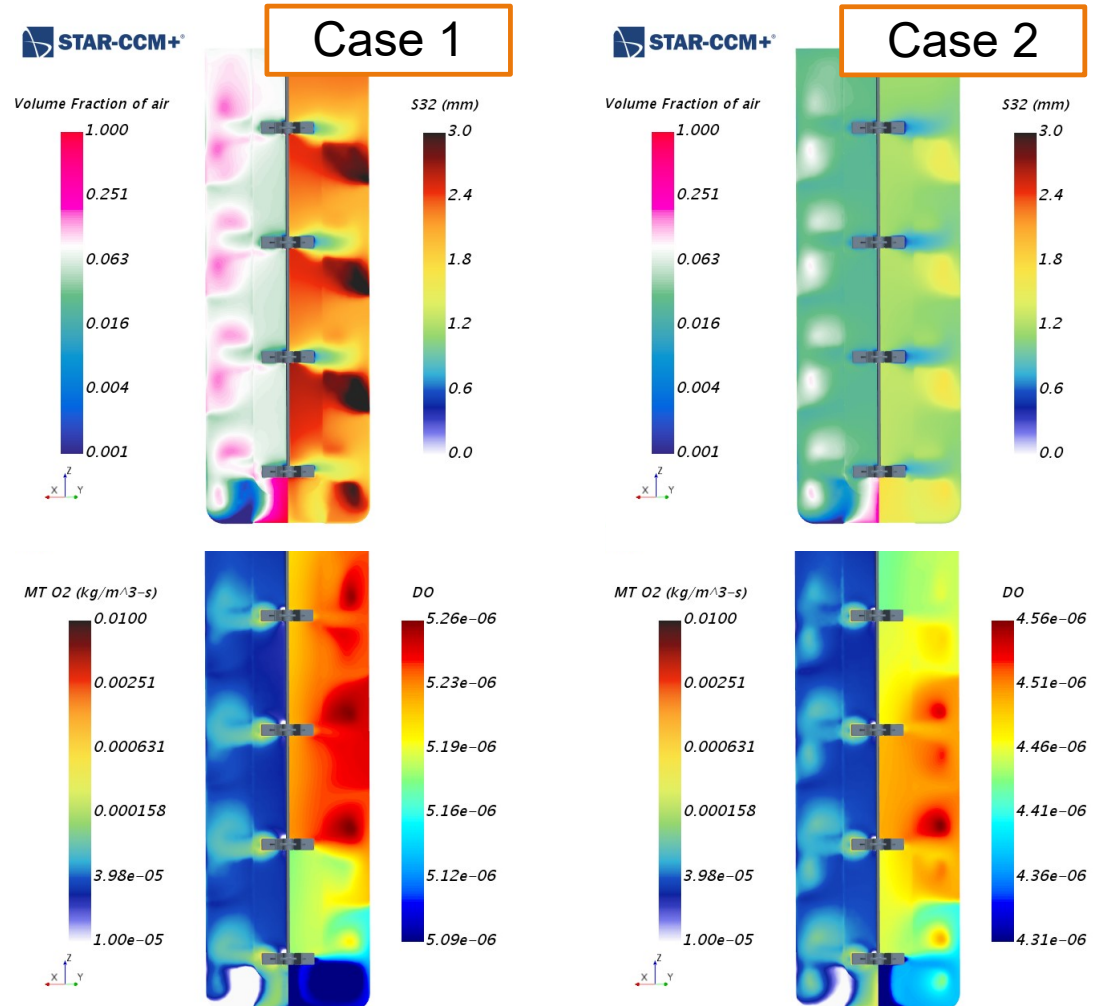
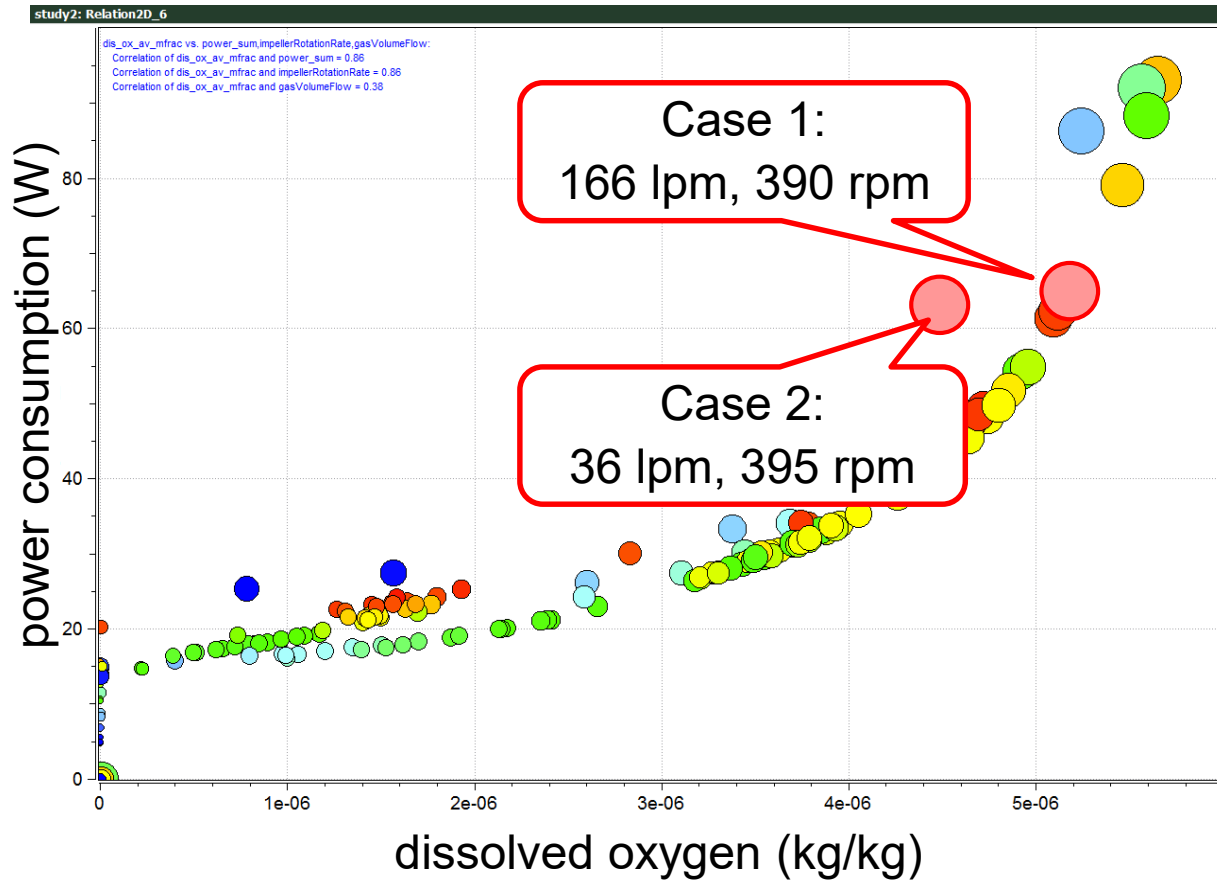


Strain rate too high due to agitation rate.  
Power consumption very high, too.

Mass transfer too small for  
given yeast oxygen uptake rate.

Good combination of sparger flow and  
agitation rate has to be chosen.

# Operating Condition Optimization





# Summary

- **Predict and understand real-world behavior**
- **Explore many design variants and operating conditions**

Complex Geometry Handling

Flexible & Robust Meshing

Multiphysics Modeling

Powerful Data Analysis

Workflow Automation

Intelligent Design Exploration

Admixtus & STAR-CCM+

- Tools to create and process parametrized CAD and generate meshes from complex geometries with ease
- Comprehensive suite of multiphase and reaction models
- Fully integrated environment allows for easy and powerful analysis and visualization of results
- Powerful design exploration and optimization tools leverage the pipelined workflow
- Admixtus to setup and handle mixing vessel simulation more efficiently

# Redefining Performance Engineering for the Digital Twin

