

Lectures on Modeling

# Reacting Flows

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in Stirred Tanks

André Bakker

2006

# Contents

Overview (3)

I. Modeling flow fields in stirred tanks (6)

II. Modeling material/species transport (46)

III. Blend times in stirred tanks (87)

IV. Modeling chemical reactions with CFD (130)

V. Fermenter specific modeling topics (175)

# Overview

## Welcome!

- This document contains the lectures that I gave for the Reacting Flows (ENGS 199) class at the Thayer School of Engineering at Dartmouth College in 2006.
- Reacting flows is a wide field, including combustion, polymerization, cracking, fermentation, etc. In this class the focus was on modeling of liquid reaction in stirred tanks as used in the process industries.
- This class had three instructors: Prof. Lee Lynd on biofuel fermentation, Richard D. LaRoche on mixing vessel design, and me on CFD modeling of mixing vessels. This document only includes my lectures on CFD.
- These lectures are provided – at no charge - for educational and training purposes only.
- You are welcome to include parts of these lectures in your own lectures, courses, or trainings, provided that you include this reference:

Bakker A. (2006) *Lectures on Modeling Reacting Flows in Stirred Tanks*. [www.bakker.org](http://www.bakker.org).

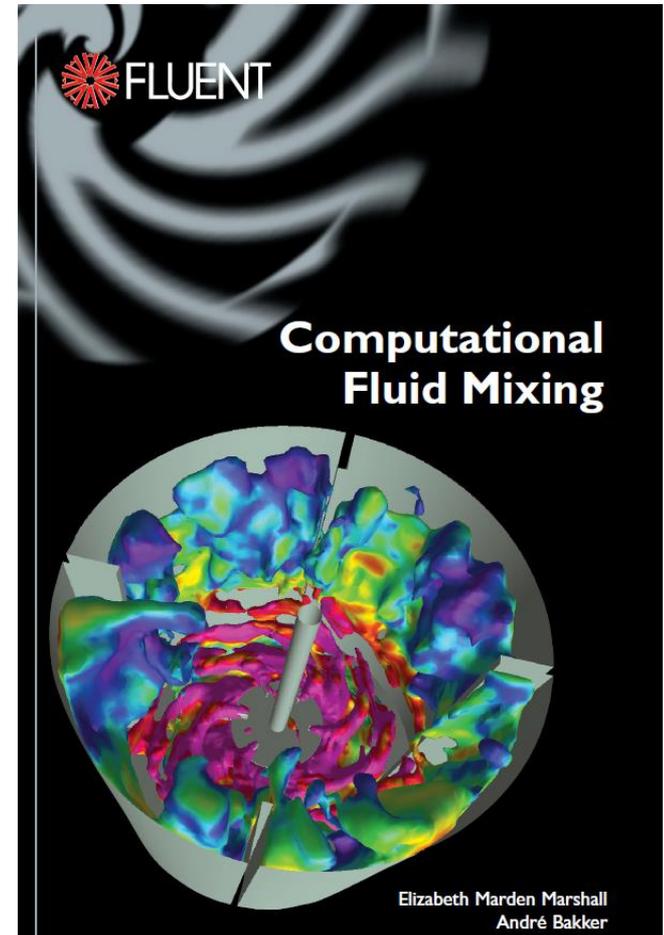
# About the author

- I received my Doctorate in Applied Physics from Delft University of Technology in the Netherlands in 1992. In addition, I obtained an MBA in Technology Management from the University of Phoenix. From 1991 to 1998 I worked at Chemineer Inc., a leading manufacturer of fluid mixing equipment. In 1998 I joined Fluent Inc., the leading developer of computational fluid dynamics software. Since 2006 I have been with ANSYS, Inc.
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# Recommended reading

- *Computational Fluid Mixing* by Marshall and Bakker. 2002. ISBN 0-9719532-0-1
- Available as a PDF file on [www.bakker.org](http://www.bakker.org) and [researchgate.net](http://researchgate.net)
- *This 154-page booklet covers many topics in the field of simulating mixing processes using CFD. A printed version of this booklet was published by Fluent Inc. The booklet starts with a great Foreword by Prof. J.M. Smith that discusses the progress of understanding of mixing throughout the ages. It continues with an easily understandable Introduction to CFD; an Introduction to Numerical Methods; a chapter on Stirred Tank Modeling Using Experimental Data; a section on Stirred Tank Modeling Using the Actual Impeller Geometry; an overview of Evaluating Mixing from Flow Field Results; a very nice suite of Application Examples; and Closing Remarks giving you useful modeling advice.*



# Modeling Flow Fields in Stirred Tanks

## Reacting Flows - Lecture I

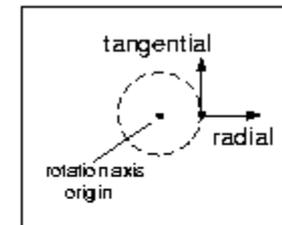
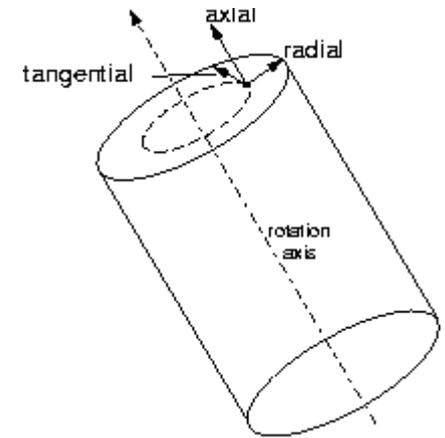
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# Outline

- Coordinate systems.
- Impeller modeling methods.
  - Transient vs. steady state.
  - Different impeller types.
- Model setup.
  - Numerics recommendations.
  - Turbulence models.
- Post-processing.
  - Power number and torque.
  - Flow rates and pumping number.
  - Shear rates.

# Coordinate systems

- Coordinate systems:
  - Cartesian: x, y, z coordinates.
  - Cylindrical: radial, tangential, axial (r,  $\theta$ , h)
  - Conversion (if h is in the z-direction):  
 $x = r \cos\theta$ ;  $y = r \sin\theta$ ;  $z = h$ .
- Velocities in the Cartesian system are usually denoted as  $v_x=u$ ,  $v_y=v$ ,  $v_z=w$  which are the velocities in the x, y, and z-direction respectively.
- Notation in the cylindrical system:
  - Axial velocity (h-direction):  $v_h=u$ .
  - Radial velocity (r-direction):  $v_r=v$ .
  - Tangential, or swirl velocity ( $\theta$ -direction):  $v_\theta=w$ .
  - Conversion (if h is in the z-direction):  
 $v_x=v_r \cos\theta - v_\theta \sin\theta$ ;  $v_y=v_r \sin\theta + v_\theta \cos\theta$ ;  $v_z=v_h$ .



# What can you calculate?

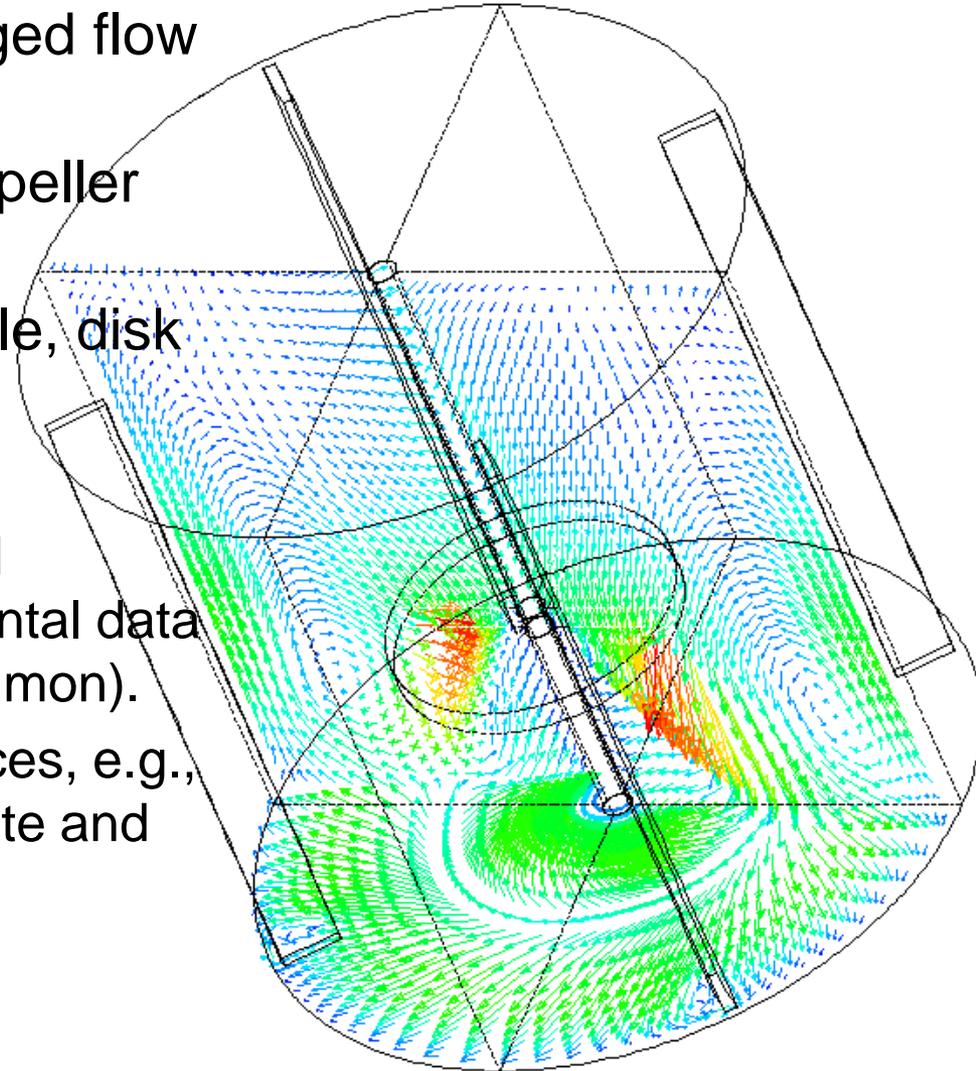
- Flow field:
  - Pumping rate.
  - Average velocities in fluid bulk, and important locations, such as near feeds, at the bottom, around cooling coils.
- Pressure field:
  - Most commonly used to calculate impeller torque and power draw.
  - Other forces: such as on baffles.
- Additional physics:
  - Particle tracking.
  - Mixing times.
  - Residence time distribution (RTD).
  - Temperature.
  - Species mixing.
  - Reactions.
  - Multiphase flow, such as solids suspension, or gas dispersion.

# Modeling the impeller

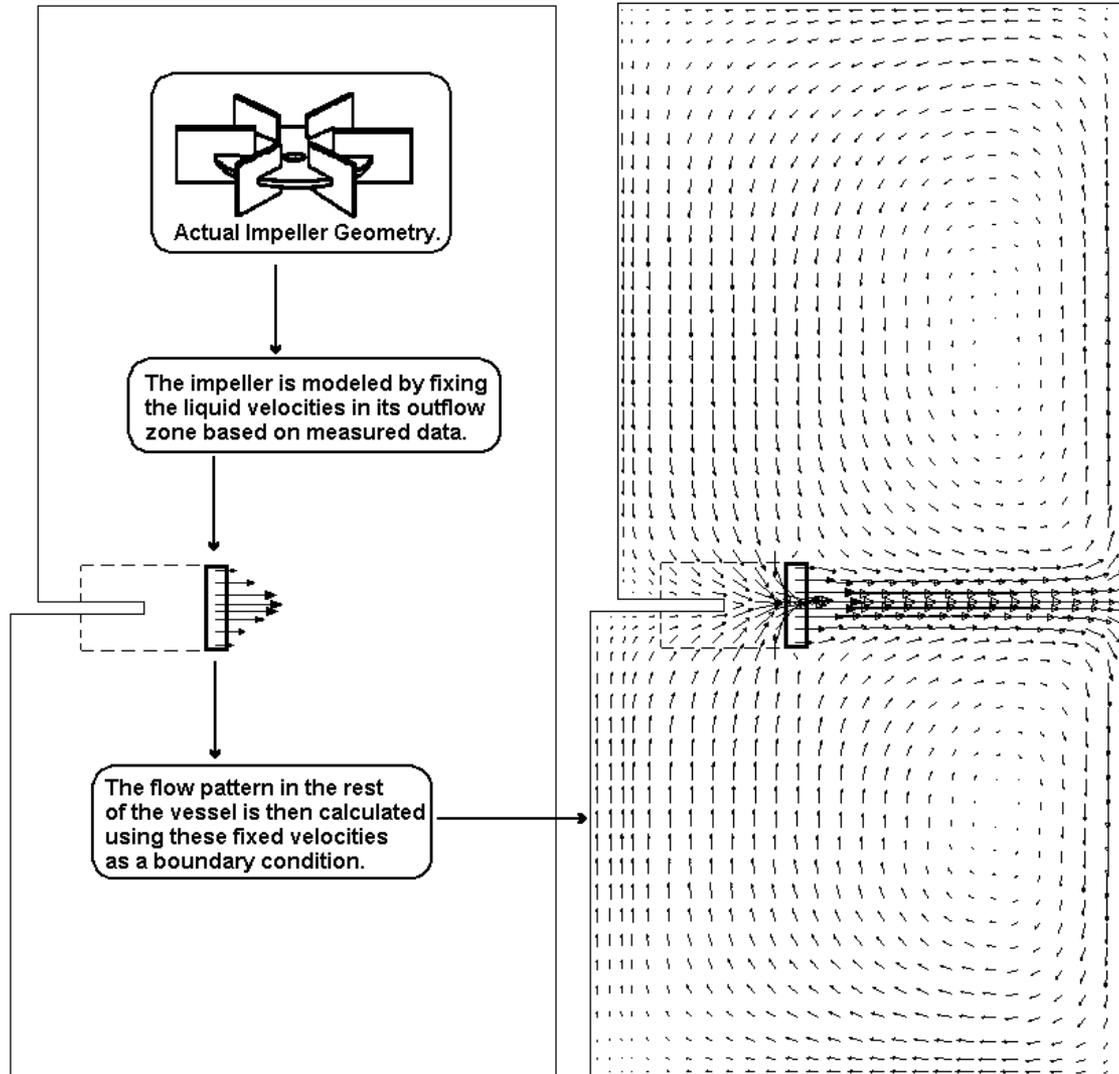
- The main difficulty lies in modeling the motion of the rotating impeller past the stationary tank walls and baffles.
- There are many different methods to do this:
  - Time averaged methods (2-D or 3-D).
    - Time averaged flow field without any details about the flow around the impeller blades.
    - With varying levels of empirical input.
  - Snapshot methods (3-D).
    - Calculate the flow field for one impeller position only.
  - Transient methods (3-D).
    - Model the actual motion of the impeller.
    - Deforming meshes or non-deforming, sliding meshes.

# Time averaged methods

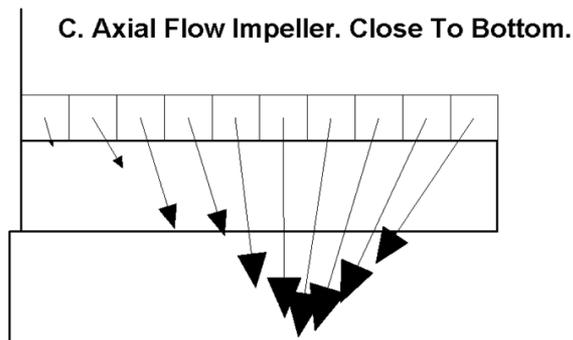
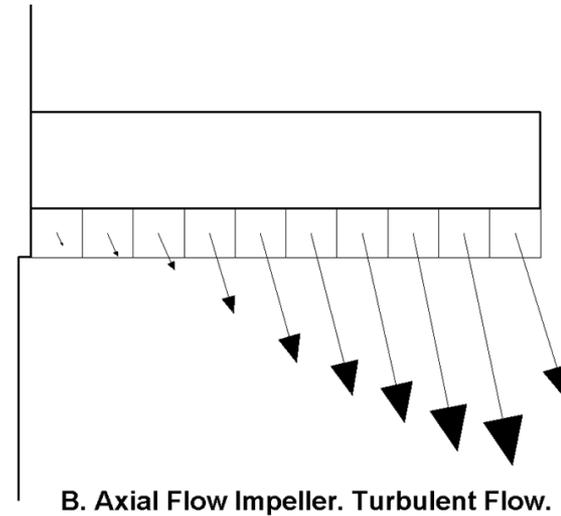
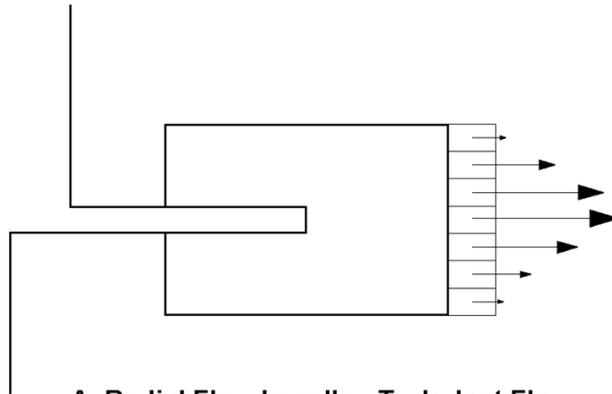
- Objective: calculate time averaged flow field in the vessel.
- Ignore details of flow around impeller blades.
- Impeller is replaced with a simple, disk style region → easy to mesh!
- In the impeller region:
  - Prescribe (“fix”) time averaged velocities, e.g., from experimental data (most accurate, and most common).
  - Or prescribe momentum sources, e.g., from airfoil theory (less accurate and less common).
- Fast and easy to solve!



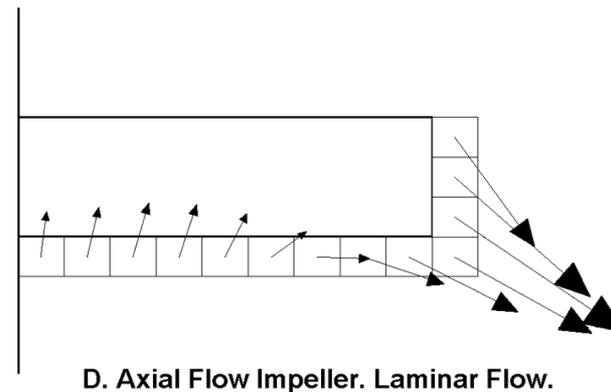
# Prescribing velocities



# Where to prescribe velocities



Pumping downwards close to the bottom: prescribing velocities at the inflow works better in practice.



At low Reynolds numbers, prescribe at two of the three surfaces.

# How to scale

- Velocities are usually measured at lab scale.

$v = \text{velocity (m/s)}$

$r = \text{radial coordinate (m)}$

$R = \text{impeller radius (m)}$

$D = 2R = \text{impeller diameter (m)}$

$N = \text{impeller rotational speed (1/s)}$

$v_{tip} = \pi ND = \text{impeller tip speed (m/s)}$

- They can be scaled to full scale as follows:

$$v_{fullscale}(r/R) = v_{lab}(r/R) \cdot \frac{v_{tip,fullscale}}{v_{tip,lab}}$$

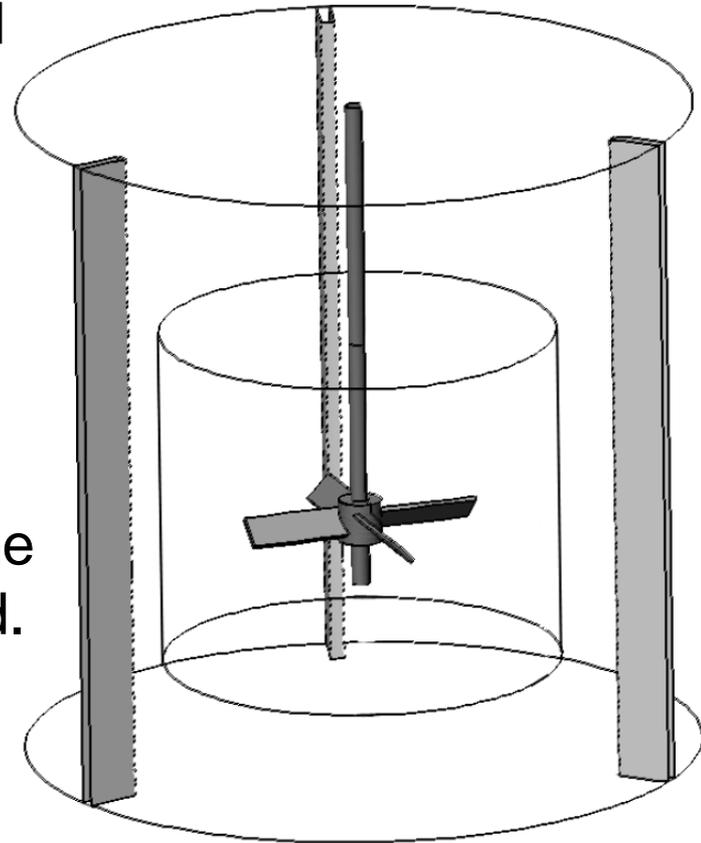
- For turbulent flows, also prescribe measured turbulence intensity.
- Ideally, velocity data are measured in a geometrically similar system, at the same Reynolds number.

# When to use a time averaged method

- It is the only impeller modeling method suitable for 2-D calculations.
- The main advantages for 3-D calculations are:
  - Easy meshing with fewer cells than other methods.
  - Fast flow field calculations.
  - Fast species mixing and particle tracking calculations.
- The main disadvantage is:
  - You need velocity data for the particular impeller at the particular Reynolds number. Note: this data can come from experiment or other CFD simulations.
  - Hard to use for multiphase flows (e.g., gas-liquid flows).
- When is it useful: if you want to do many parametric reaction studies for the same system.

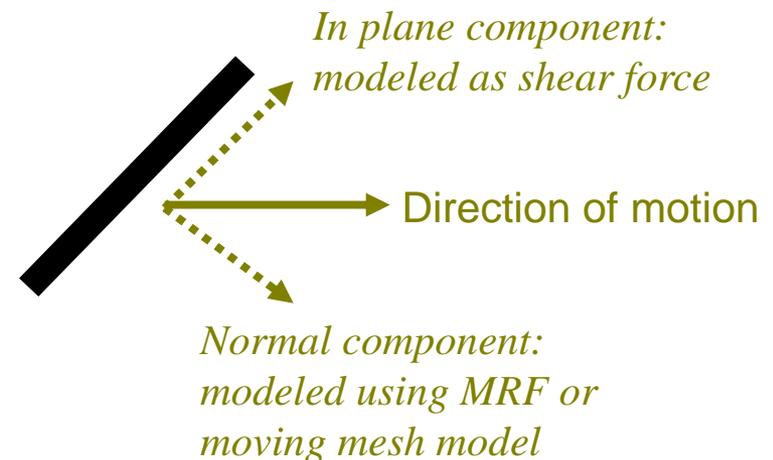
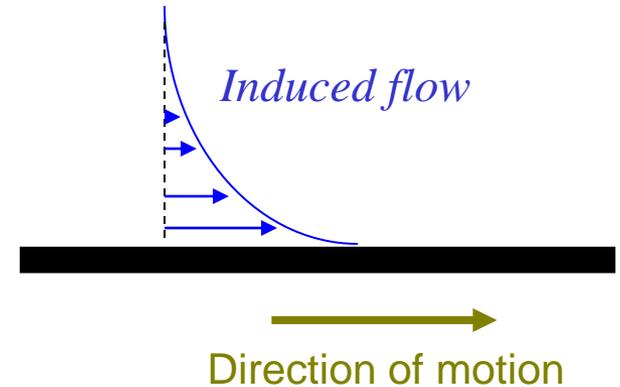
# Steady-state methods

- Calculate one flow field for one given impeller position.
- Steady state calculation: ignores flow field history effects.
- Mesh the actual shape of the impeller.
- No need to input experimental data.
- In FLUENT this is done by having a separate fluid region that contains the impeller.
- For this region, a Moving Reference Frame (MRF) with a rotational motion is specified.



# Wall motion

- In plane motion:
  - The direction of motion is parallel to the wall.
  - Flow is induced by shear forces.
  - This can be modeled by simply specifying a wall velocity.
- Out of plane motion.
  - The direction of motion is not parallel to the wall.
  - Flow is induced by shear forces and by normal forces (“pushing”).
  - The effect of the shear forces is modeled by specifying a wall velocity.
  - The effect of the normal forces requires the use of a moving reference frame (steady-state) or moving mesh condition (transient) for the fluid region in which the wall is contained.

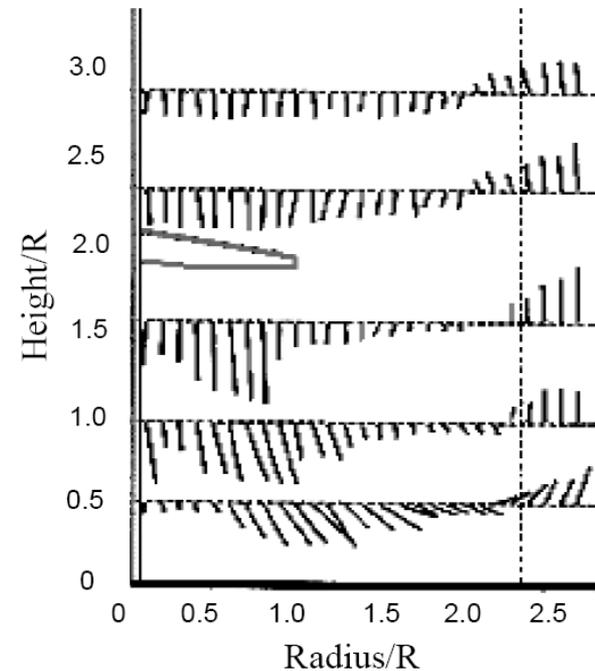
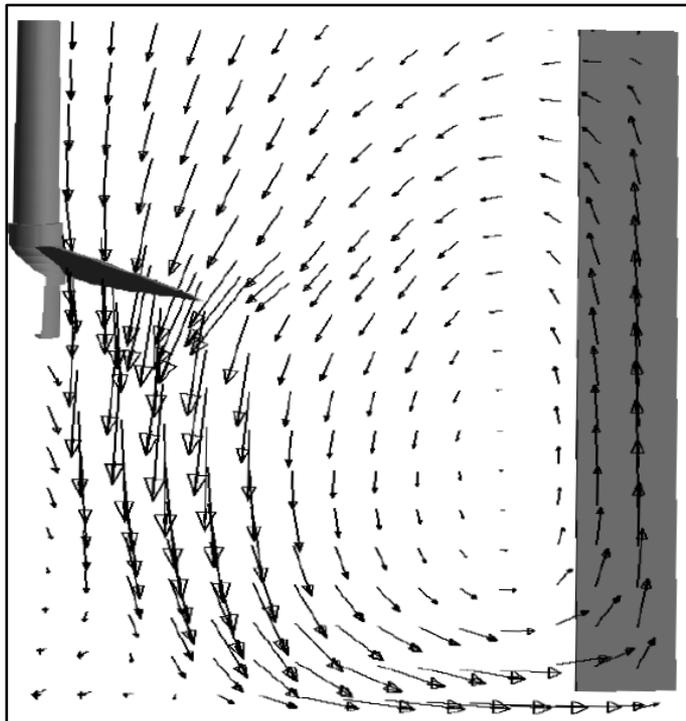
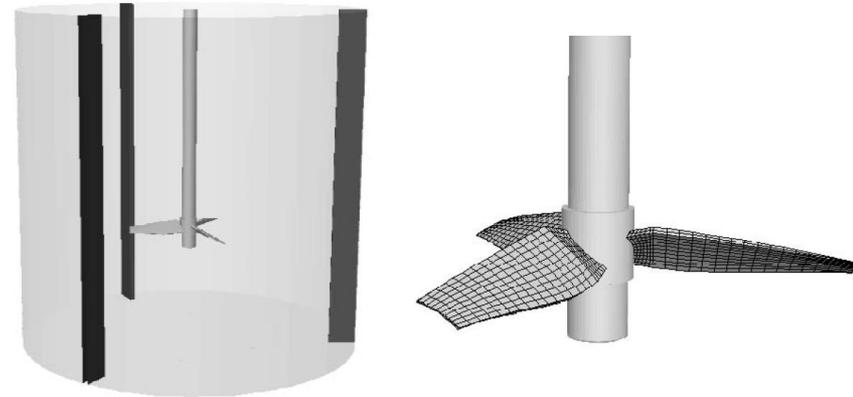


# MRF method

- Solving:
  - In the MRF zone, the flow field is calculated by solving the Navier-Stokes equations in a rotating reference frame.
  - In the remainder of the vessel, the flow is calculated by solving the equations in a stationary reference frame.
  - The flow fields are connected at the interior surfaces separating the two regions.
- Requirements:
  - The impeller zone needs to be a volume of revolution around the impeller shaft (e.g., a cylinder or sphere).
  - It is acceptable if stationary surfaces are part of the MRF zone, if they are a surface of revolution around the axis (e.g., the tank bottom or cylindrical vessel walls; but not the baffles). Need to specify zero velocity in the absolute reference frame for such surfaces.

# MRF method - validation

- Marshall et al. (1999).
- A310 impeller in a 1.2m vessel.
- Predicted power number of 0.29 compared to 0.30 in experiment.
- Predicted pumping number of 0.52 compared to 0.56 in experiment.



Marshall, E. M., Y. Tayalia, L. Oshinowo, and R. Weetman, *Comparison of Turbulence Models in CFD Predictions of Flow Number and Power Draw in Stirred Tanks*, Presented at Mixing XVII, Banff, Alberta, Canada, August 15-20, 1999

# When to use MRF

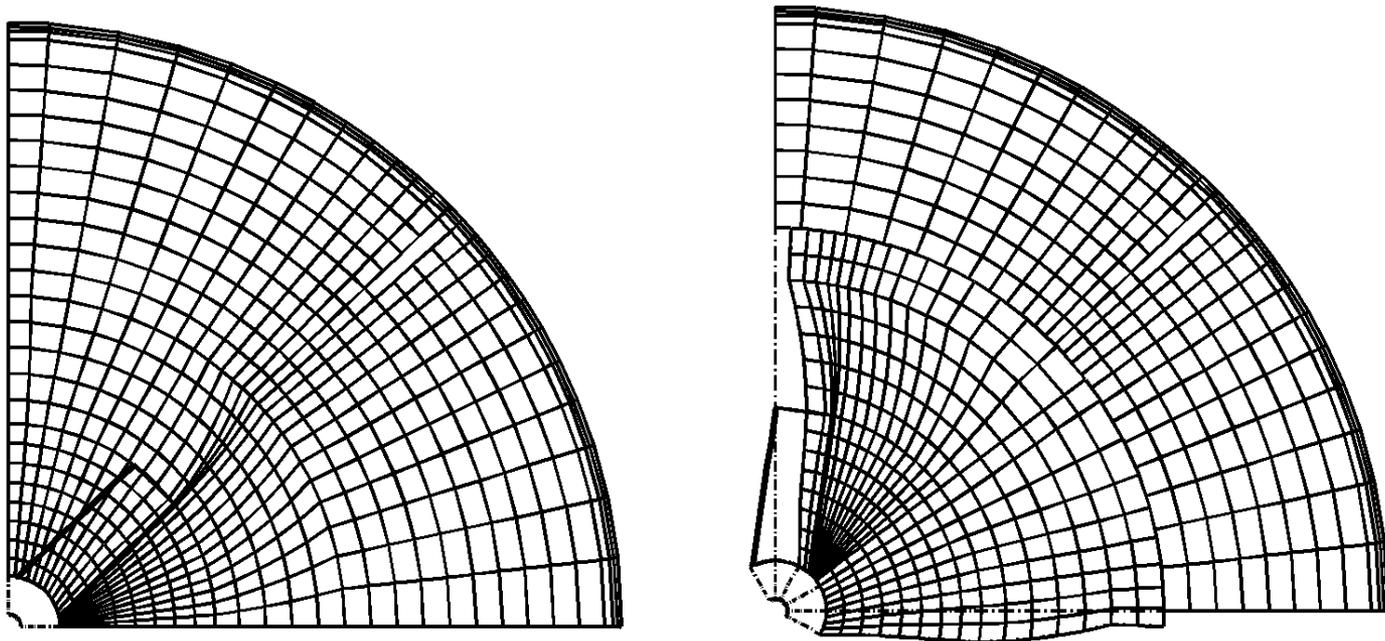
- When experimental impeller data is not available.
- When the impeller geometry is known.
- When relatively short calculation times are desired.
- When transient flow field effects are not important:
  - Impellers on a central shaft in an unbaffled cylindrical vessel.
  - In baffled vessels when impeller-baffle interaction effects are of minor importance.
- Initialize with a zero-velocity field in the absolute reference frame or a solution of a prior calculation (e.g., from a lower Reynolds number simulation).
- For turbulent flows, it is best to initialize with low values of the turbulence properties (e.g., 0.01 and 0.001 for  $k$  and  $\epsilon$ ).

# Unsteady methods

- A full time-dependent calculation is performed.
- Mesh the actual shape of the impeller.
- During the calculations, the impeller actually moves with respect to the stationary geometry components, such as the baffles.
- Because the geometry changes during the calculations, the mesh has to change as well.
- How to do this:
  - Moving/deforming mesh (MDM) method: Have one mesh and deform or remesh this every time step for the new impeller position.
  - Overset mesh method: Have a mesh for the solid geometry of the impeller, move this through the stationary mesh for the fluid, and calculate intersections every time step.
  - Sliding mesh method (called Moving Mesh in FLUENT).

# Sliding mesh method

- Method used in FLUENT.
- Define a separate fluid region for the impeller.
- Similar to the MRF model, with one exception: the impeller region mesh should be disconnected from the mesh for the tank region.
- This allows the impeller mesh to slide past the tank mesh.
- Data is interchanged by defining grid interfaces.

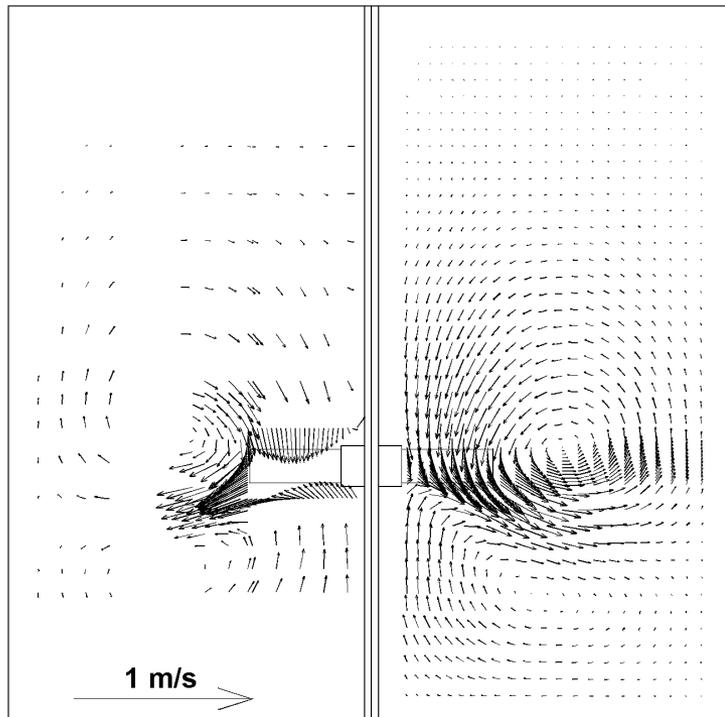
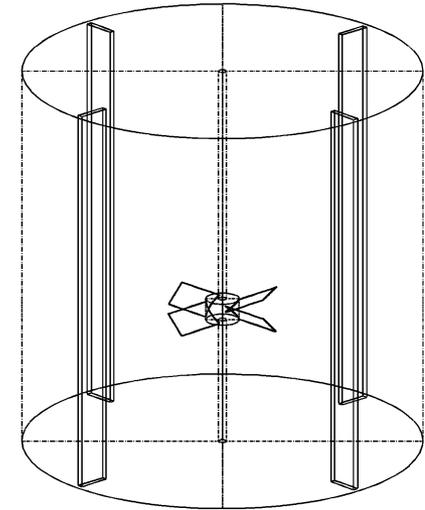


# When to use the sliding mesh method

- Advantages:
  - Fewest assumptions: suitable for widest range of cases.
  - Time-dependent solution is good for:
    - Impeller-baffle interaction.
    - Start-up or periodic transient flow details.
- Disadvantages:
  - CPU intensive.
  - Requires many cycles to reach “steady-state”.
  - Time scales for sliding mesh may not be compatible with time scales of other processes (blending, solid suspension, etc.).
- Use when:
  - When there is strong interaction between impeller and walls or baffles (e.g., systems with off-center or angled shafts).
  - Certain species or particle tracking calculations.

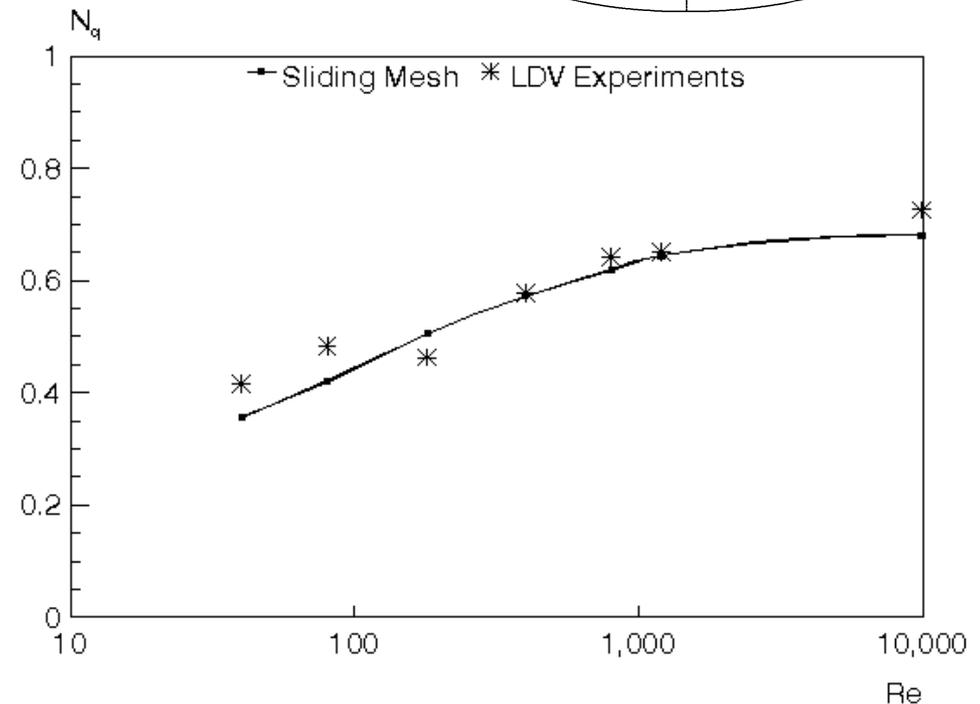
# Sliding mesh validation

- Pitched blade turbine for a range of Reynolds numbers.
- Bakker A., LaRoche R.D., Wang M.H., Calabrese R.V. (1997) *Sliding Mesh Simulation of Laminar Flow in Stirred Reactors*, Trans IChemE, Vol. 75, Part A., January 1997, page 42-44.



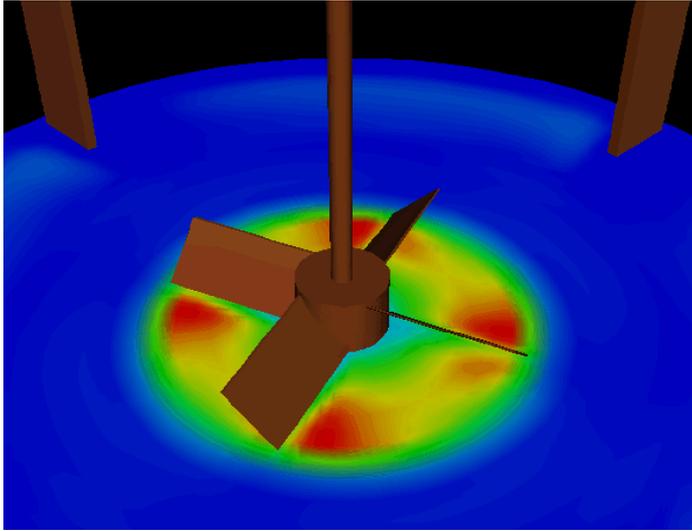
LDV Data

Simulation

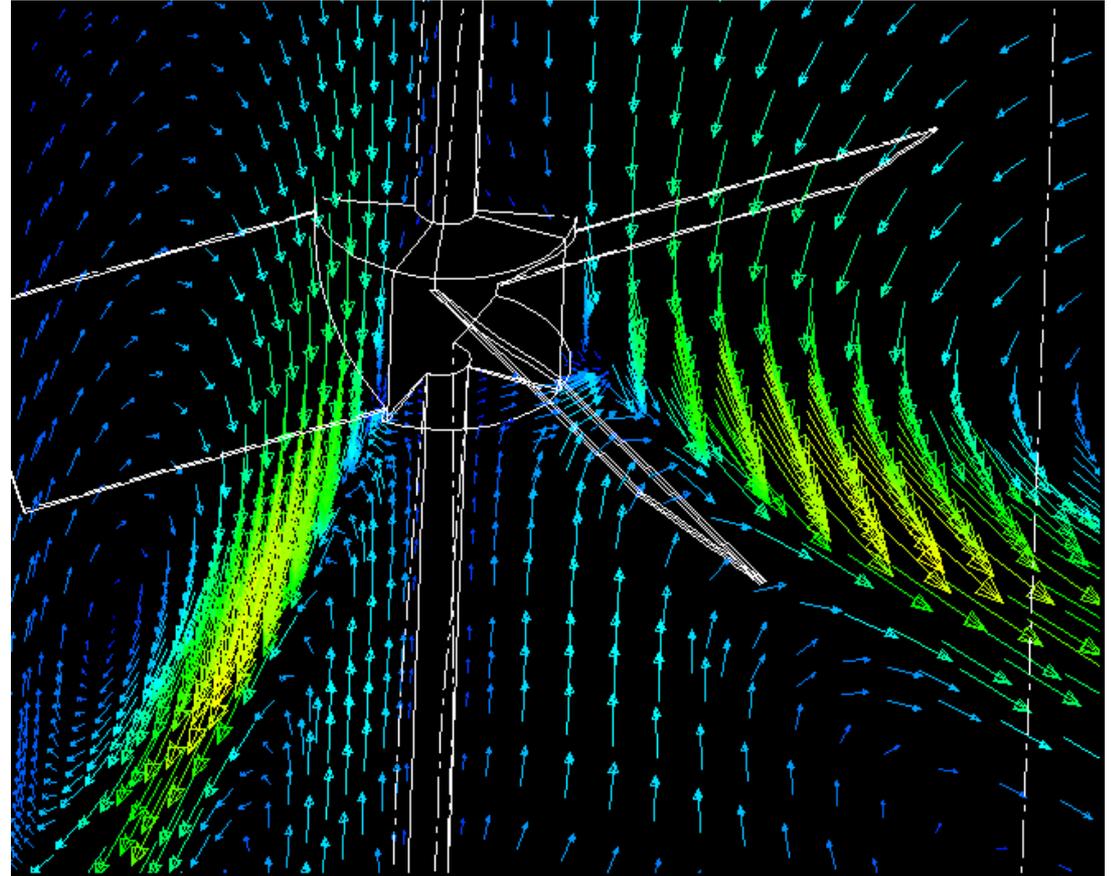


Pumping Number  $N_q = Q_1(\text{m}^3/\text{s}) / (ND^3)$

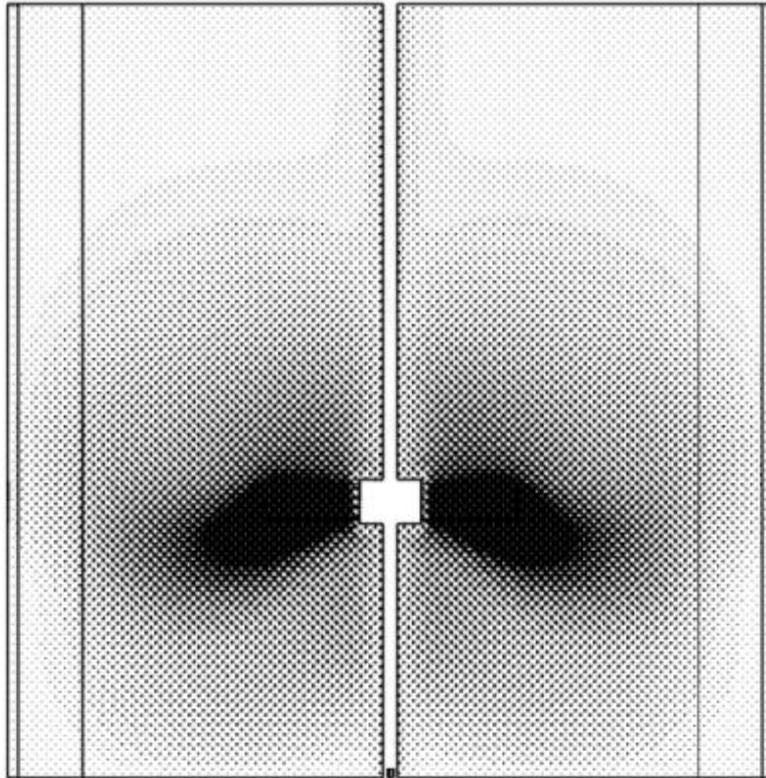
# Impeller flow pattern



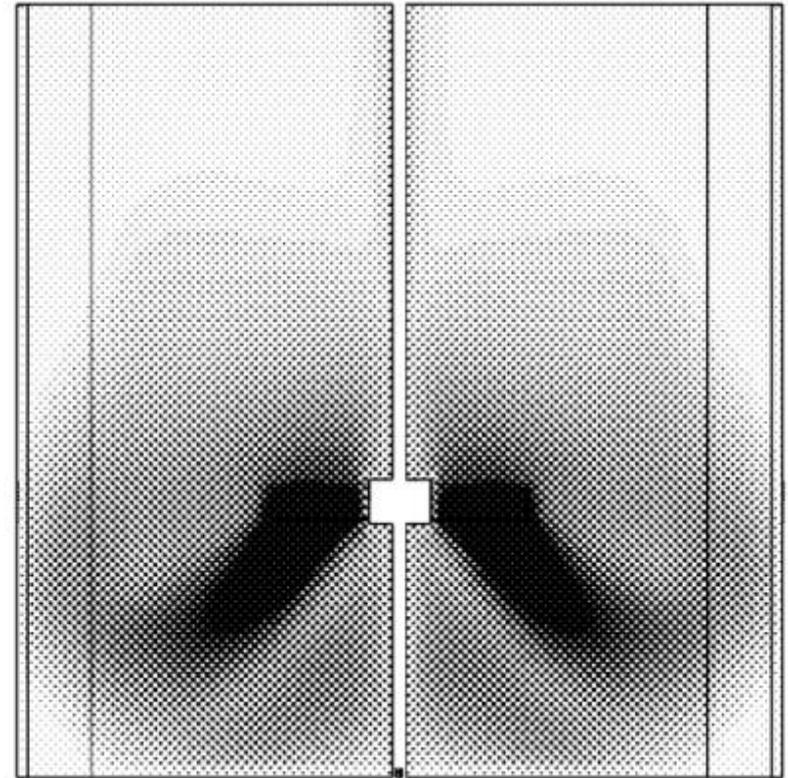
$Re = 40$



# Velocity magnitude

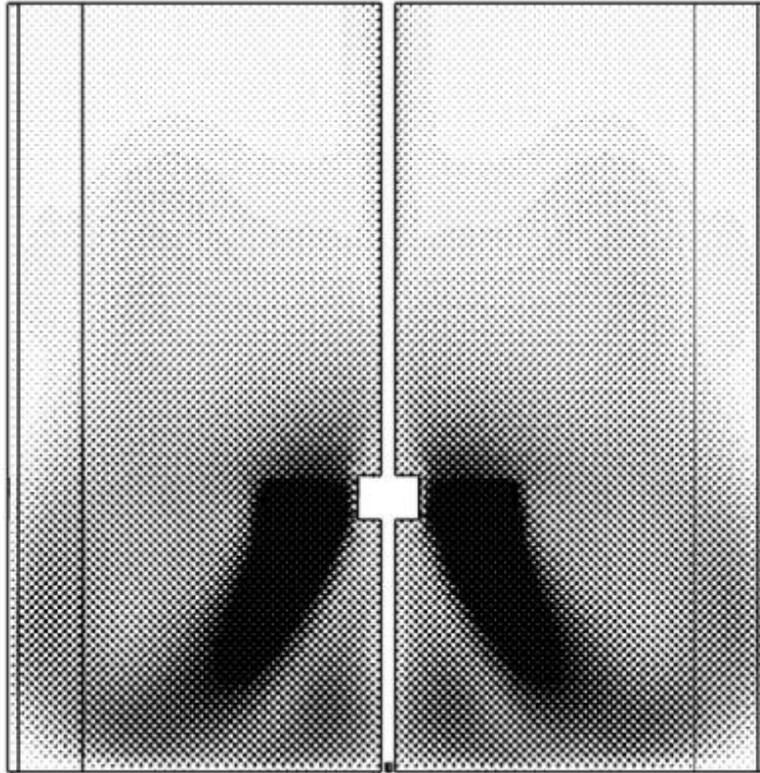


$Re = 40$

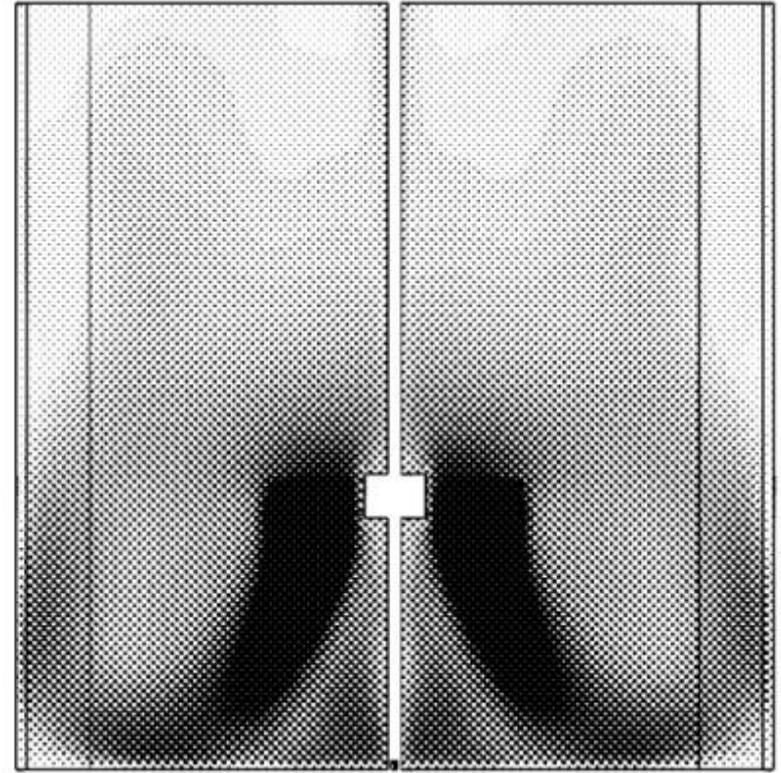


$Re = 180$

# Velocity magnitude

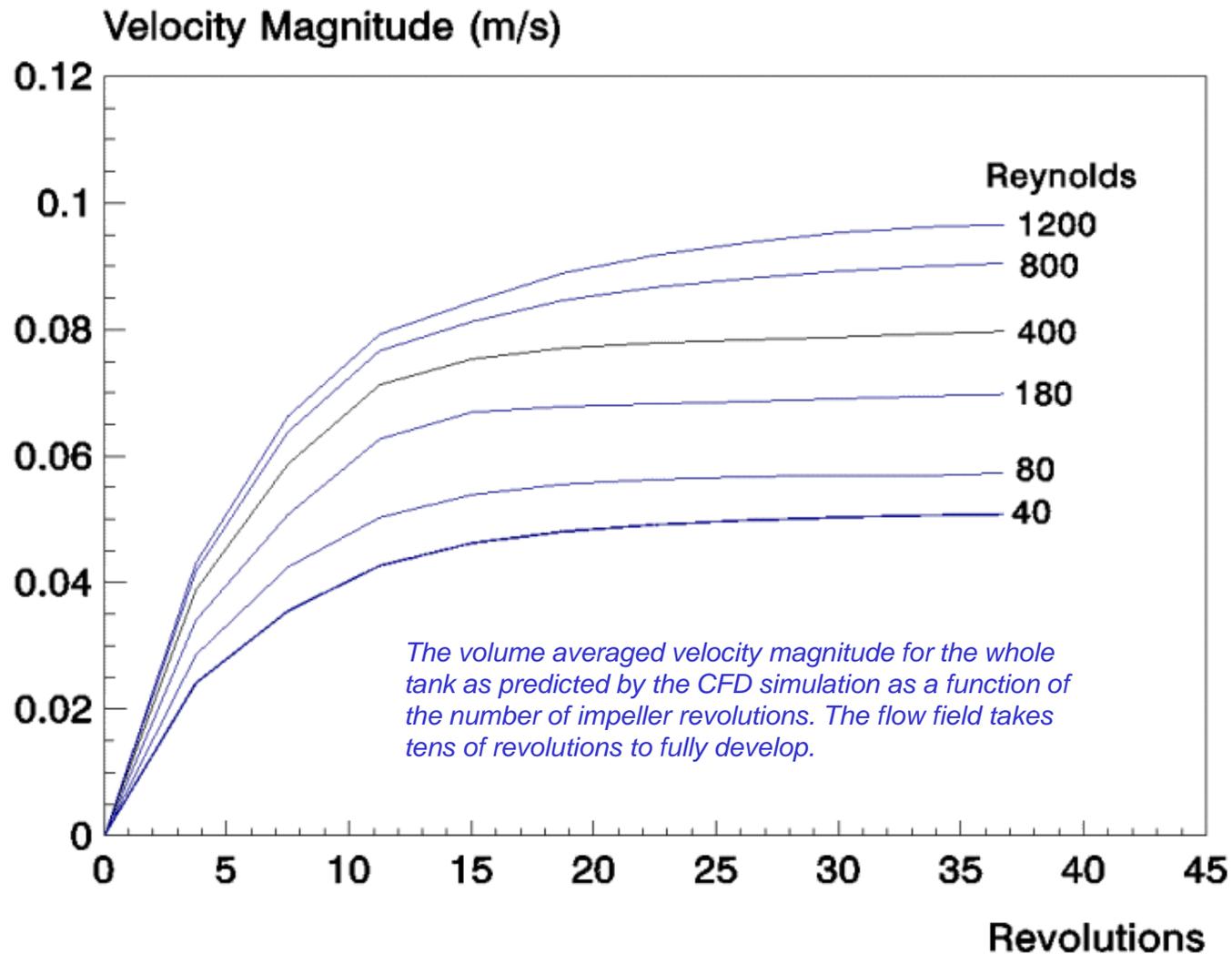


$Re = 400$

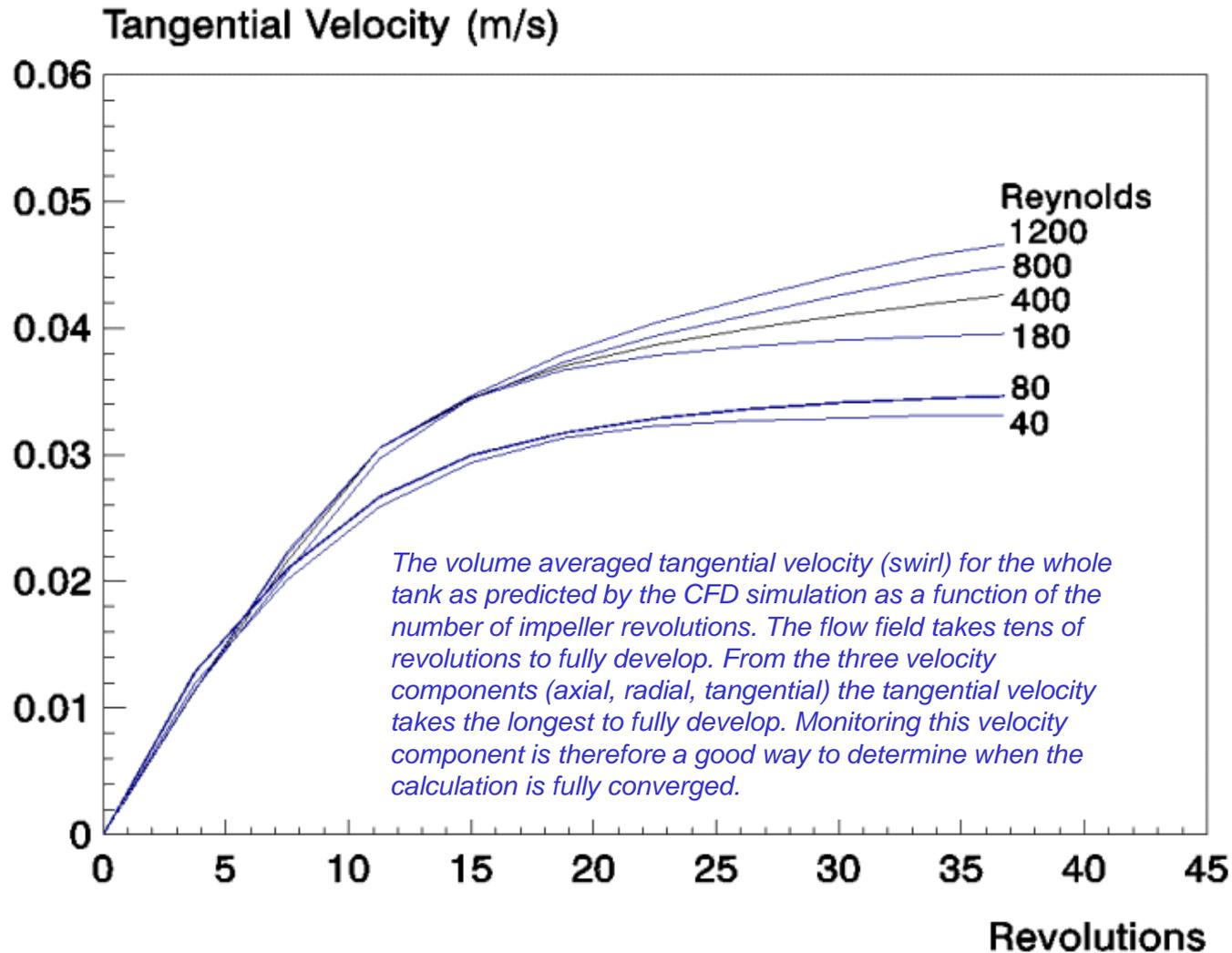


$Re = 1200$

# Average velocity magnitude



# Average tangential velocity



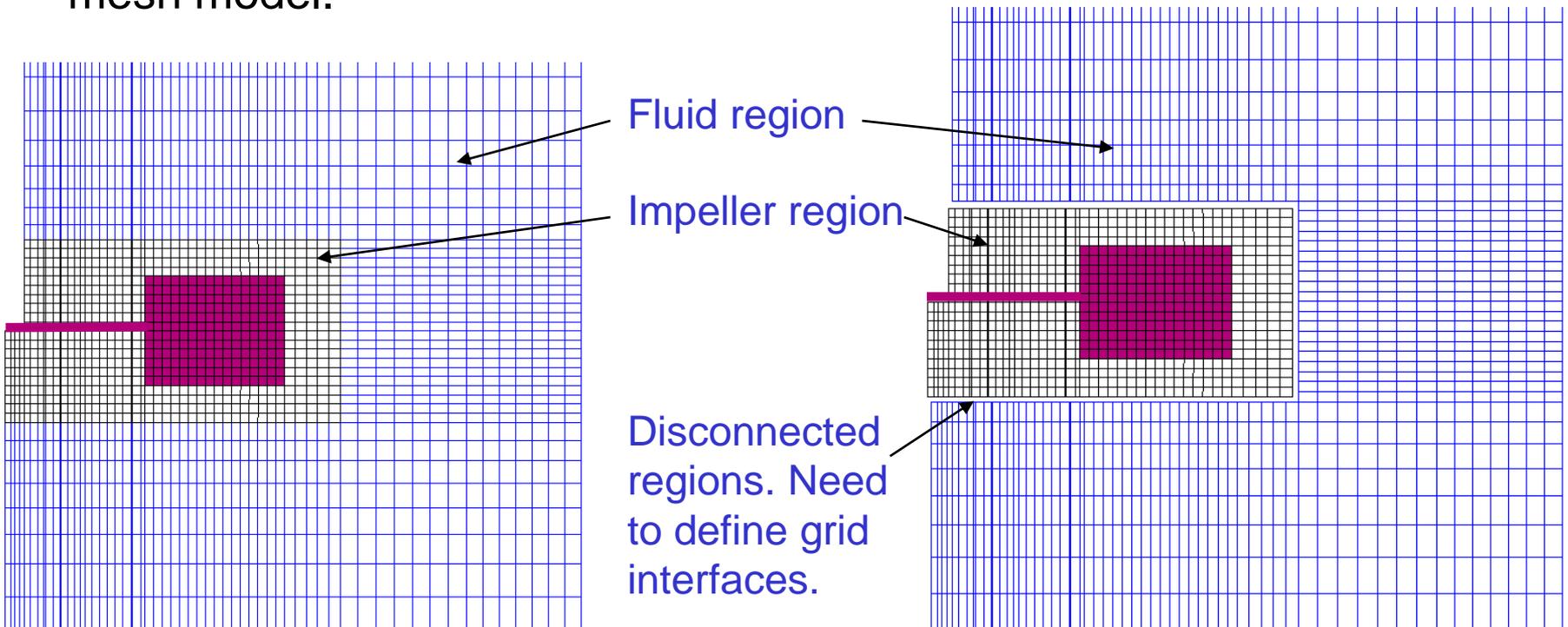
# Sliding mesh calculation

- There need to be separate, disconnected mesh zones for the rotating and stationary regions.
- Define “Grid Interfaces” between these two zones so that data can be exchanged.
- Set-up as unsteady model.
- Define impeller region as “moving mesh”.
- Define rotational axis and rotational velocity.
- Define other boundary conditions and model settings.
- Initialize either with a zero-velocity field in the absolute reference frame or a solution of a prior calculation (e.g., a steady MRF calculation).
- For turbulent flows, it is best to initialize with low values of the turbulence properties (e.g., 0.01 and 0.001 for  $k$  and  $\epsilon$ ).
- Perform transient simulation.

# Mesh options

- Meshes for the fluid region and impeller region are connected.
- Suitable for steady-state calculations using the MRF model.
- Cannot be used with the sliding mesh model.

- Meshes for the fluid region and impeller region are disconnected.
- Information is exchanged by defining grid interfaces.
- Necessary for the sliding mesh model. Will also work for MRF.



# Impeller region size

- The fluid region containing the impeller should be a surface of revolution around the axis, e.g., a cylinder.
- In principle, it can be any size.
  - With sliding mesh models, convergence is most robust if the region is relatively small, so that all the fluid in the rotating region moves with a velocity that it is not too much different from the impeller itself.
  - With MRF models, species transport calculations are most accurate if the impeller region size is as small as possible.
  - A region with an interface about one impeller blade height removed from the impeller usually works well.

# Periodicity

- In many cases, it is not necessary to model the full tank and only a periodic section needs to be modeled.
- The periodicity, or number of sections to be modeled, is equal to the greatest common denominator of the number of impeller blades and baffles:

| Impeller blades | Baffles | Periodicity | Section (degrees) |
|-----------------|---------|-------------|-------------------|
| any             | 1       | 1           | 360               |
| 2               | 4       | 2           | 180               |
| 3               | 3       | 3           | 120               |
| 3               | 4       | 1           | 360               |
| 4               | 4       | 4           | 90                |
| 6               | 4       | 2           | 180               |

- Note: if feed pipes are present, one usually has to model the full vessel.

# Liquid surface

- The liquid surface usually deforms as a result of the liquid motion.
- If the deformation is large, and strong surface vortices form, air may be entrained from the headspace.
  - This may or may not be desirable.
  - Usually, the system is designed to prevent this.
- In most baffled vessels, this deformation is usually small compared to the scale of the vessel.
- The liquid surface can in most cases be modeled as flat and frictionless (e.g., with a zero-shear or symmetry boundary condition).
- For systems where surface deformation is important, a free-surface multiphase model (e.g., VOF) has to be used.
  - This is very CPU time intensive and should be avoided if possible.

# Model setup and convergence

- Turbulence models:
  - Unbaffled vessels: always use the Reynolds stress model (RSM).
  - Fully baffled vessels: the k- $\varepsilon$  realizable model works well for most flows.
- Numerics:
  - Always use second order or higher numerics for the final solution.
  - For tetrahedral meshes, use the node-based gradient scheme.
- Initialization:
  - Initialize velocities to zero (in absolute reference frame).
  - Initialize k and  $\varepsilon$  to lower values than FLUENT default, e.g., 0.01 and 0.001 respectively (instead of 1).
- Convergence:
  - Default residual convergence criteria are usually not tight enough.
  - Monitor torque (moment) on the impeller, average tangential velocity, and average velocity magnitude.

# Flow field results

- Flow field can be visualized by means of vector plots, contour plots, iso-surfaces and pathlines.
  - Quickly shows if the number of impellers is sufficient.
  - Shows if material from feed pipes will go to the impeller or not.
- Quantitative data that can be extracted from the flow field and used in standard design procedures is:
  - Impeller torque and power draw.
  - Impeller pumping rate.
  - Shear rates, and effective viscosities.
  - Average velocities, and local velocities in regions of interest.

# The power number

- Calculate power number of the impeller:
  - As data needed for your other analysis.
  - Or, if already known, as validation of the simulation result.
- Calculate power draw from the torque  $M(Nm)$  on the impeller (in FLUENT called the moment):

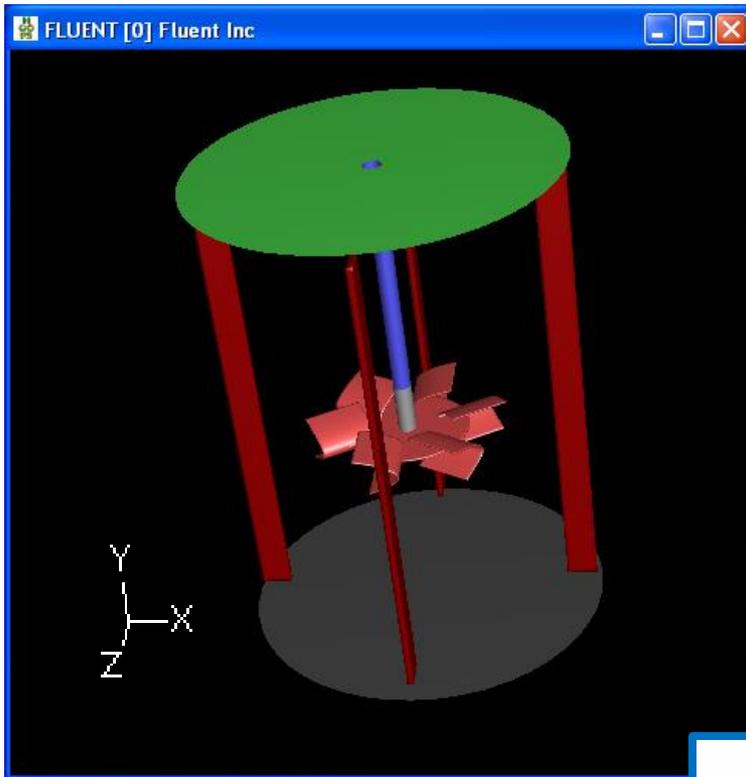
$$P(W) = 2 \pi N(s^{-1}) M(Nm)$$

- And calculate the power number  $Po$ :

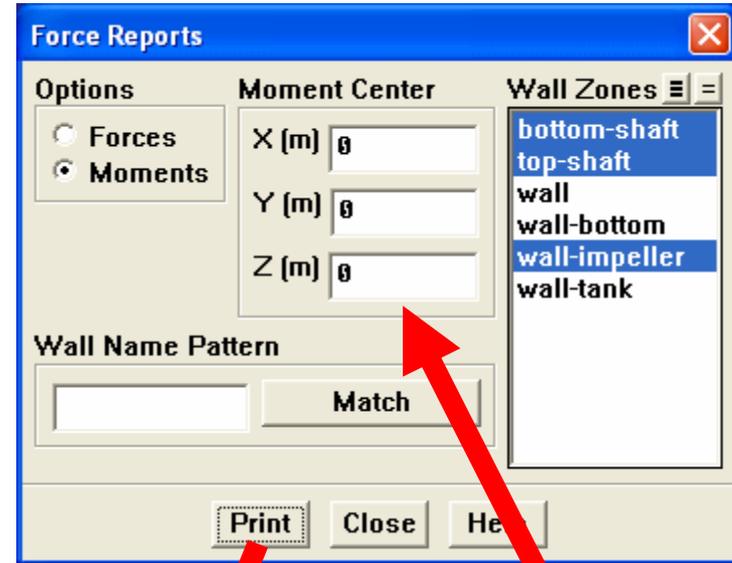
$$Po = \frac{P(W)}{\rho(kg\ m^{-3}) N(s^{-1})^3 D(m)^5}$$

- Note: in principle the power draw can also be calculated as the volume integral of the energy dissipation rate  $\varepsilon$ , but this is usually less reliable.

# Calculate the impeller torque in FLUENT



*In this example, the impeller rotates around the y-axis, and the y-axis moment is then the torque on the impeller. For periodic domains, reported torque is for the one modeled section only!*



| total moment    |                |                |
|-----------------|----------------|----------------|
| n-m             |                |                |
| (-3.9358653e-06 | 2.4544759e-06  | 1.06714e-05)   |
| (9.8104629e-05  | -1.3150549e-05 | 0.00028933252) |
| (0.00028774214  | 0.093091597    | 9.842025e-05)  |
| (0.00038191091  | 0.093080901    | 0.00039842417) |

Moment around the x y z axis

*Make sure the moment center lies on the axis of rotation of the impeller.*

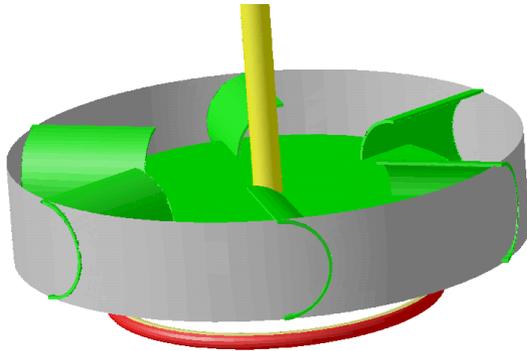
# Impeller pumping number

- Calculate the pumping number of the impeller:
  - As data needed for your other analysis.
  - Or, if already known, as validation of the simulation result.
- Calculate the flow rate through the impeller  $Q(\text{m}^3\text{s}^{-1})$ .
- The pumping number is defined as:

$$N_q = \frac{Q(\text{m}^3\text{s}^{-1})}{N(\text{s}^{-1}) D(\text{m})^3}$$

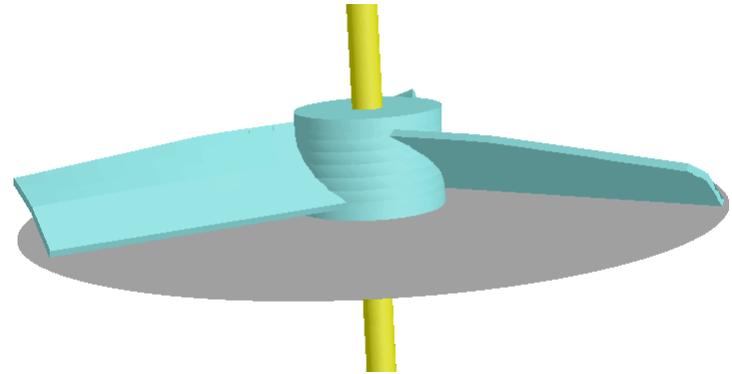
# Surfaces to create to calculate flow rate

- Radial flow impeller.



- Create a cylindrical surface around the impeller.
  - Iso-surface of constant radial coordinate.
  - Clip to axial extents of impeller.
- Calculate the mass flow.

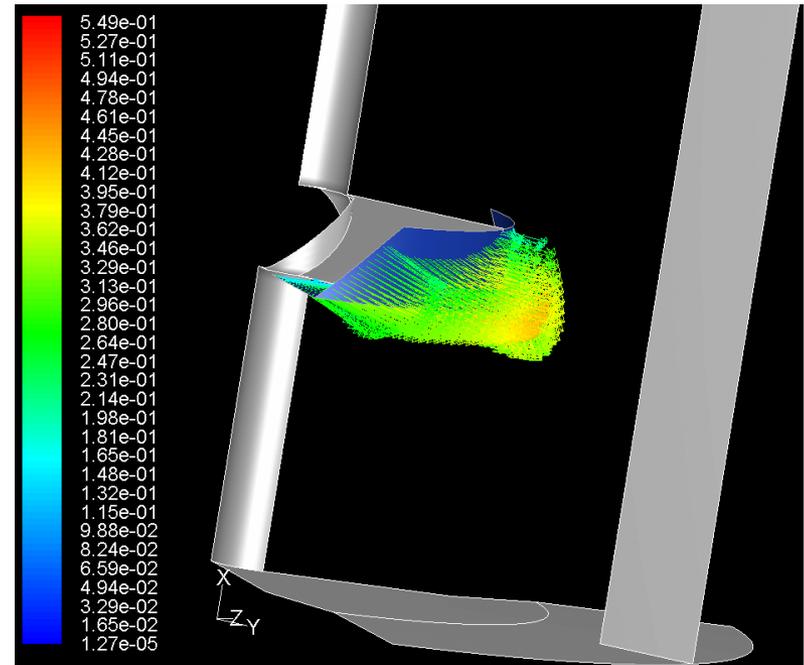
- Axial flow impeller.



- Create a disk surface in the impeller outflow.
  - Iso-surface of constant axial coordinate.
  - Clip to radial extents of impeller.
- Calculate the mass flow.

# Surfaces for mixed flow impeller

- A PBT in laminar flow gives a combined radial/axial flow pattern.
- Need to calculate mass flow out of the impeller both at the side and the bottom.
- Create radial surface on side and clip to positive radial velocities.
- Create surface below and clip to downwards velocities.
- Calculate mass flow through both surfaces.



Example: PBT45 - W/D = 0.27 - Re = 40 - T = 0.49m

$Mass\ flow = 4 * (0.425\ (side) + 0.496\ (bottom)) = 3.684\ kg / s\ total$

Multiplied by 4 because only 90° section modeled!

$D = 0.2\ m; \quad 60\ RPM; \quad \rho = 1000\ kg / m^3$

$$N_q = \frac{3.684 / 1000}{1 * 0.2^3} = 0.46$$

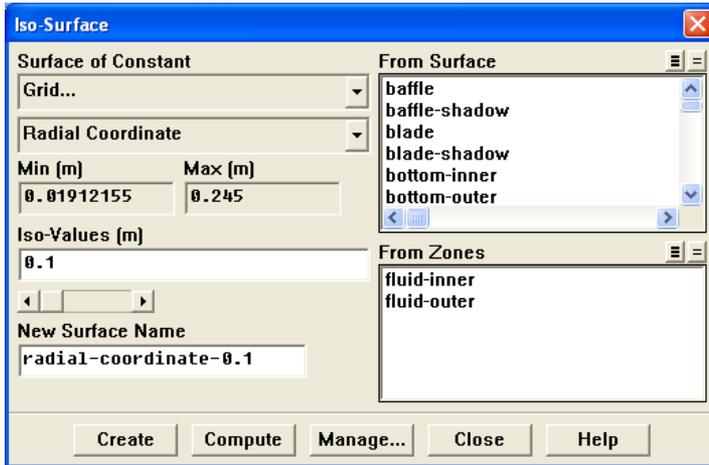
Power number calculation:

$M = 4 * 0.03263 = 0.1305\ Nm$

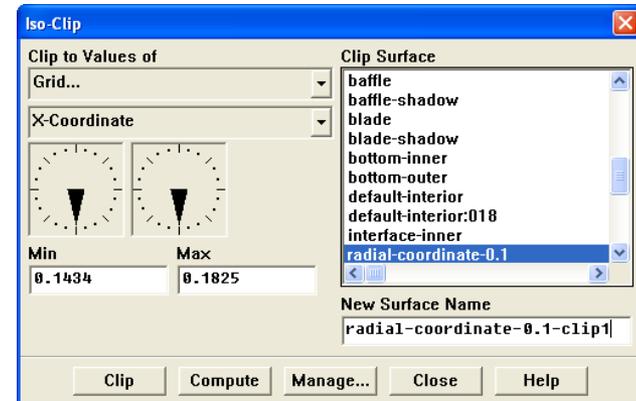
$$Po = \frac{2\pi N M}{\rho N^3 D^5} = 2.56$$

# Example radial flow calculation (PBT at $Re=40$ )

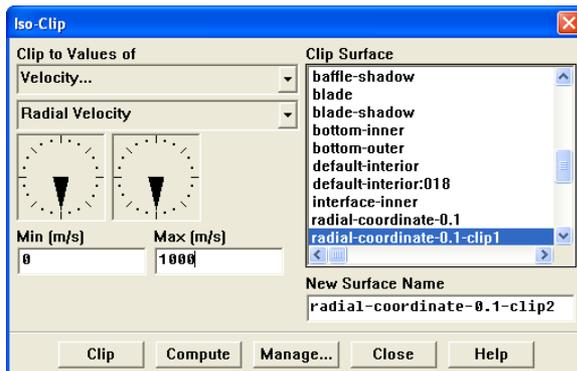
- Fluent example from previous slide (pbt-Re040).
- 1. Use Surface | Iso-Surface to create an iso-surface of radial coordinate at  $D/2$ . Here  $D=0.2$ , so create at radial coordinate=0.1.



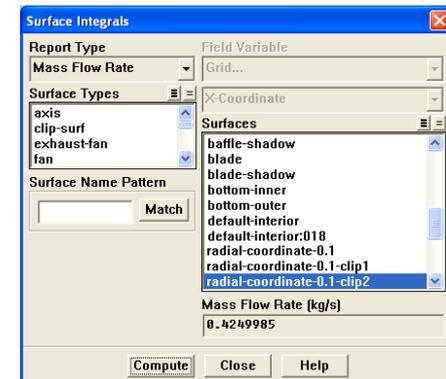
- 2. Use Surface | Iso-Clip. Clip the resulting surface to the axial extents of the impeller. Here that is from  $0.1434 < x < 0.1825$ . You can get that by first selecting in the From Surface list, the “blade”. Click “Compute”. Then select the surface from Step 1 in the “From Surface” list and then use “Clip.”



- 3. Clip the surface resulting from step 2, to positive radial velocities.

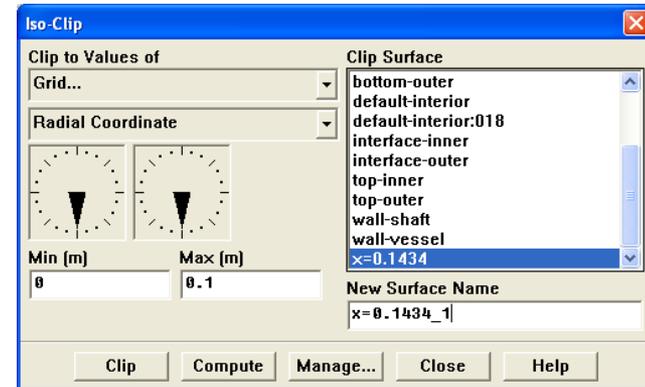
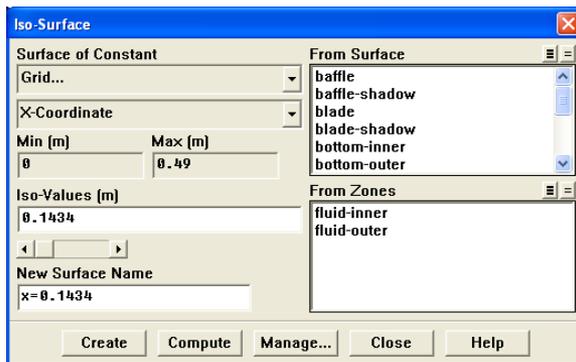


- 4. Calculate the Mass Flow Rate. Use Results | Surface Integrals. Note that this is for the one periodic section of the domain only.

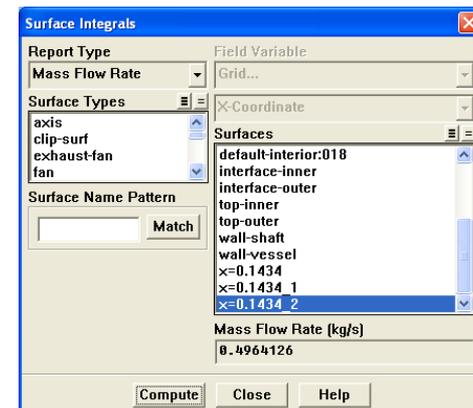
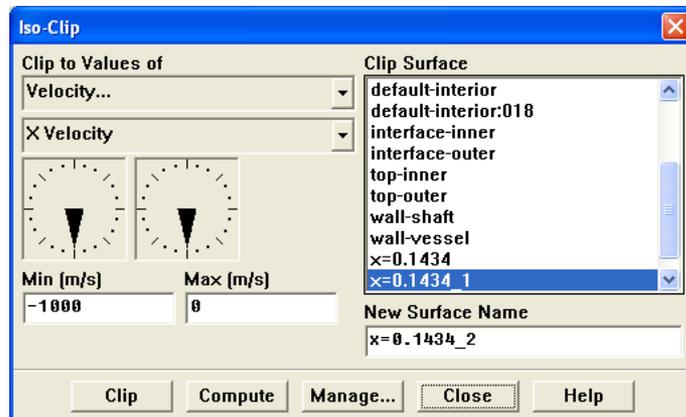


# Example axial flow calculation (PBT at $Re=40$ )

- 1. Use Surface | Iso-Surface to create an iso-surface of axial coordinate at bottom of impeller. Here that is at  $x=0.1434$ .
- 2. Use Surface | Iso-Clip. Clip the resulting surface from step 1 to the radial extents of the impeller. Here that is for radial coordinate  $< 0.1$ .



- 3. Clip the surface resulting from step 2, to downward axial velocities. Here that is for  $x$ -velocities  $< 0$ .
- 4. Calculate the Mass Flow Rate. Use Results | Surface Integrals. Note that this is for the one periodic section of the domain only.



# Computing shear rate

- To calculate shear rate (units 1/s),
  - Report → Volume Integrals, Check Volume-Average
  - Select Field variable Derivatives/Strain Rate
    - Select the impeller or tank volumes depending on where you want the shear rates calculated
- Comparable to Metzner and Otto\* shear rates calculated from

$$S \text{ (s}^{-1}\text{)} = k.N$$

- For PBT example (60RPM, Re=40):
  - Impeller swept volume:  $S = 18.8 \text{ s}^{-1}$ .
  - Whole tank:  $S = 2.1 \text{ s}^{-1}$ .

\* Metzner, A.B.; Otto, R.E. Agitation of non-Newtonian Fluids. AIChE J. 1957. 3 (1), 3.

# Conclusion

- Main problem is the modeling of the impeller.
- Different impeller models are available.
  - Time averaged (e.g., “fix velocity”)
  - Steady state MRF.
  - Unsteady sliding mesh.
- In addition to flow fields, parameters needed as inputs to empirical correlations can be obtained:
  - Power number.
  - Pumping number.
  - Shear rates.

# Modeling Material/Species Transport

## Reacting Flows - Lecture II

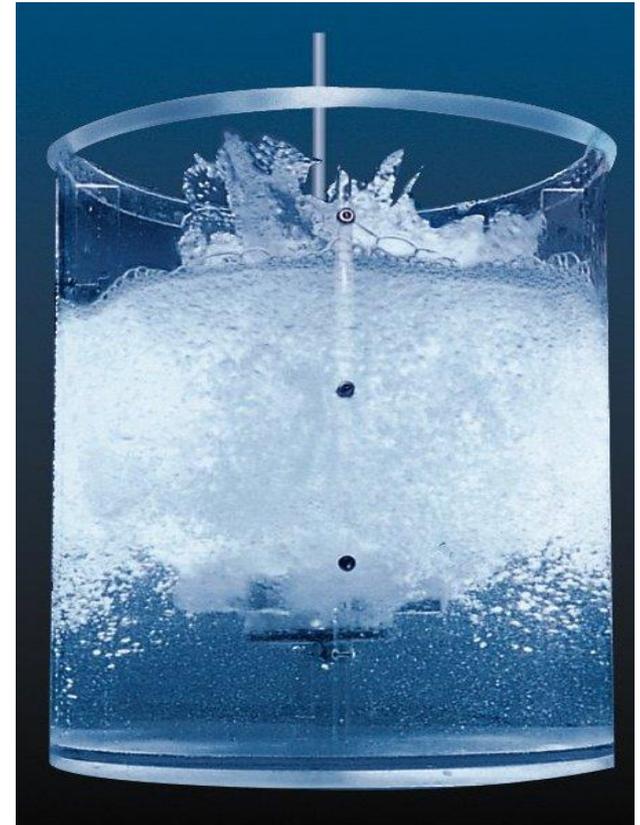
André Bakker

# Outline

- In addition to flow fields, we often need to model additional physics.
- The fluid velocities transport a number of properties:
  - Mass of one or more materials.
  - Momentum.
  - Energy.
- Proper modeling of material transport is necessary if we want to model mixing or reaction.
- Methods to model material transport:
  - Discrete phase modeling (DPM), aka particle tracking.
  - Species transport, aka scalar transport.
  - Multiphase flow modeling, e.g., Eulerian flow models.

# Multiphase flow → multiple momentum eqns.

- Multiphase flow is simultaneous flow of:
  - Materials with different states or phases (i.e., gas, liquid or solid).
  - Materials in the same state or phase, but that are immiscible (i.e., liquid-liquid systems such as oil droplets in water).
- Each phase has its own velocity field and its own momentum.
- It is therefore often necessary to solve multiple sets of momentum equations, one set for each phase.
- Interaction between the phases requires the introduction of momentum exchange terms.
- Models are often complex, and time consuming to solve.
- Will not discuss here.



# Systems with single set of momentum eqns.

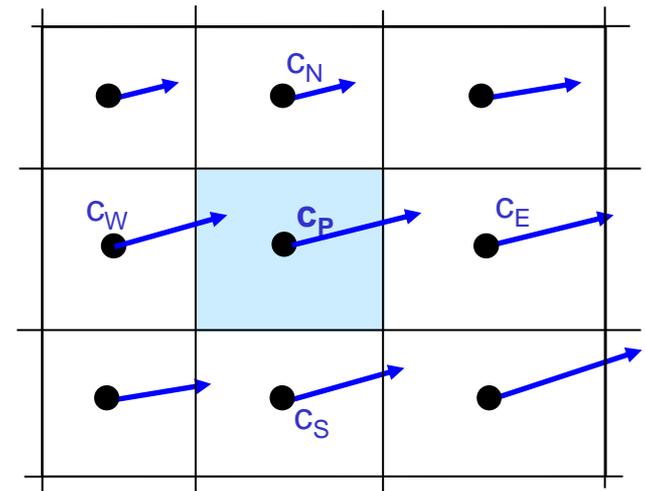
- We will discuss material transport in systems that are adequately described by a single set of momentum equations:
  - Species or scalar transport.
  - Particle tracking / discrete phase modeling (DPM).
- One fluid flow field is solved.
- The rate of transport of the species or particles is derived from that single fluid flow field.
- The local concentration of species or particles may affect the flow field itself.

# Species transport

- The species transport equation (constant density, incompressible flow) is given by:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left( \mathbf{D} \frac{\partial c}{\partial x_i} \right) + S$$

- The concentration of the chemical species is  $c$ .
- The velocity is  $u_i$ .
- $\mathbf{D}$  is the diffusion coefficient.
- $S$  is a source term.
- This equation is solved in discretized form to calculate the transport and local species concentrations.

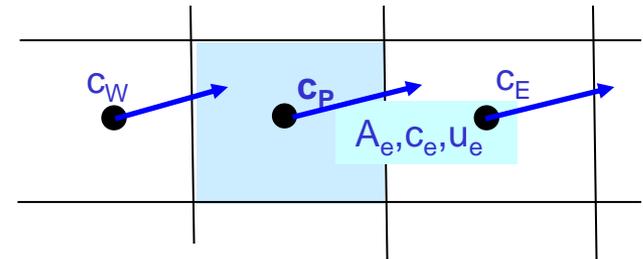


# Species transport – the convective term

- Convection is transport of material due to the velocity of the fluid.

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left( \mathbf{D} \frac{\partial c}{\partial x_i} \right) + S$$

- Flux from one grid cell to the next is area times normal-velocity times concentration.
- From cell “p” to “E”:  $A_e \cdot u_e \cdot c_e$ .



- Values at cell faces required!
- Implication: for best accuracy, use higher order discretization.

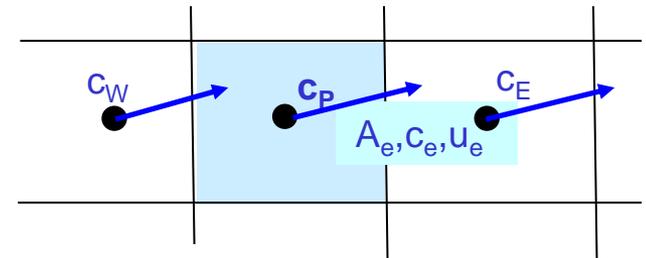
# Species transport – the diffusive term

- Diffusion is transport resulting from concentration gradients.

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left( \mathbf{D} \frac{\partial c}{\partial x_i} \right) + S$$

- Diffusion flux from one grid cell to the next is area times the concentration gradient times the diffusion coefficient.
- From cell “p” to “E”:

$$\mathbf{D} A_e \frac{dc}{dx} \Big|_e$$



- Gradient at interface between cells is easily calculated.
- The main difficulty is the calculation of the diffusion coefficient.

# The diffusion term - molecular

- Molecular diffusion:
  - As a result of concentration gradients: mass diffusion.
  - As a result of temperature gradients: thermodiffusion.
- Mass diffusion coefficient:
  - Constant dilute approximation: same constant for all species.
  - Dilute approximation: different constant for each species.
  - Multi-component: a separate binary diffusion coefficient  $\mathbf{D}_{ij}$  for each combination of species “i” into species “j”.
- Thermodiffusion: flux is proportional to thermal diffusion coefficient  $\mathbf{D}_T$  and temperature gradients:

$$\mathbf{D}_T \frac{\nabla T}{T}$$

- Not usually important in industrial chemical reactors.

# The diffusion term - turbulence

- Turbulent diffusion: transport due to the mixing action of the chaotic turbulent velocity fluctuations.
- The turbulent diffusion coefficient is calculated from the turbulent viscosity  $\mu_t$ :

$$\mathbf{D}_t = \frac{\mu_t}{\rho Sc_t}$$

- The turbulent Schmidt number  $Sc_t$  is a model constant. Recommended values are:
  - 0.7 if an eddy viscosity turbulence model is used, e.g., k- $\epsilon$ .
  - 1.0 if the Reynolds stress model (RSM) is used.

# Species transport – source terms

- The source term:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i} (u_i c) = \frac{\partial}{\partial x_i} \left( \mathbf{D} \frac{\partial c}{\partial x_i} \right) + S$$

- This describes all other effects:
  - Creation or destruction of species due to chemical reaction.
  - Any other physical phenomena the user wants to implement.

# Model setup

- Model setup:
  - Specify which species are present in the mixture.
  - Specify properties of all species.
  - If N species are present, N-1 equations are solved. The concentration of the Nth species follows from the fact that all mass fractions  $Y_i$  should sum to unity.

$$\sum_i Y_i = 1$$

$$\text{mass fraction: } Y_i = \frac{c_i (\text{kg} / \text{m}^3)}{\rho_{\text{mixture}} (\text{kg} / \text{m}^3)}$$

$$\text{mixture density: } \rho_{\text{mixture}} = \sum_i c_i$$

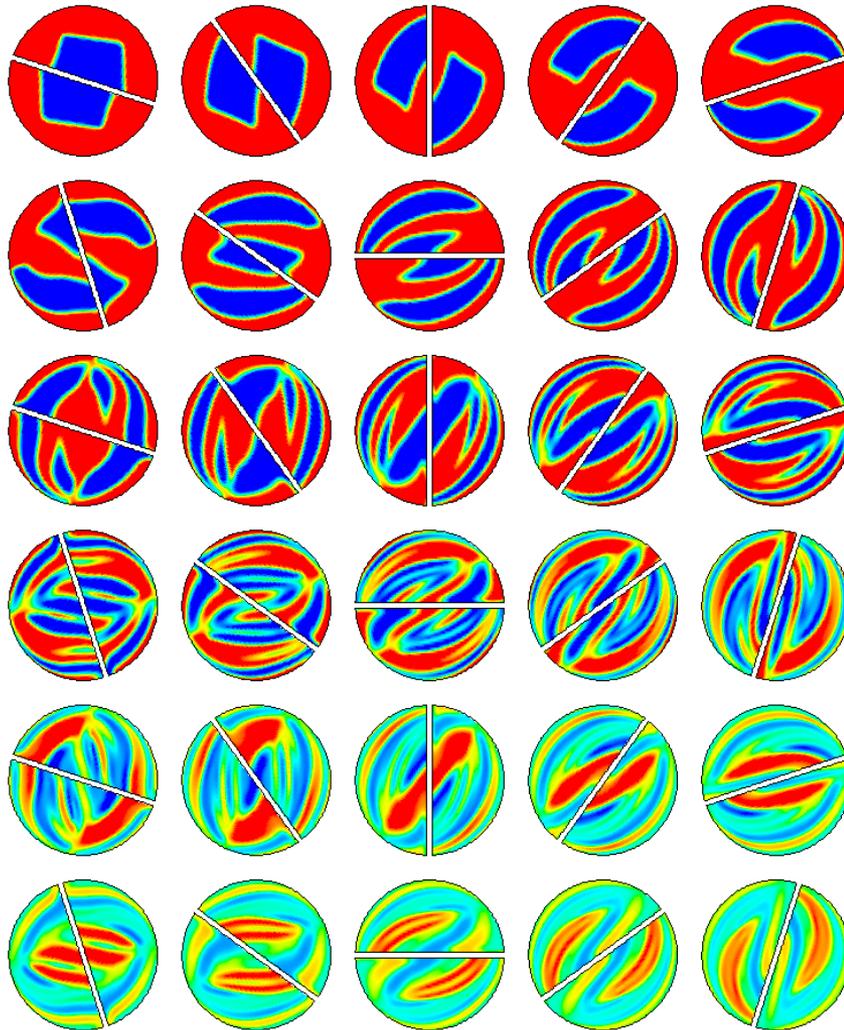
# Boundary conditions

- Wall boundary conditions:
  - Either specified mass fraction, or zero flux.
- Inlet boundary conditions:
  - At inlets, the inlet flux is calculated as:  $u_n c - \mathbf{D} \frac{\partial c}{\partial x_n}$ 
    - Need to specify inlet concentration/mass fraction.
    - The inlet diffusion flux depends on the concentration gradient. Value cannot be predicted beforehand. If a fixed mass flow rate is desired, this term should be disabled.
- Outlet boundary conditions: specify species mass fraction in case backflow occurs at outlet.

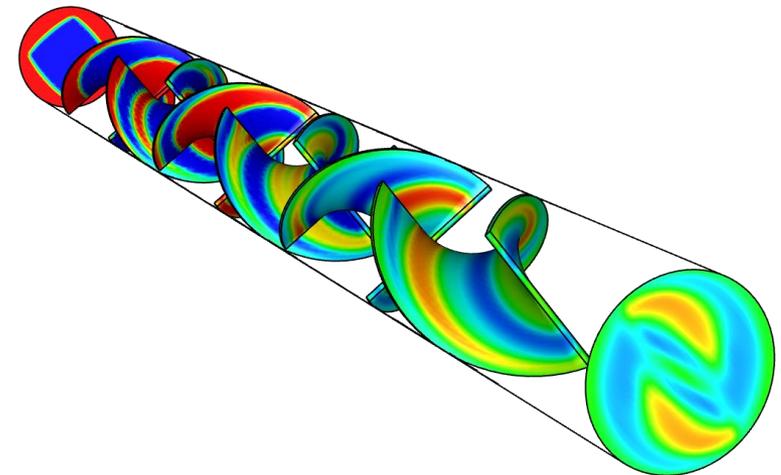
# Species equation is one-way!

- All species have the same convective velocity.
- Diffusion usually reduces concentration gradients → mixing.
- As a result, the diffusion equation cannot usually be used to model separation!
- To model separation, multiphase models where the phases have different velocities are necessary.
- Exceptions:
  - Some laminar flow, thermal diffusion dominated cases.
  - Cases with complex transport models implemented through source terms.

# Mixing mechanism



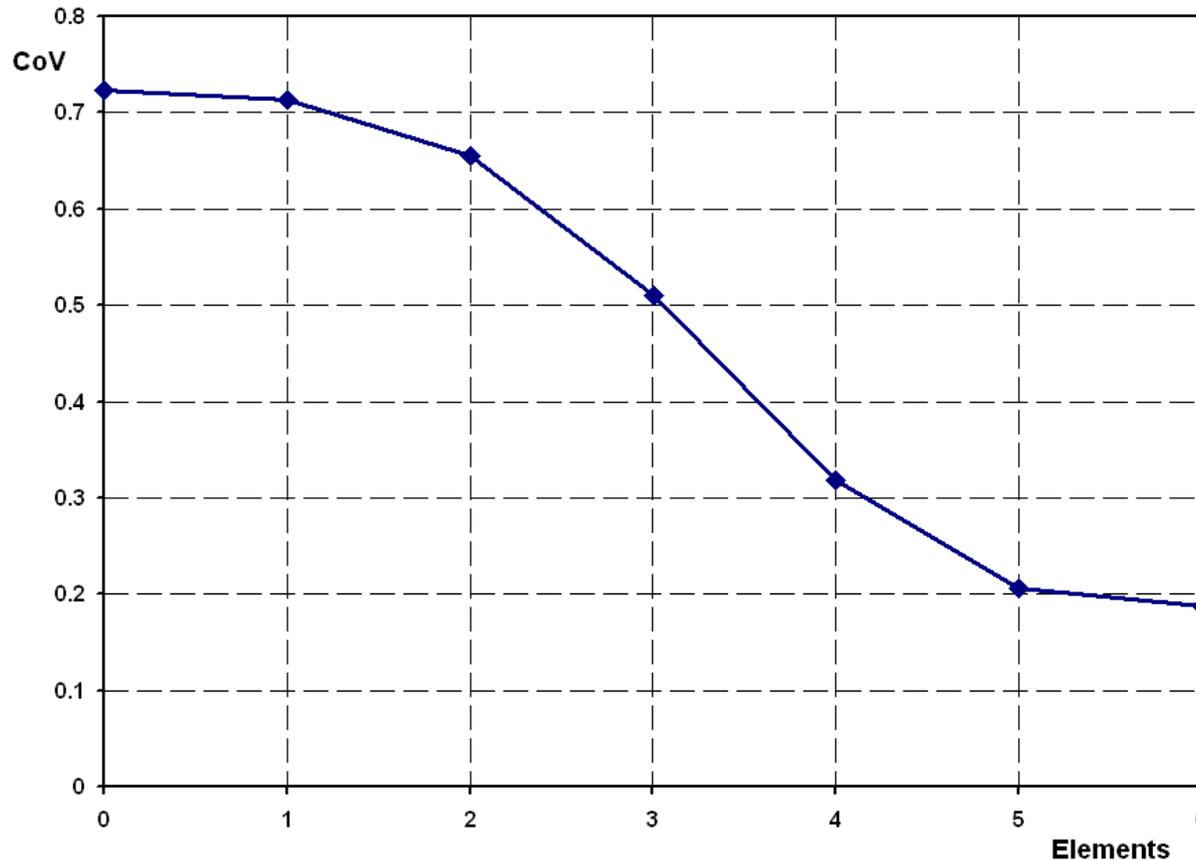
- Kenics helical-element static mixer.
- Laminar mixing.
- CFD simulation.
- Six elements.
- Each element splits, stretches and folds the fluid parcels.
- Every two elements the fluid is moved inside-out.



# Mixing quantification

- Species concentration in sample points at different axial locations.
- Coefficient of variance:

$$CoV = \frac{stdev(c)}{average(c)}$$



Kenics mixer

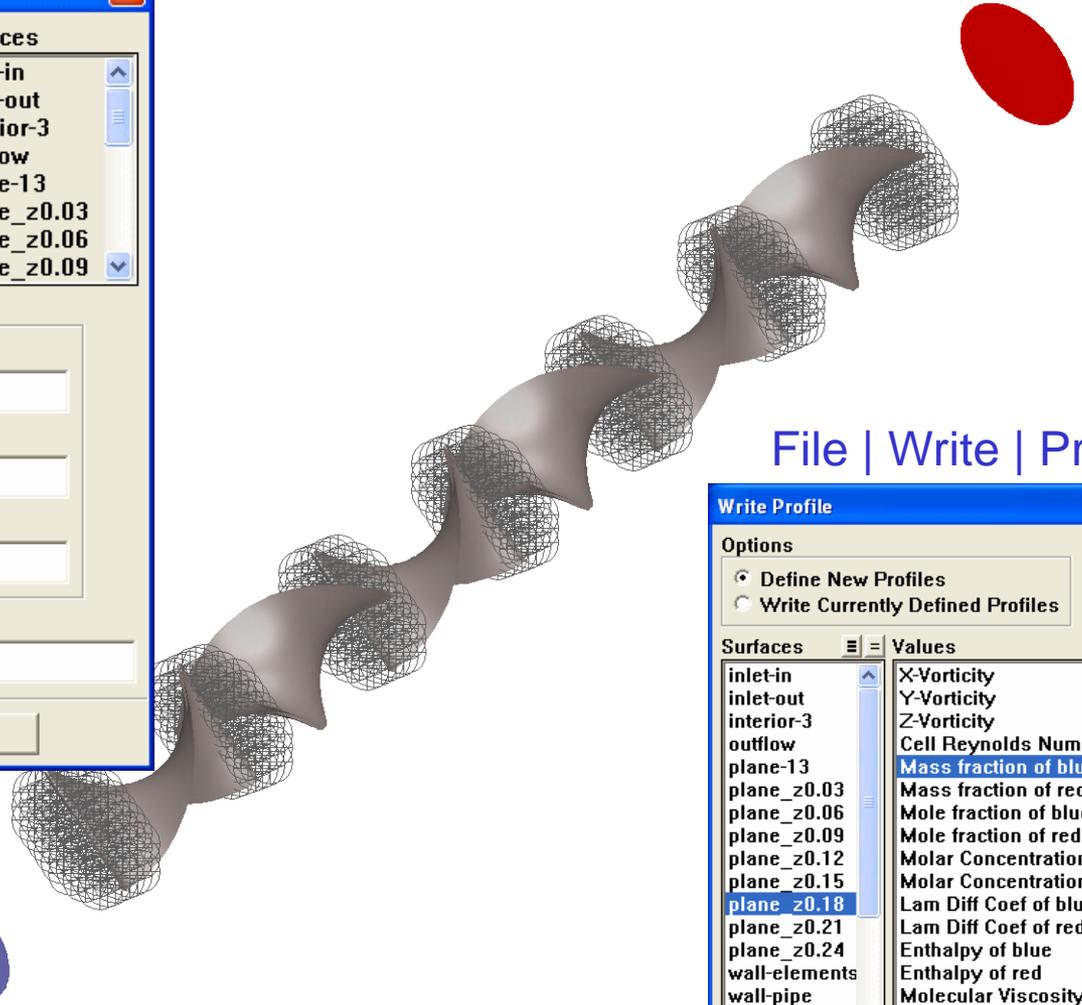
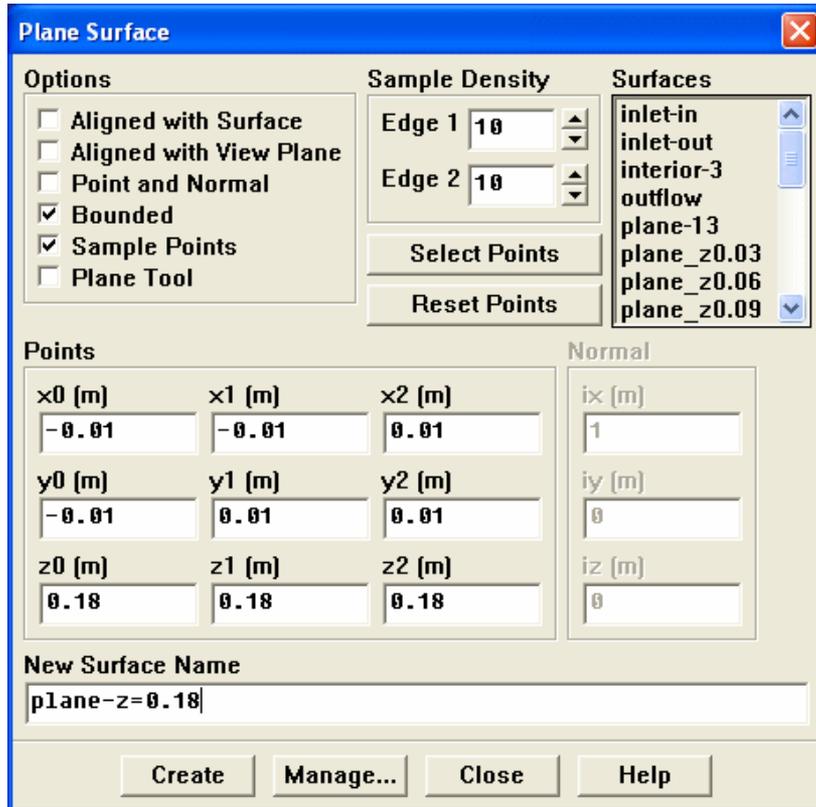
Six elements

Re=10

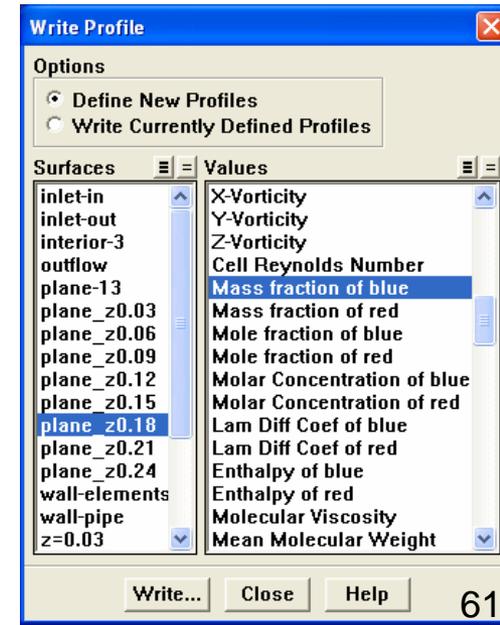
88 evenly spaced  
sample points in  
each axial plane.

# Locations of sample plane points

## Surfaces | Plane

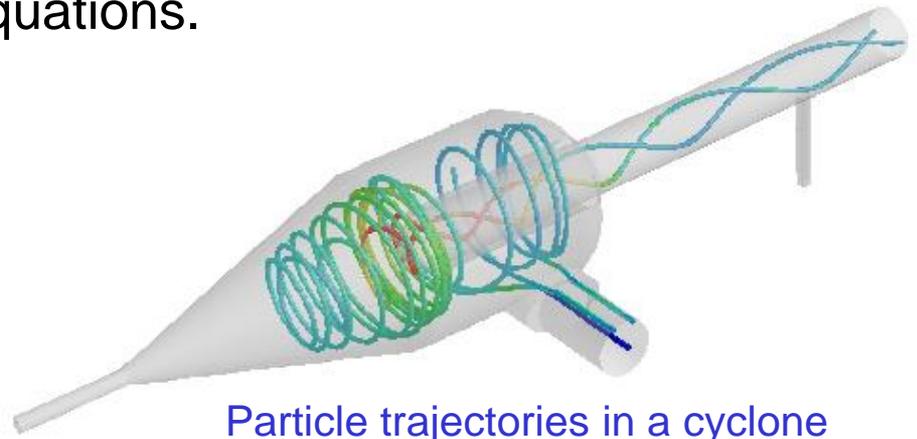


## File | Write | Profile



# Particle tracking

- Solve one set of momentum equations for the fluid flow.
  - In an Eulerian reference frame, i.e., on the grid locations.
- Simulate a second, discrete phase consisting of individual particles.
  - Known as discrete phase modeling (DPM).
  - In a Lagrangian frame of reference, i.e., following the particles.
  - Trajectories are calculated, as well as particle heat and mass transfer.
  - Particles may affect fluid flow field. This is done by introducing source terms in the fluid flow equations.



# DPM theory

Trajectory is calculated by integrating the particle force balance equation:

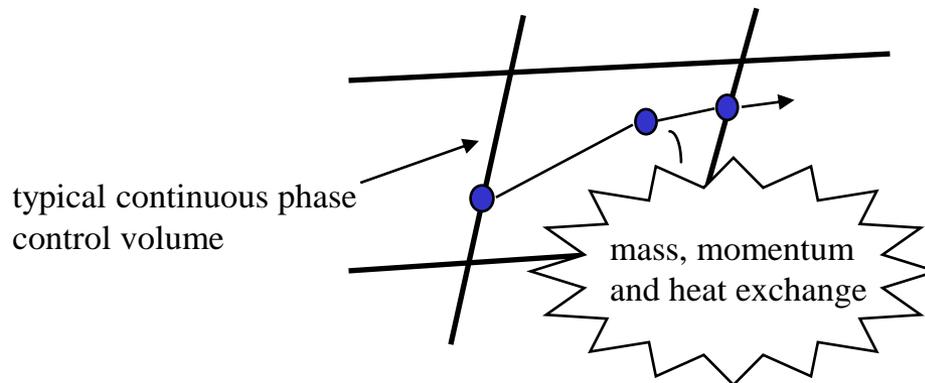
$$\frac{du_i^p}{dt} = F_D(u_i - u_i^p) + g_i(\rho_p - \rho) / \rho_p + F_i / \rho_p$$

Drag force is  
a function of the  
relative velocity

Gravity force

Additional forces:

- Pressure gradient
- Thermophoretic
- Rotating reference frame
- Brownian motion
- Saffman lift
- Other (user defined)

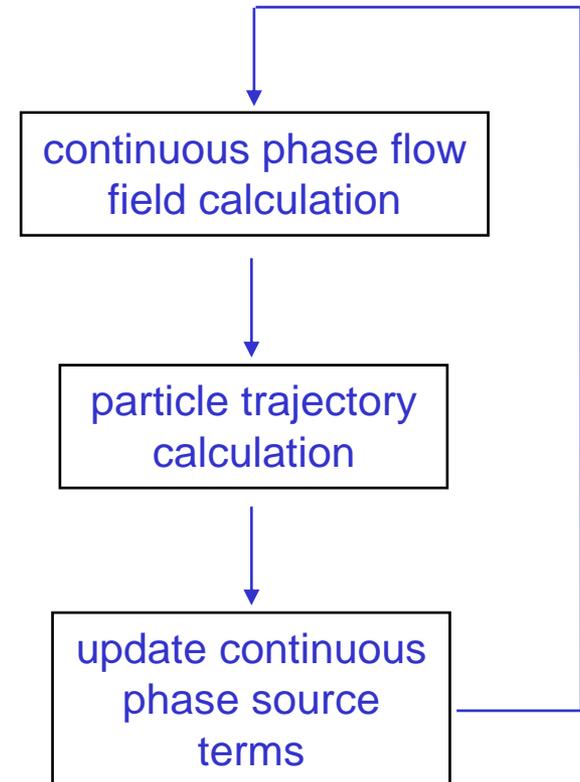


# Coupling between phases

- One-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase has no influence on the gas phase.
- Two-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase influences fluid phase via source terms of mass, momentum, and energy.
  - Examples include:
    - Inert particle heating and cooling.
    - Droplet evaporation.
    - Droplet boiling.
    - Devolatilization.
    - Surface combustion.

# Discrete phase model

- Trajectories of particles/droplets are computed in a Lagrangian frame.
  - Exchange (couple) heat, mass, and momentum with Eulerian frame gas phase.
- Discrete phase *volume* fraction should preferably be less than 10%.
  - Mass loading can be large (+100%).
  - No particle-particle interaction or break up.
- Turbulent dispersion modeled by:
  - Stochastic tracking.
  - Particle cloud model.
- Model particle separation, spray drying, liquid fuel or coal combustion, etc.



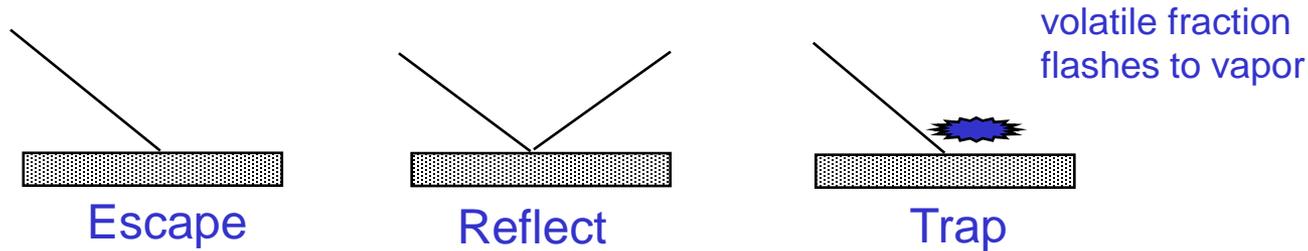
# Particle types

- Particle types are inert, droplet and combusting particle.

| <b>Particle Type</b>     | <b>Description</b>   |
|--------------------------|--|
| Inert.                   | Inert/heating or cooling   |
| Droplet (e.g., oil).     | Heating/evaporation/boiling.<br>Requires modeling of heat transfer and species.  |
| Combusting (e.g., coal). | Heating.<br>Evolution of volatiles/swelling.<br>Heterogeneous surface reaction.<br>Requires modeling of heat transfer and species. |

# Particle-wall interaction

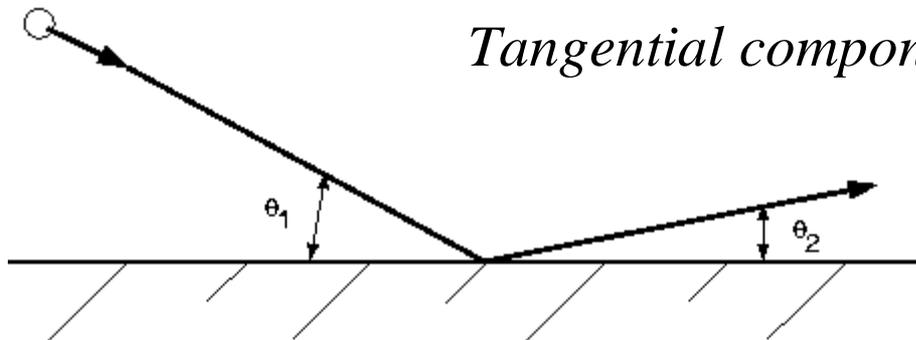
- Particle boundary conditions at walls, inlets, and outlets:



- For particle reflection, a restitution coefficient  $e$  is specified:

$$\text{Normal component: } e_n = \frac{v_{2,n}}{v_{1,n}}$$

$$\text{Tangential component: } e_t = \frac{v_{2,t}}{v_{1,t}}$$



# Particle fates

- “Escaped” trajectories are those that terminate at a flow boundary for which the “escape” condition is set.
- “Incomplete” trajectories are those that were terminated when the maximum allowed number of time steps was exceeded.
- “Trapped” trajectories are those that terminate at a flow boundary where the “trap” condition has been set.
- “Evaporated” trajectories include those trajectories along which the particles were evaporated within the domain.
- “Aborted” trajectories are those that fail to complete due to numerical/round-off reasons. If there are many aborted particles, try to redo the calculation with a modified length scale and/or different initial conditions.

# Turbulence: discrete random walk tracking

- Each injection is tracked repeatedly in order to generate a statistically meaningful sampling.
- Mass flow rates and exchange source terms for each injection are divided equally among the multiple stochastic tracks.
- Turbulent fluctuations in the flow field are represented by defining an instantaneous fluid velocity:

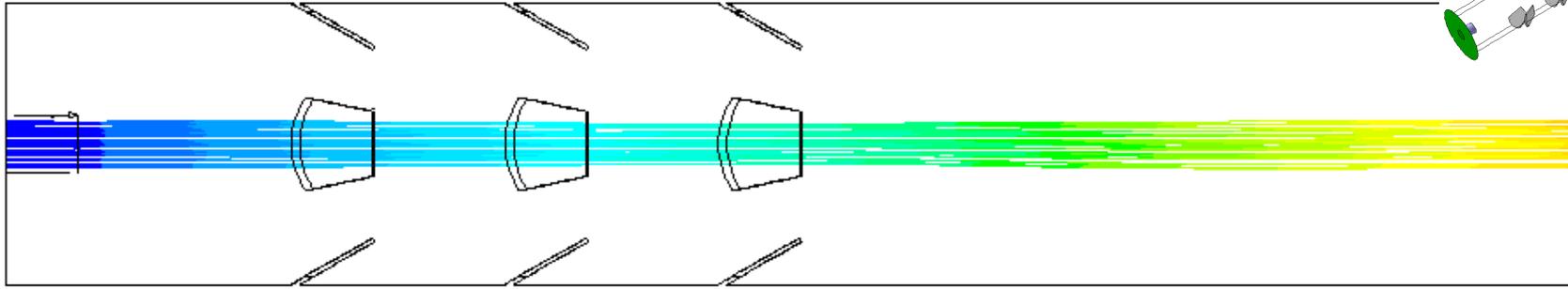
$$u_i = \overline{u_i} + u'_i$$

- where  $u'_i$  is derived from the local turbulence parameters:

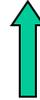
$$u'_i = \zeta \sqrt{\frac{2k}{3}}$$

- and  $\zeta$  is a normally distributed random number.

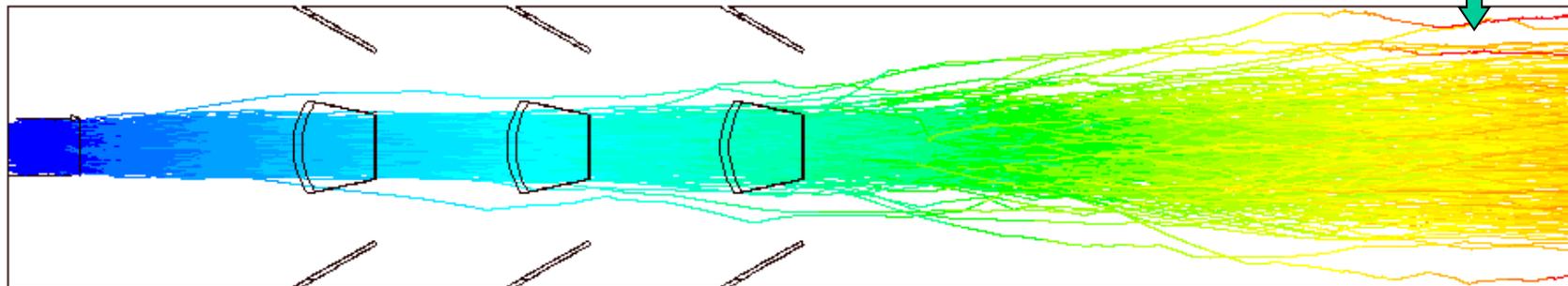
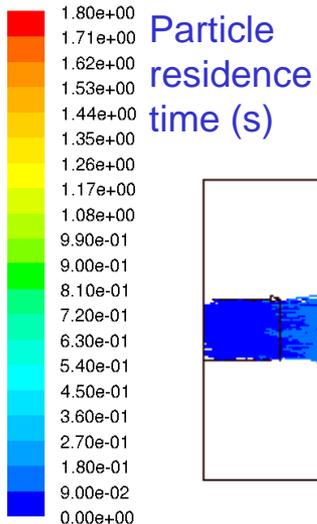
# Stochastic tracking – static mixer



- Stochastic tracking turned off.
- One track per injection point.
- Uses steady state velocities only and ignores effect of turbulence.

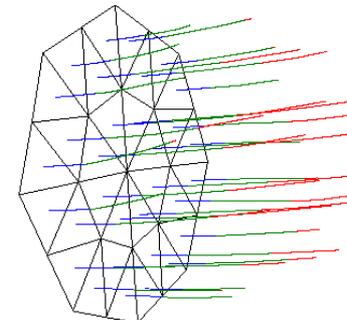
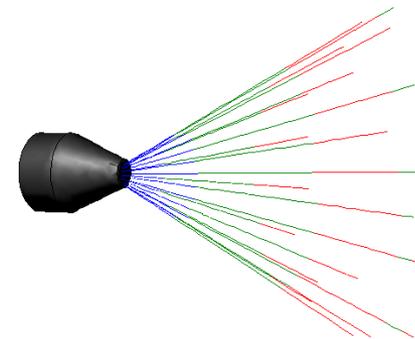
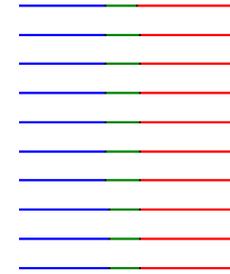


- Stochastic tracking turned on.
- Ten tracks per injection point.
- Adds random turbulent dispersion to each track.
- Tracks that start in the same point are all different.



# Injection set-up

- Injections may be defined as:
  - Single: a particle stream is injected from a single point.
  - Group: particle streams are injected along a line.
  - Cone: (3-D) particle streams are injected in a conical pattern.
  - Surface: particle streams are injected from a surface (one from each face).
  - File: particle streams injection locations and initial conditions are read in from an external file.



# Injection definition

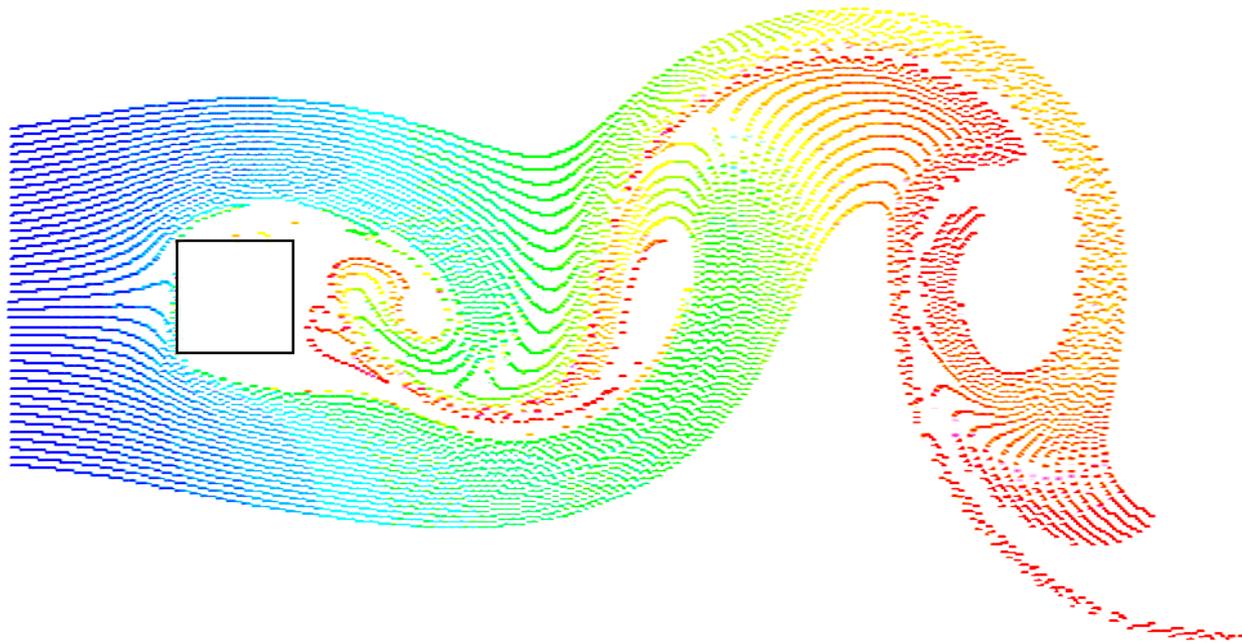
- Every injection definition includes:
  - Particle type (inert, droplet, or combusting particle).
  - Material (from data base).
  - Initial conditions (except when read from a file).
- Combusting particles and droplets require definition of destination species.
- Combusting particles may include an evaporating material.
- Turbulent dispersion may be modeled by stochastic tracking.

# Solution strategy: particle tracking

- Cell should be crossed in a minimum of two or three particle steps. More is better.
- Adjust step length to either a small size, or 20 or more steps per cell.
- Adjust “Maximum Number of Steps.”
- Take care for recirculation zones.
- Heat and mass transfer: reduce the step length if particle temperature wildly fluctuates at high vaporization heats.

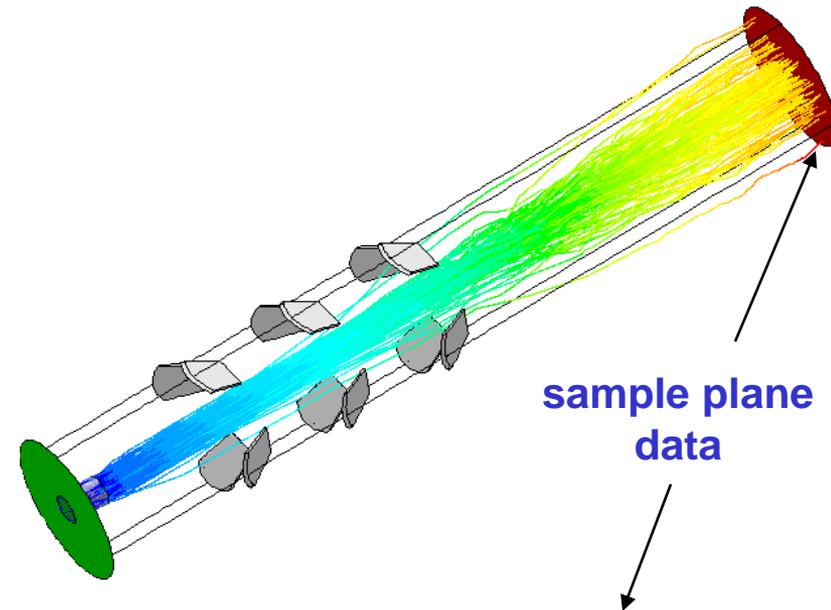
# Particle tracking in unsteady flows

- Each particle advanced in time along with the flow.
- For coupled flows using implicit time stepping, sub-iterations for the particle tracking are performed within each time step.
- For non-coupled flows or coupled flows with explicit time stepping, particles are advanced at the end of each time step.



# Sample planes and particle histograms

- Track mean particle trajectory as particles pass through sample planes (lines in 2D), properties (position, velocity, etc.) are written to files.
- These files can then be read into the histogram plotting tool to plot histograms of residence time and distributions of particle properties.
- The particle property mean and standard deviation are also reported.
- Files can be imported into Excel for additional plotting.

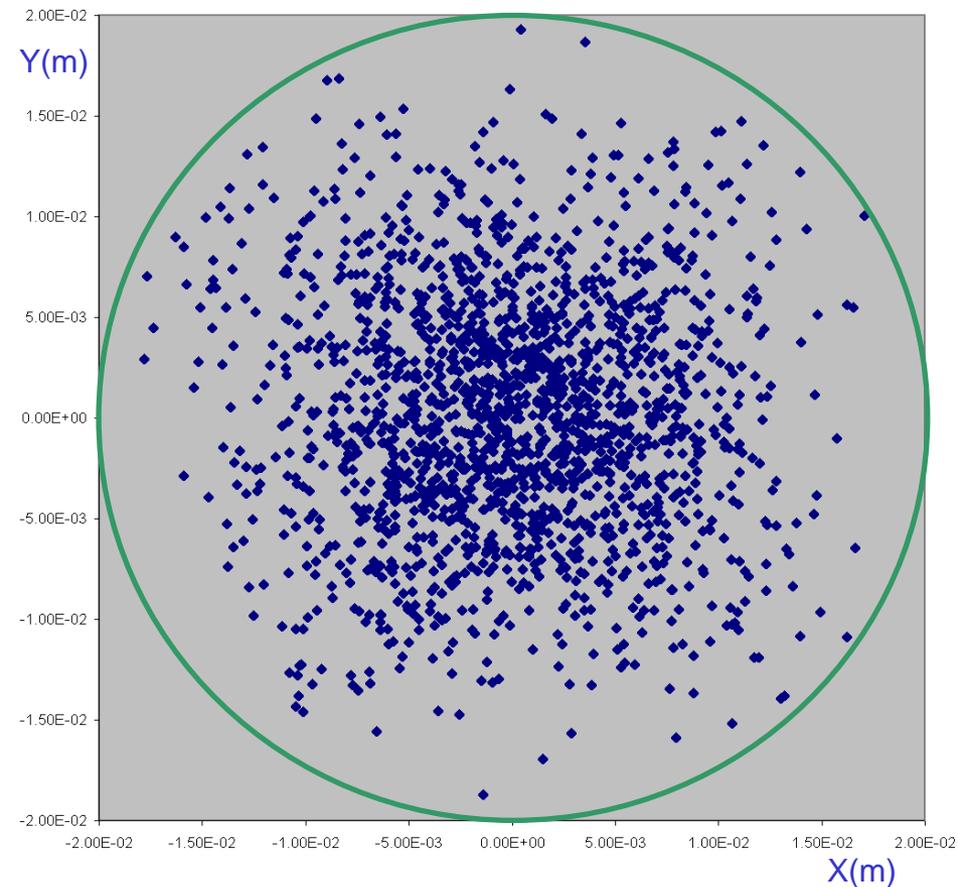


Microsoft Excel - p-outlet-frombiginlet.xls

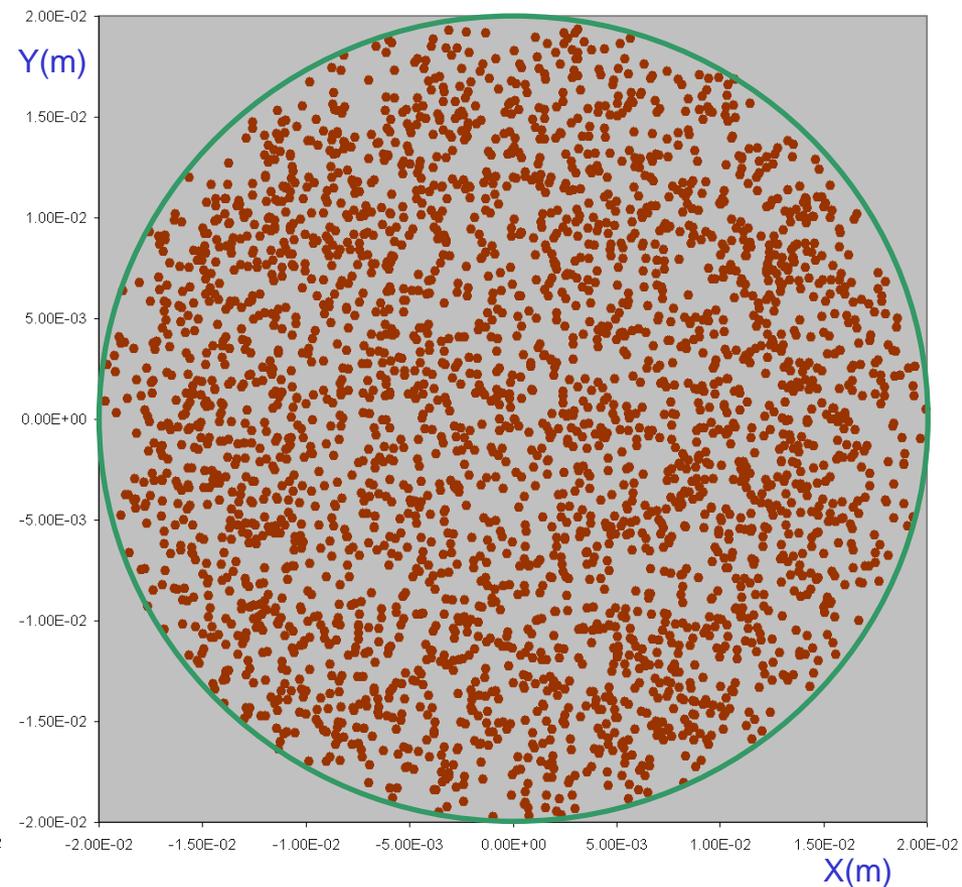
|    | B         | C         | D        | E         | F         | G        | H        | I        | J         | K           | L                    |
|----|-----------|-----------|----------|-----------|-----------|----------|----------|----------|-----------|-------------|----------------------|
| 1  | p-outlet  |           |          |           |           |          |          |          |           |             |                      |
| 2  | X         | Y         | Z        | U         | V         | W        | diameter | T        | mass-flow | time        | name                 |
| 3  | -1.65E-03 | -1.37E-02 | 1.80E-01 | 3.13E-02  | 3.33E-03  | 1.20E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.7625e+000 | biginlet-turbdisp:0  |
| 4  | -5.16E-03 | -1.73E-02 | 1.80E-01 | 1.21E-02  | -1.46E-02 | 8.60E-02 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 2.1119e+000 | biginlet-turbdisp:1  |
| 5  | 4.23E-03  | 1.71E-02  | 1.80E-01 | 7.08E-03  | 1.41E-02  | 9.31E-02 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5966e+000 | biginlet-turbdisp:2  |
| 6  | 1.75E-02  | 5.29E-03  | 1.80E-01 | -1.83E-02 | 1.69E-02  | 9.51E-02 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 2.3321e+000 | biginlet-turbdisp:3  |
| 7  | 1.28E-02  | 1.09E-02  | 1.80E-01 | 1.03E-02  | -2.07E-02 | 1.45E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4862e+000 | biginlet-turbdisp:4  |
| 8  | -1.21E-02 | -5.80E-03 | 1.80E-01 | -3.56E-03 | 1.31E-02  | 1.62E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5323e+000 | biginlet-turbdisp:5  |
| 9  | -8.84E-03 | -1.22E-02 | 1.80E-01 | -2.12E-02 | -9.28E-03 | 1.36E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5029e+000 | biginlet-turbdisp:6  |
| 10 | 6.43E-03  | 7.95E-03  | 1.80E-01 | 9.40E-04  | -3.27E-02 | 1.41E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5547e+000 | biginlet-turbdisp:7  |
| 11 | 4.73E-03  | -5.75E-03 | 1.80E-01 | 5.85E-03  | -1.58E-02 | 1.21E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4525e+000 | biginlet-turbdisp:8  |
| 12 | -8.46E-03 | 1.42E-02  | 1.80E-01 | -5.92E-03 | -9.73E-03 | 1.32E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.8950e+000 | biginlet-turbdisp:9  |
| 13 | -5.92E-03 | 9.29E-03  | 1.80E-01 | -8.97E-03 | -1.13E-03 | 1.37E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.6813e+000 | biginlet-turbdisp:10 |
| 14 | -1.17E-02 | 8.35E-03  | 1.80E-01 | 1.94E-03  | -1.22E-02 | 1.30E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4796e+000 | biginlet-turbdisp:11 |
| 15 | 1.18E-02  | -1.13E-02 | 1.80E-01 | -8.66E-03 | -1.37E-02 | 1.37E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5689e+000 | biginlet-turbdisp:12 |
| 16 | 1.04E-02  | -6.59E-04 | 1.80E-01 | -1.09E-02 | 1.95E-02  | 1.33E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.3931e+000 | biginlet-turbdisp:13 |
| 17 | -1.88E-02 | 3.81E-03  | 1.80E-01 | -1.21E-03 | -1.09E-02 | 5.16E-02 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.5971e+000 | biginlet-turbdisp:14 |
| 18 | -2.71E-03 | -1.58E-03 | 1.80E-01 | -3.18E-02 | -2.02E-02 | 1.37E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 2.2104e+000 | biginlet-turbdisp:15 |
| 19 | 5.42E-04  | -8.26E-03 | 1.80E-01 | -1.26E-02 | 1.96E-02  | 1.35E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.6430e+000 | biginlet-turbdisp:16 |
| 20 | 7.86E-03  | 2.31E-04  | 1.80E-01 | -1.15E-02 | 1.40E-02  | 1.52E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.7527e+000 | biginlet-turbdisp:17 |
| 21 | 1.27E-02  | 1.31E-02  | 1.80E-01 | -4.26E-03 | 8.12E-03  | 8.09E-02 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.7755e+000 | biginlet-turbdisp:18 |
| 22 | 1.00E-02  | 8.15E-03  | 1.80E-01 | 7.16E-03  | -2.68E-03 | 1.43E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4351e+000 | biginlet-turbdisp:19 |
| 23 | -1.05E-02 | -1.56E-02 | 1.80E-01 | -7.89E-03 | -7.71E-03 | 1.46E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.6010e+000 | biginlet-turbdisp:20 |
| 24 | -8.44E-03 | -9.87E-03 | 1.80E-01 | 1.76E-02  | 1.01E-02  | 1.53E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4710e+000 | biginlet-turbdisp:21 |
| 25 | 1.29E-04  | -3.94E-05 | 1.80E-01 | -1.99E-02 | -8.63E-03 | 1.43E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.4557e+000 | biginlet-turbdisp:22 |
| 26 | -8.84E-03 | -1.36E-02 | 1.80E-01 | -1.29E-02 | 4.39E-03  | 1.20E-01 | 1.00E-06 | 3.00E+02 | 0.00E+00  | 1.6535e+000 | biginlet-turbdisp:23 |

# Particle locations at outlet (HEV)

- Flow following particles.



Particles from small center inlet

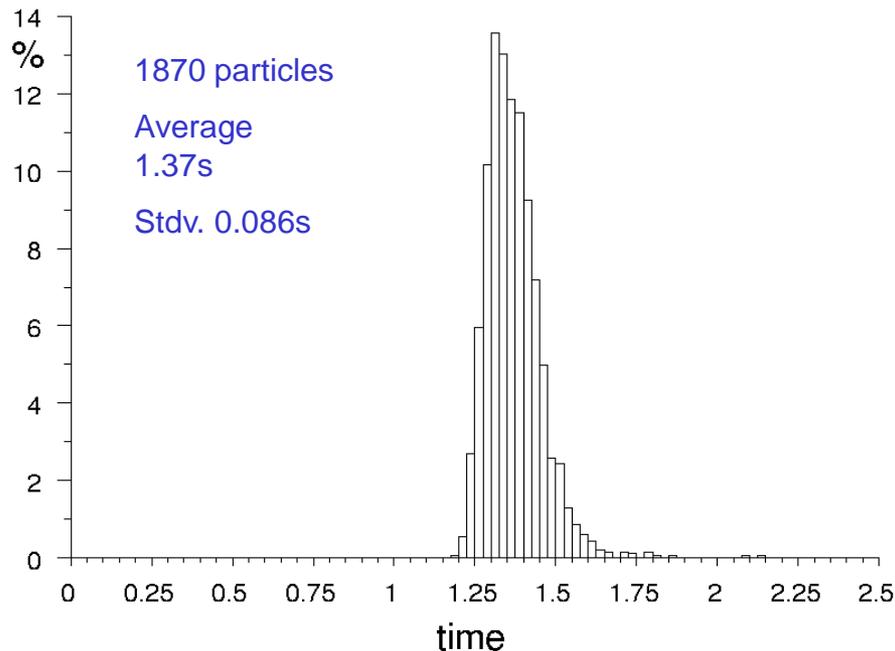


Particles from large outer inlet

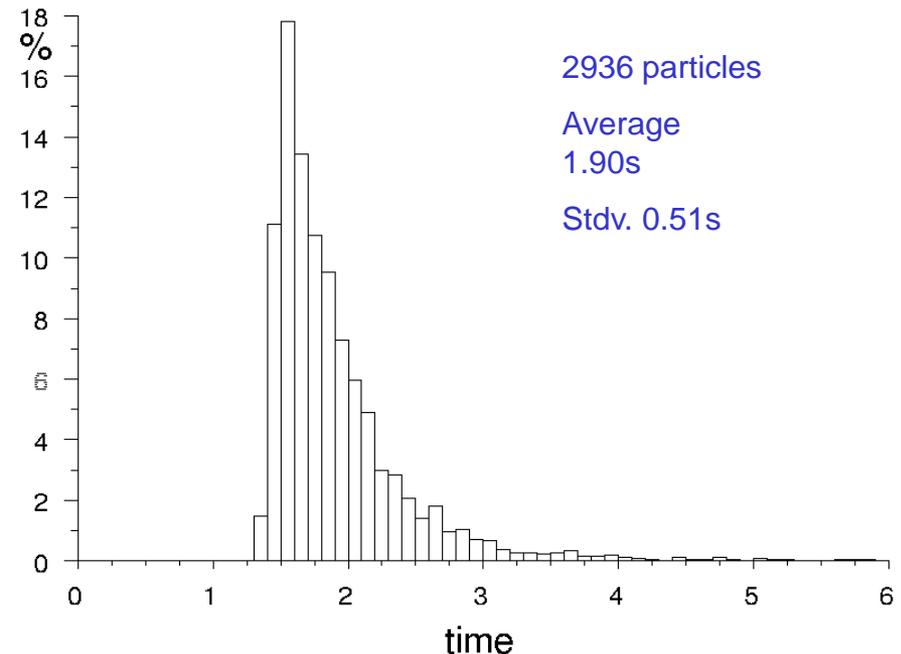
*These graphs show where the particle trajectories intersect with a plane (in this case the outlet). Such intersection graphs are also called Poincaré maps.*

# Residence time distribution

- Residence time histograms can be made from particle times at outlet for flow following particles.
- For this mixer, volume is 0.275 l, total volumetric flow rate is 0.152 l/s, and an average residence time of 1.8 s is expected.



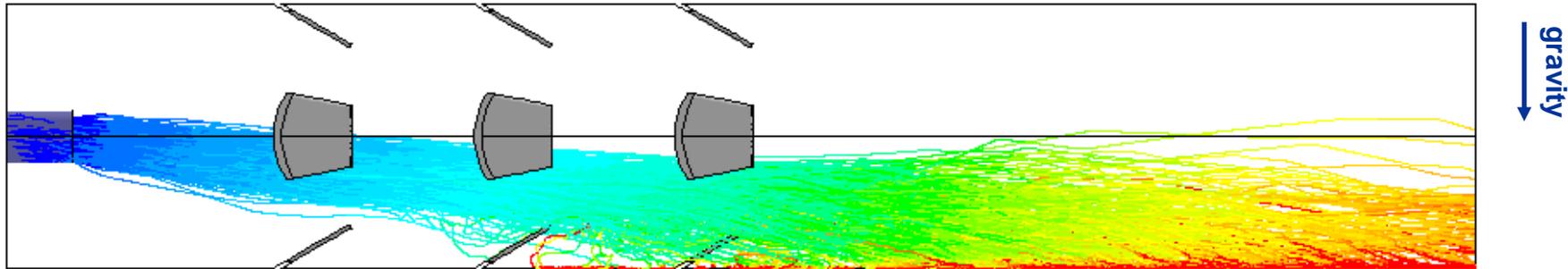
Particles from small center inlet



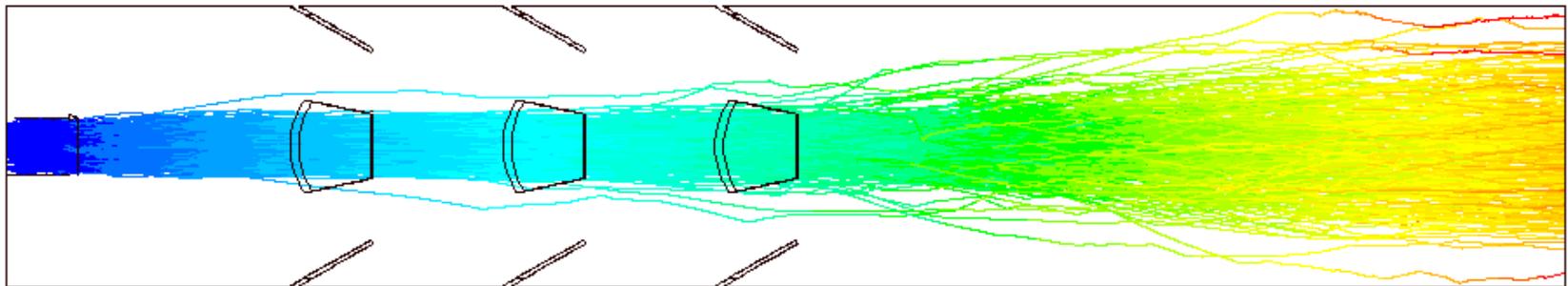
Particles from large outer inlet

# Effect of particle properties

- Sand particles (0.2mm, 2000 kg/m<sup>3</sup>).



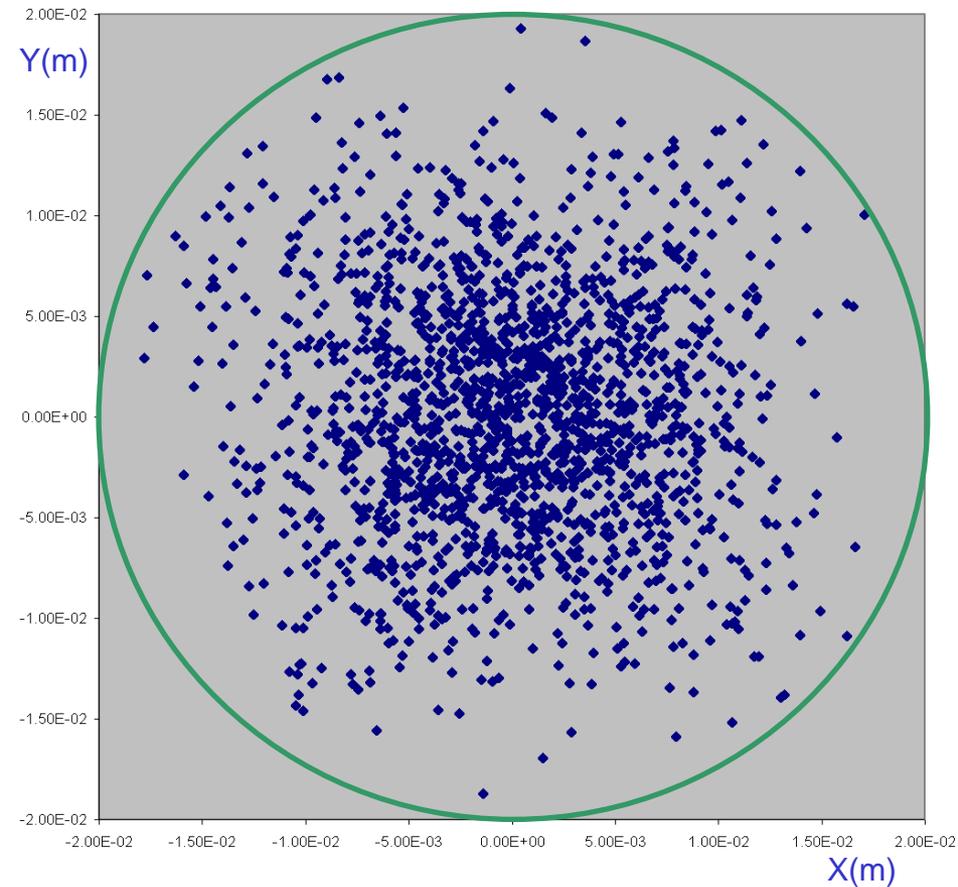
- Flow following particles.



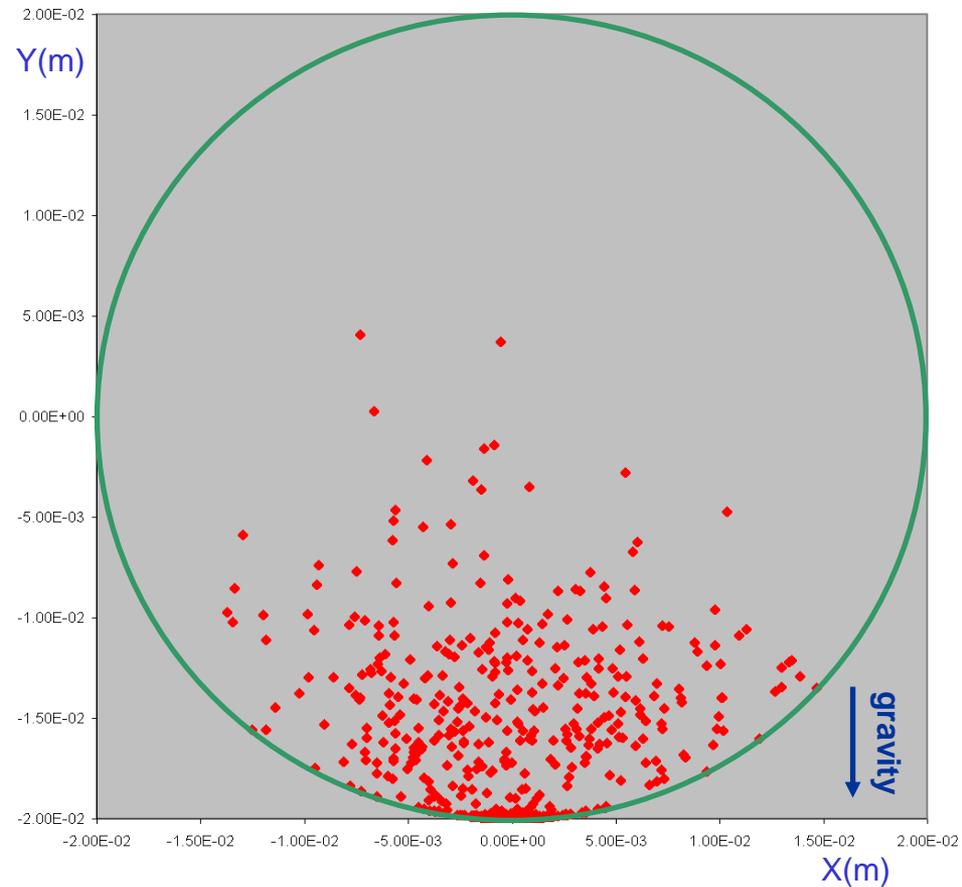
# Effect of particle properties

- Flow following particles.

- Sand particles (in water).



Particles from small center inlet



Particles from small center inlet.

# Particle tracking accuracy

- There are three types of errors: discretization, time integration, and round-off.
- Research has shown that in regular laminar flows the error in the particle location increases as  $t^2$ , and in chaotic flows almost exponentially.
- Errors tend to align with the direction of the streamlines in most flows.
- As a result, even though errors multiply rapidly (e.g., 0.1% error for 20,000 steps is  $1.001^{20,000} = 4.8E8$ ), qualitative features of the flow as shown by the deformation of material lines can be properly reproduced. But the length of the material lines may be off by as much as 100%.
- Overall, particle tracking, when properly done, is less diffusive than solving for species transport, but numerical diffusion does exist.

# Summary

- There are different main ways to model material transport:
  - Multiphase flow: multiple momentum equations.
  - Species flow: one set of momentum equations.
  - Discrete phase modeling (DPM; particle tracking): one set of momentum equations for the fluid flow. Additional force balance for the individual particles.
- Species mixing:
  - Material distribution, mixing parameters.
  - Basis for chemical reaction calculations.
- DPM:
  - Heat and mass transfer from particles.
  - Mixing analysis.
  - Unlike species, do not necessarily follow fluid flow exactly.

# Blend Times in Stirred Tanks

## Reacting Flows - Lecture III

André Bakker

# Evaluation of mixing performance

- Methods to evaluate mixing performance:
  - Characterization of homogeneity.
  - Blending time.
- General methods to characterize homogeneity:
  - Visual uniformity.
  - Quantitative change in local concentration as a function of time.
  - Review instantaneous statistics about the spatial distribution of the species.
    - Average concentration
    - Minimum and maximum
    - Standard deviation in the concentration.
    - Coefficient of variation  $CoV = \text{standard deviation}/\text{average}$ .

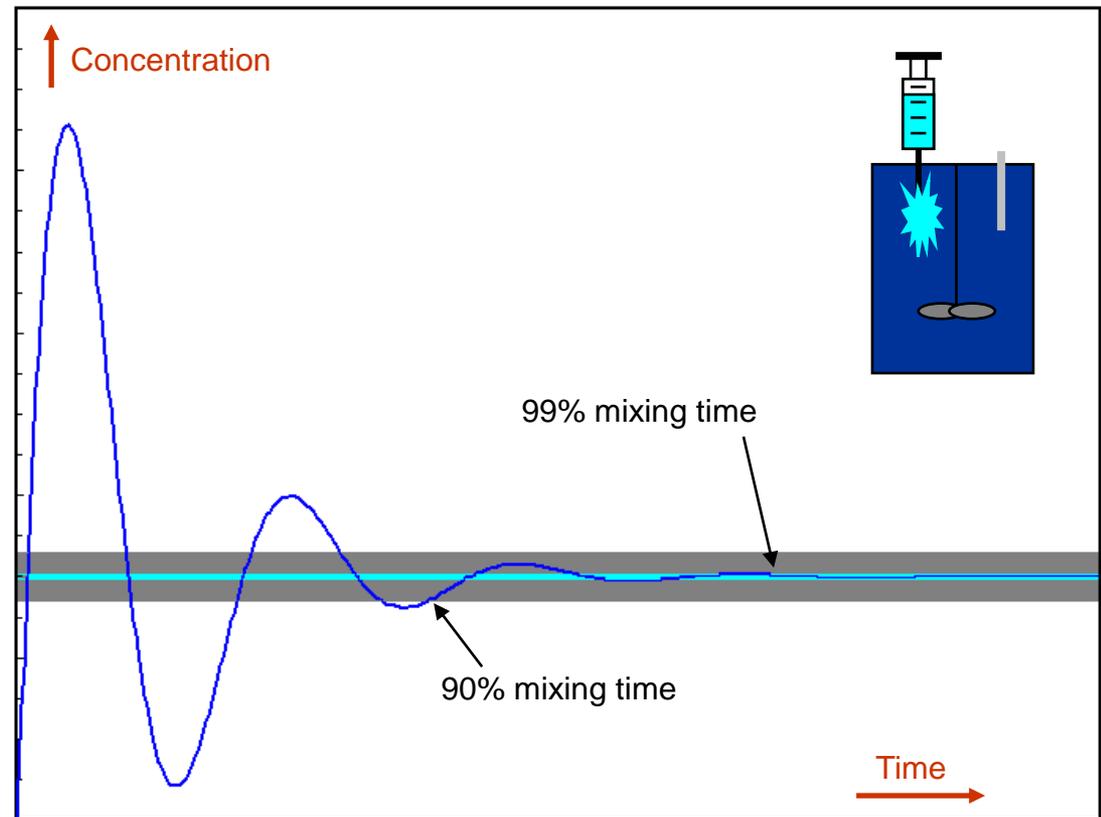
# Visual uniformity

- Experimentally measure the time it takes to obtain visual uniformity.
- Can be done with acid-base additions and a pH indicator.
- Offers good comparisons between performance of different mixing systems.
- Not a suitable approach for CFD.



# Quantitative variation in a point

- Measuring the tracer concentration as a function of time  $c(t)$  in one or more points in the vessel, is a common experimental method.
- The mixing time is then the time it takes for the measured concentration  $c(t)$  to stay within a certain range of the final concentration  $c_\infty$ .
- Advantage: easy to use in experiments.
- Disadvantage: uses only one or a few points in the vessel.
- Does not use all information present in a CFD simulation.



# Blend time calculations with CFD

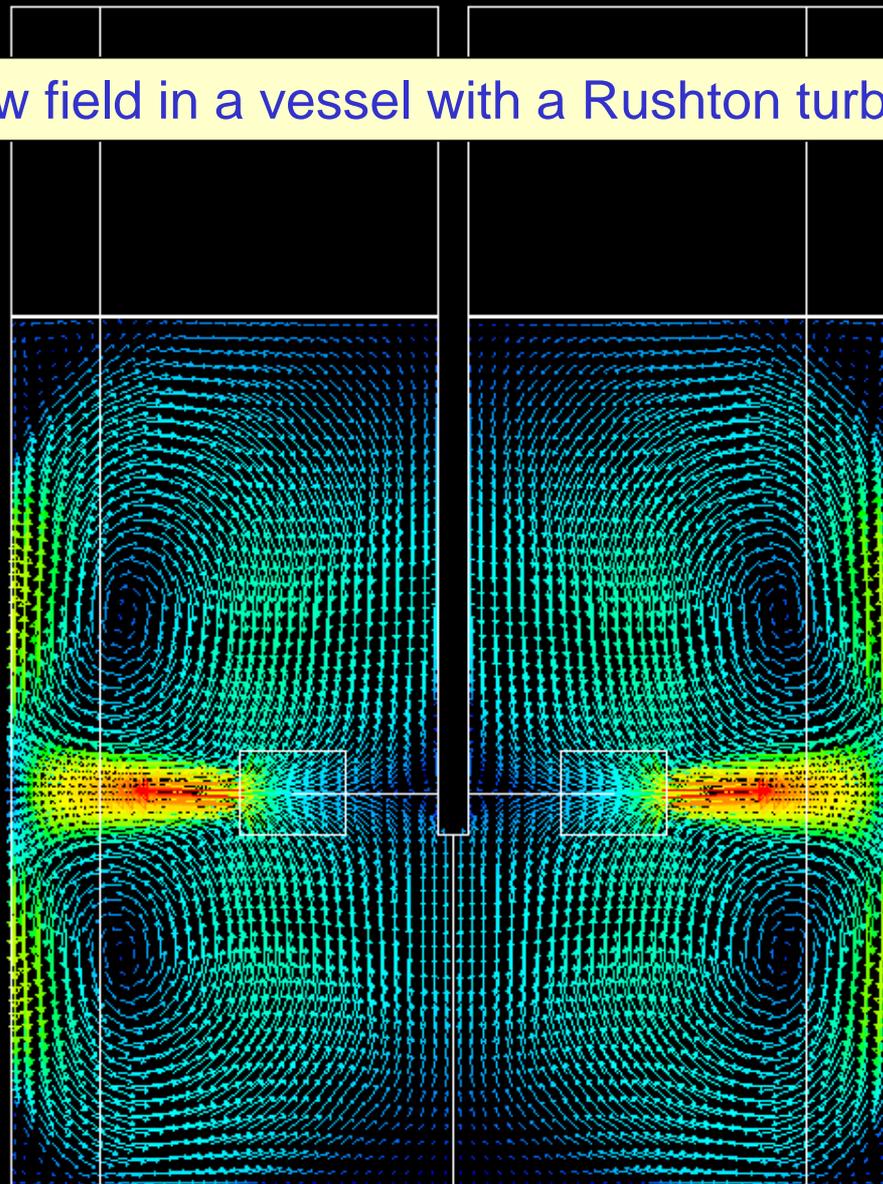
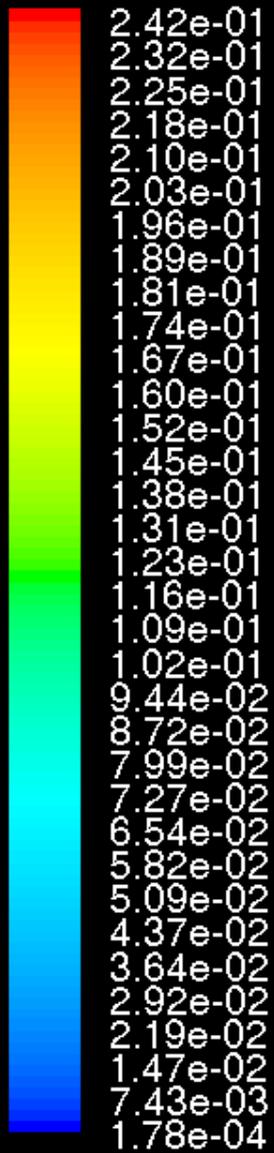
- Transport and mixing of a tracer:
  - Add tracer to the domain.
  - Mass fraction of tracer calculated and monitored as a function of time.
  - Determine blend time based on the mass-fraction field satisfying a pre-specified criterion.
- Flow field required can be steady, frozen unsteady or unsteady.
- Benefit of CFD:
  - The full concentration field is known.
  - Can use more data to determine blend time than what can be measured experimentally using probes.
- Main question: what should be the mixing criterion?

# CFD analysis for blend time

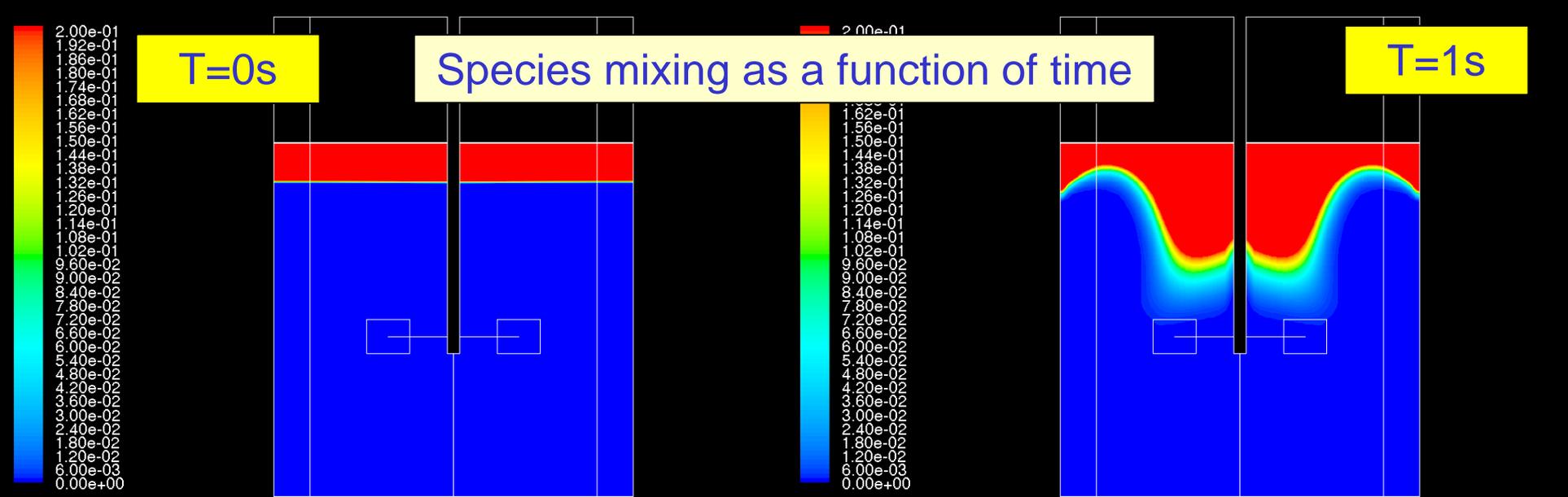
|   |                  | <i>Physical Lab</i> | <i>CFD Lab</i> |
|---|------------------|---------------------|----------------|
| <b><i>Addition of Tracer</i></b>                  | Volume of Tracer | Controlled          | Exact          |
|   | Delivery Time    | finite              | zero           |
|   | Location         | variable            | fixed          |
| <b><i>Concentration Measurement of Tracer</i></b> | Conductivity     | Yes                 | No             |
|   | Color            | Yes                 | No             |
|   | Mass Fraction    | inferred            | Yes            |

- We will now:
  - Illustrate the blend time analysis using a 2-D Rushton turbine flow field example.
  - Tracer added and its transport and mixing calculated. Mass fractions are monitored as a function of time.
  - Blend time is calculated using different criteria.

## Example: flow field in a vessel with a Rushton turbine

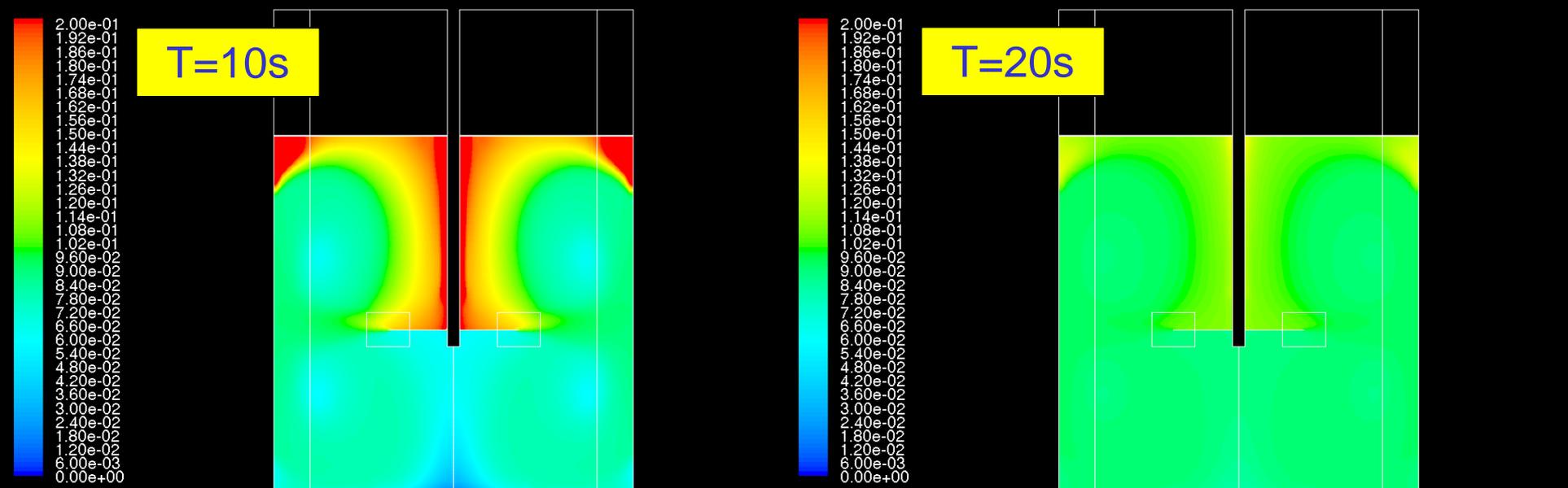


Rushton Impeller - 50 RPM - 31.6l Vessel  
Velocity Vectors Colored By Velocity Magnitude (m/s)



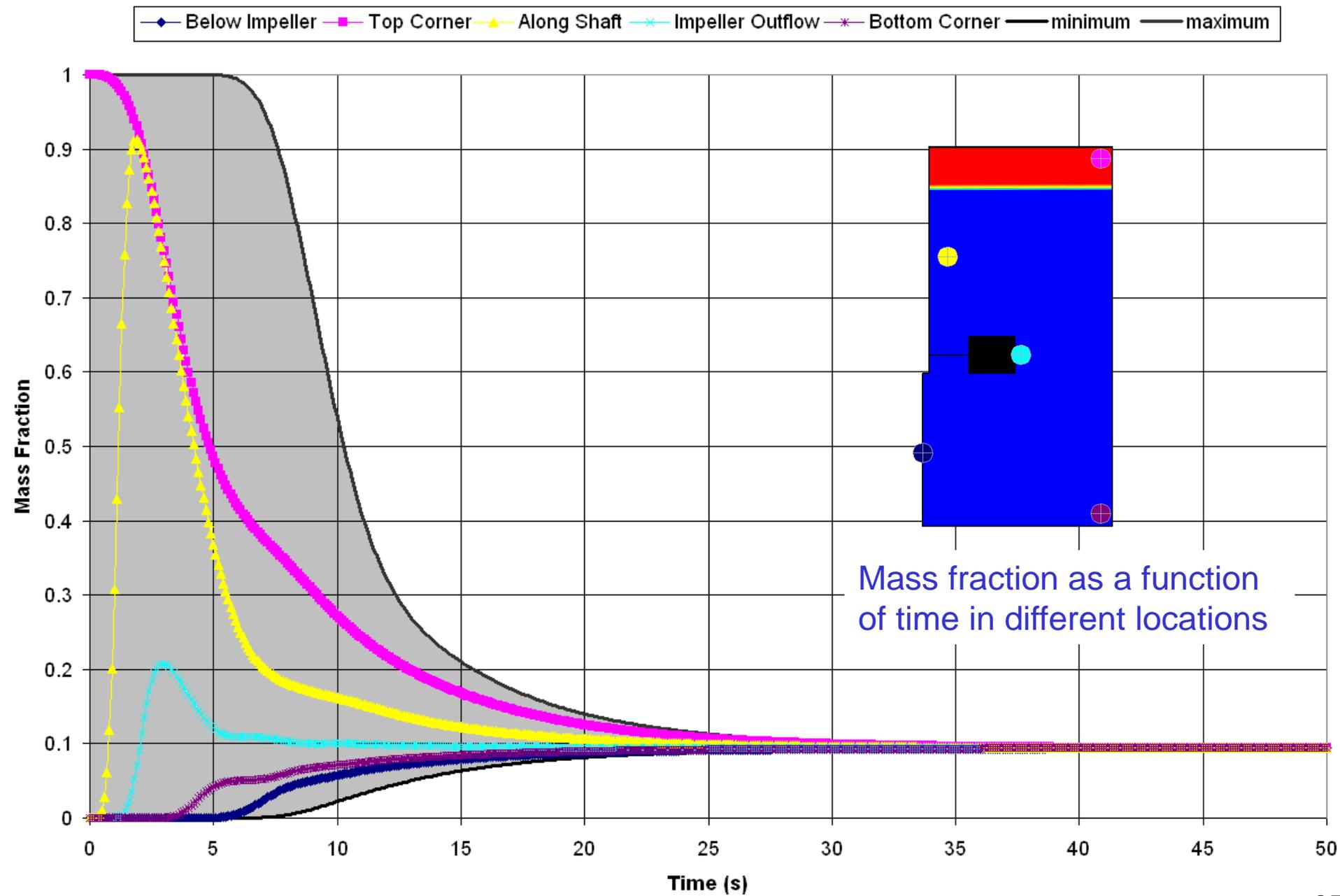
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



# Measures of variation

- Variations in  $Y$ , the mass fraction of tracer, can be measured in several ways. For all measures, greater numbers indicate a greater variation with no upper bound.
- Coefficient of variation. Ratio between standard deviation  $\sigma_Y$  and the average  $\langle Y \rangle$ :

$$CoV = \frac{\sigma_Y}{\langle Y \rangle}$$

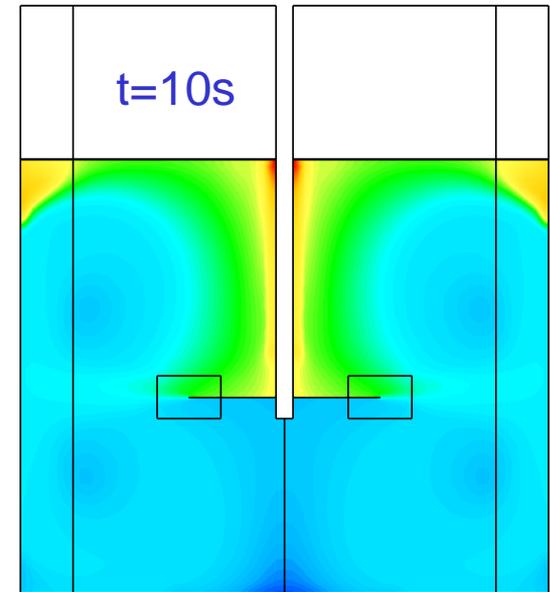
- Ratio between maximum and minimum mass fractions  $Y_{\max}/Y_{\min}$ .
- Largest deviation between extremes in the mass fraction and the average:

$$\Delta_{\max} = \max(Y_{\max} - \langle Y \rangle, \langle Y \rangle - Y_{\min})$$

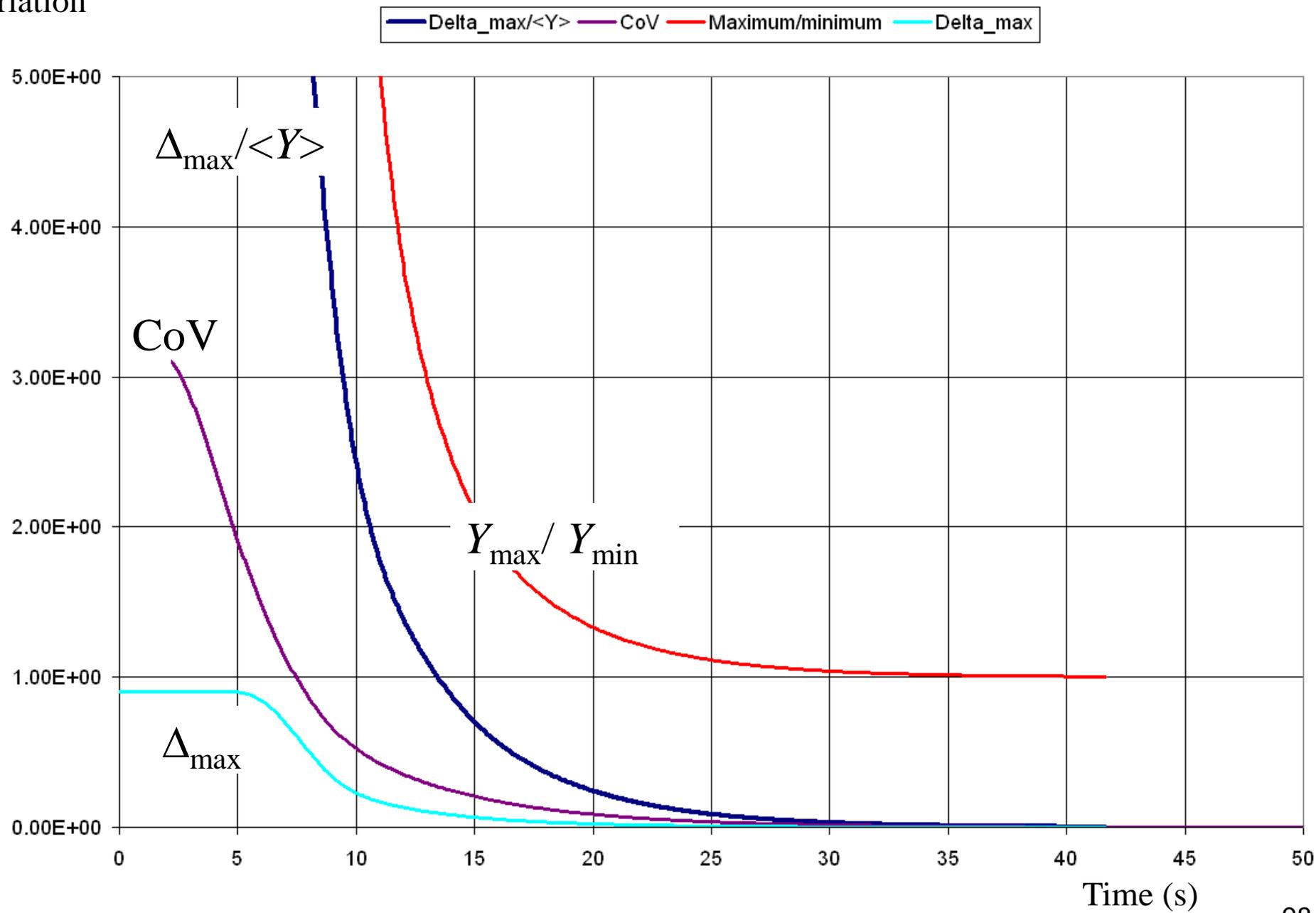
Can also be normalized over  $\langle Y \rangle$ .

# Variation calculation example

- Mass fraction data:
  - Min-max anywhere: 0.0223-0.539
  - Min-max from probes: 0.0574-0.272
  - Average: 0.0943
  - Standard deviation: 0.0493
  
- Measures of variation:
  - $\text{Max/min} = 0.539/0.0223 = 24.2$  (anywhere)
  - $\text{Max/min} = 0.272/0.0574 = 4.7$  (from probes)
  - $\text{CoV} = 0.0493/0.0943 = 0.52$
  - $\Delta_{\text{max}} = \max(0.539-0.0943, 0.0943-0.0223) = 0.44$
  - $\Delta_{\text{max}}/\langle Y \rangle = 0.44/0.0943 = 4.7$



## Variation



# Measures of uniformity - absolute

- There is a need to have an absolute measure of uniformity  $U$  that is  $\leq 1$  with 1 (or 100%) indicating perfect uniformity.

- Ratio between the minimum and maximum mass fractions.

- Bounded between 0 and 1.

$$U_{\min/\max} = \frac{Y_{\min}}{Y_{\max}}$$

- Based on coefficient of variance CoV:

- Not bounded: can be less than 0.

$$U_{CoV} = 1 - CoV$$

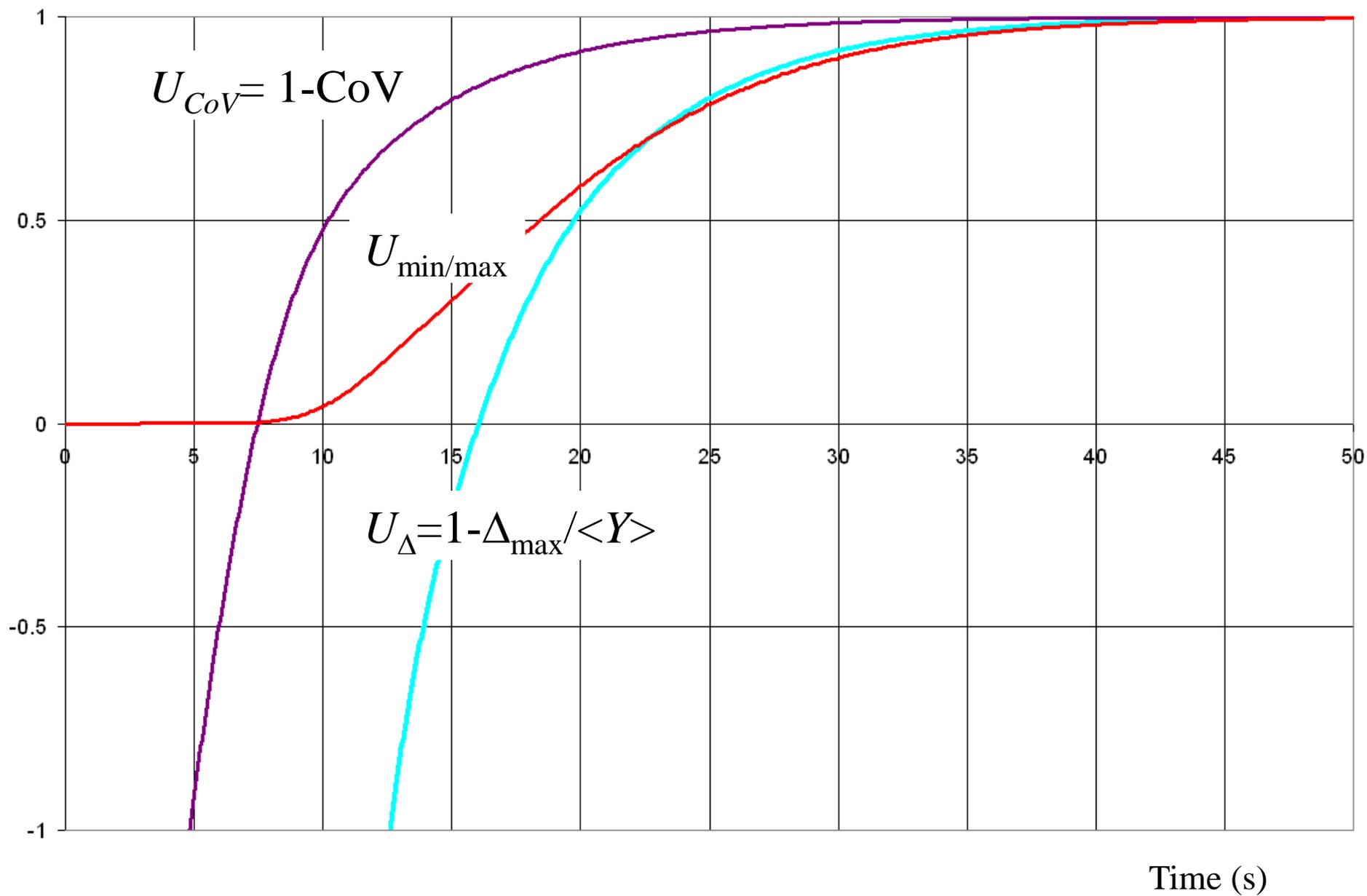
- Based on largest deviation from the average:

- Conceptually closer to common experimental techniques.

- Not bounded: can be less than 0.

$$U_{\Delta} = 1 - \frac{\Delta_{\max}}{\langle Y \rangle}$$

Uniformity

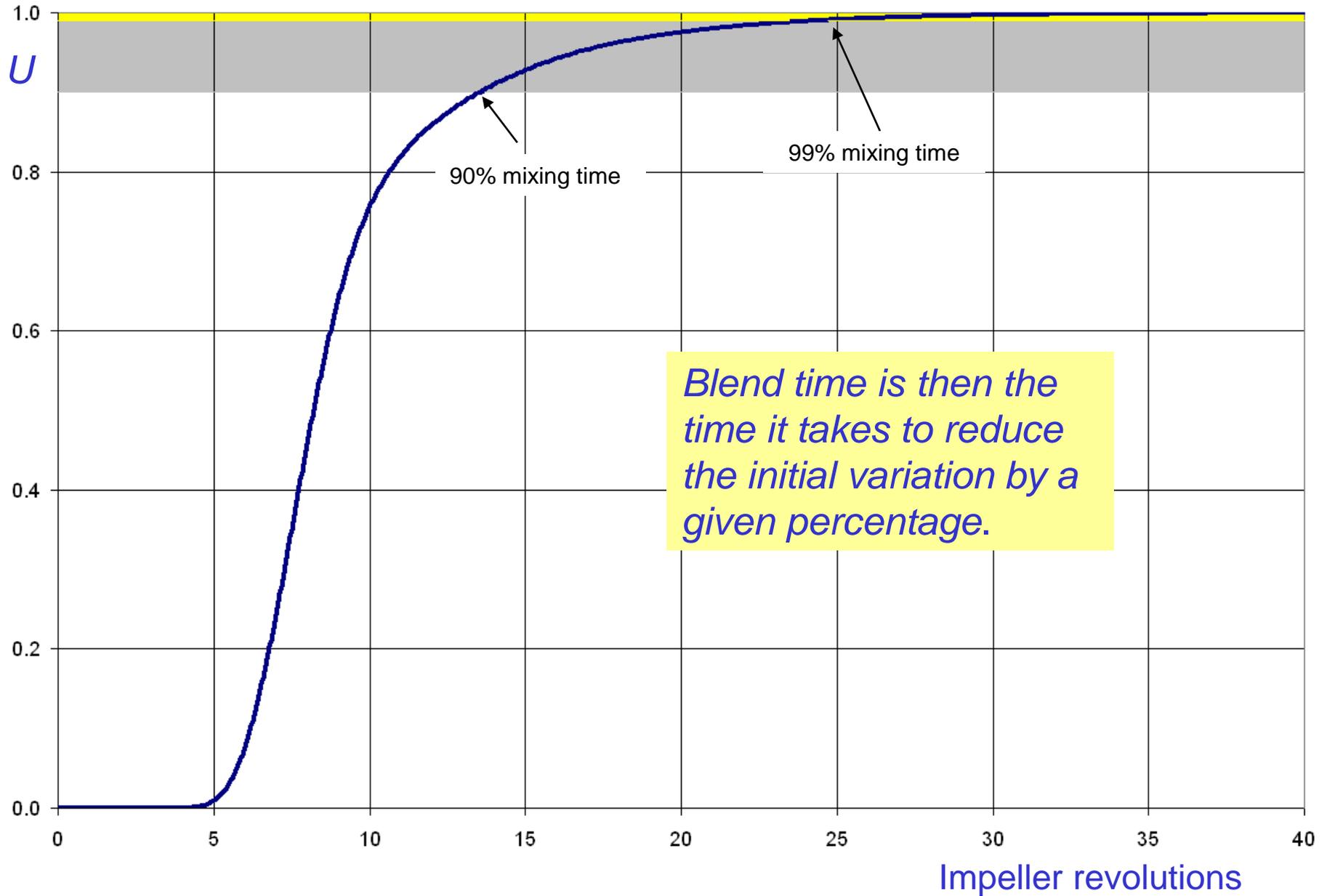


# Uniformity

- These measures of uniformity:
  - All indicate perfect uniformity at values of 1.
  - Are not all bounded between 0 and 1.
  - Do not take initial conditions into account.
- Generally, it is most useful to be able to predict the time it takes to reduce concentration variations by a certain amount.
- This is then done by scaling the largest deviation in mass fraction at time  $t$  by the largest deviation at time  $t=0$ .

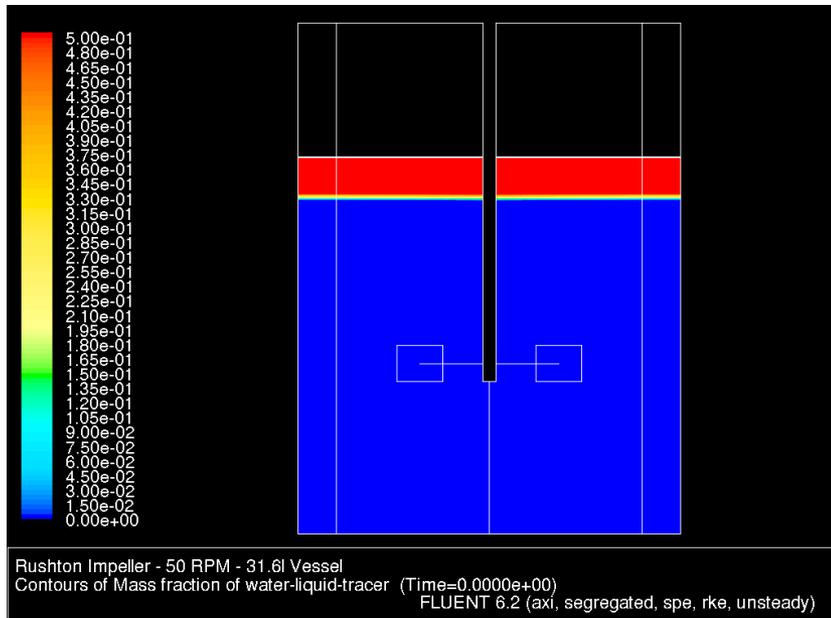
$$U(t) = 1 - \frac{\Delta_{\max}(t)}{\Delta_{\max}(t=0)}$$

- e.g., for the example case:
  - At  $t=0\text{s}$ ,  $Y_{\max}=1$  and  $\langle Y \rangle=0.0943 \rightarrow \Delta_{\max}(t=0) = 0.906$ .
  - At  $t=10\text{s}$ ,  $\Delta_{\max}(10\text{s}) = 0.44 \rightarrow U(10\text{s}) = 0.51$ .
- Data are often correlated in terms of number of impeller revolutions, at  $t=10\text{s}$  and 50RPM, there were  $10 \cdot \text{RPM}/60=8.33$  impeller revolutions.

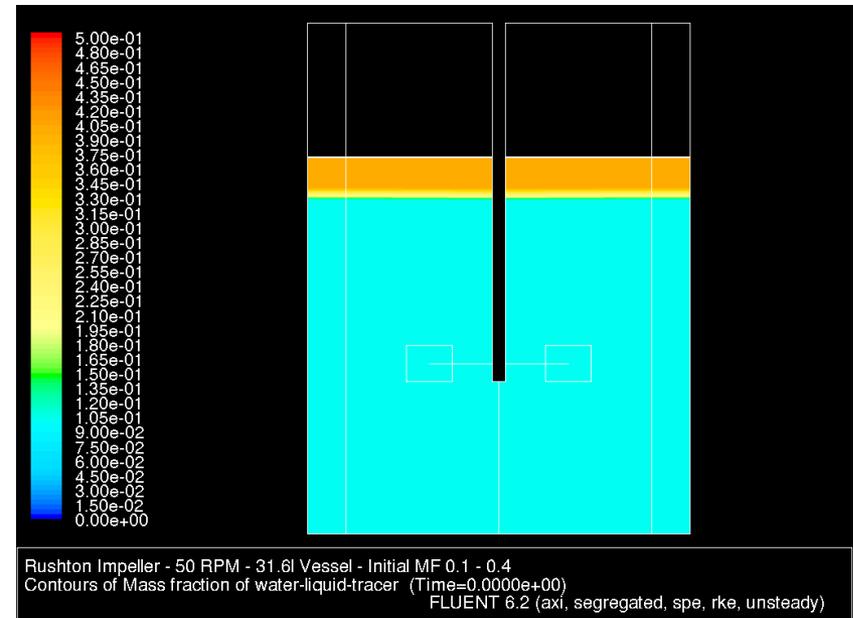


# Comparison between systems

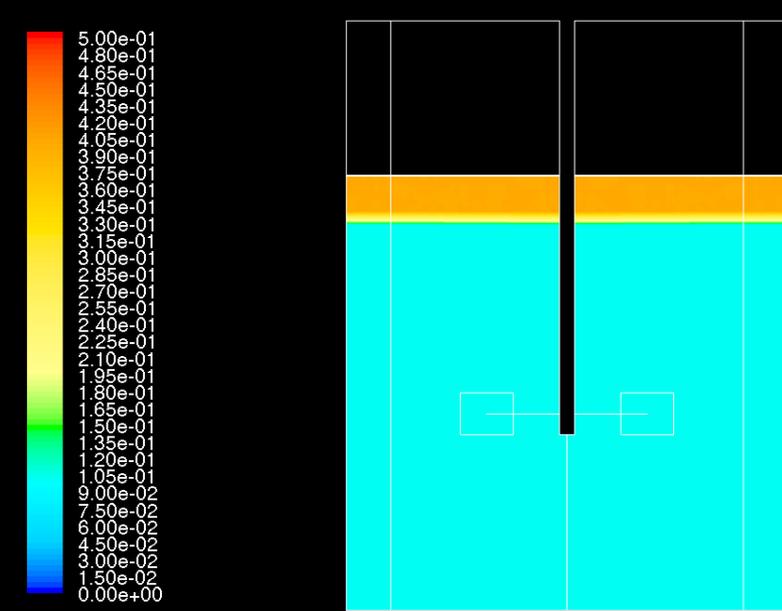
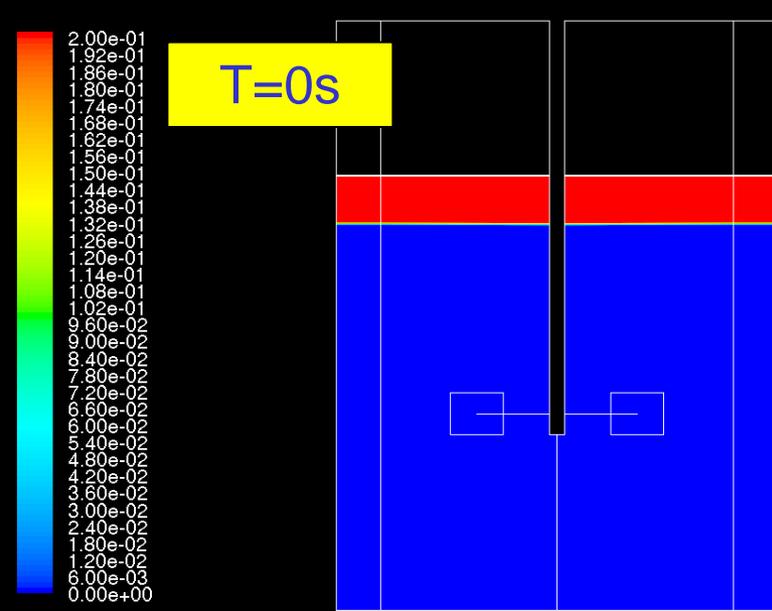
- Let's compare two systems with:
  - The same flow field.
  - The same spatial distribution of species.
  - But different initial mass fractions of species.



Layer with  $Y_{tracer}=1$  on top of fluid  
with  $Y_{tracer}=0$ .  $\langle Y \rangle = 0.094$ .

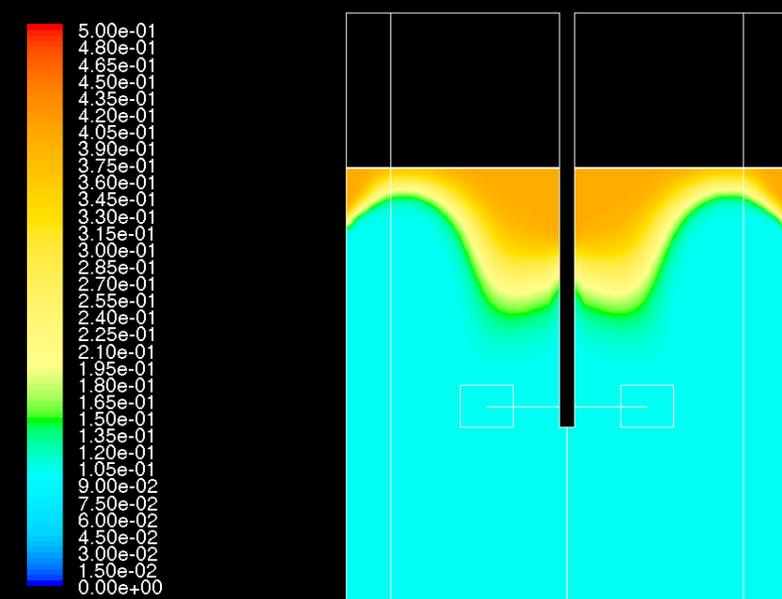
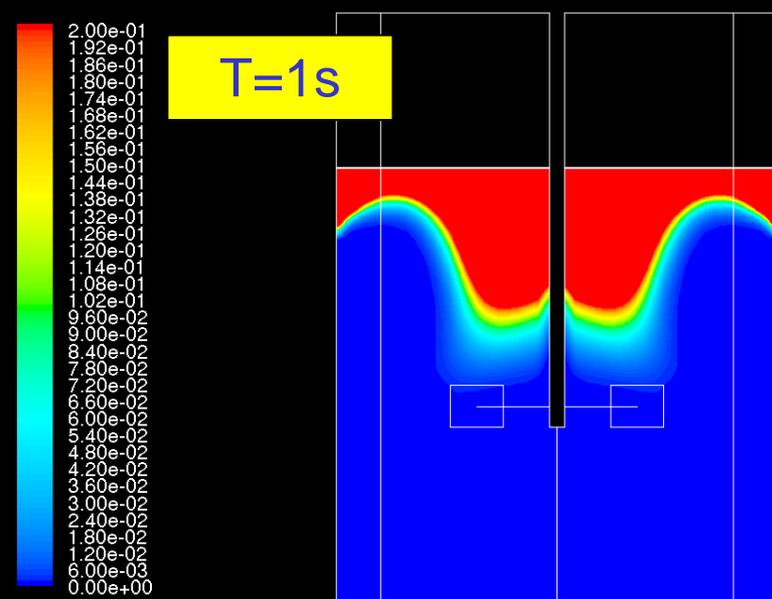


Layer with  $Y_{tracer}=0.4$  on top of fluid  
with  $Y_{tracer}=0.1$ .  $\langle Y \rangle = 0.13$ .



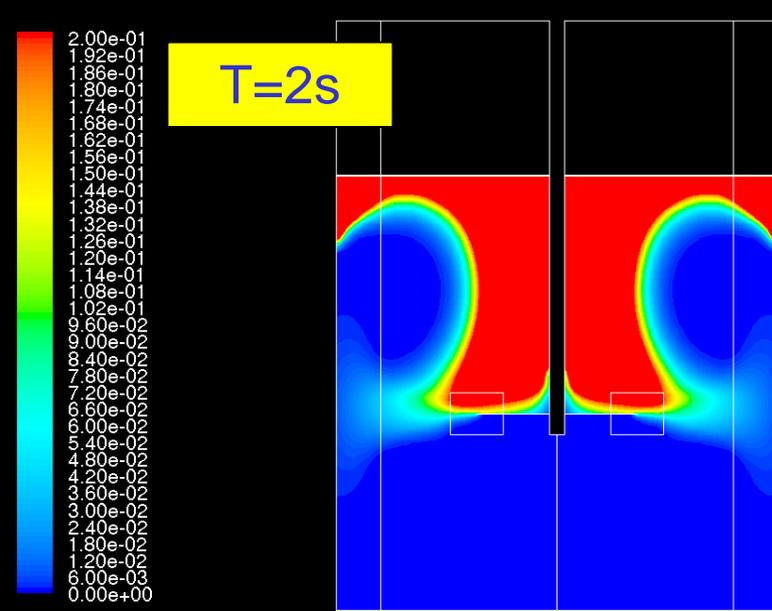
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

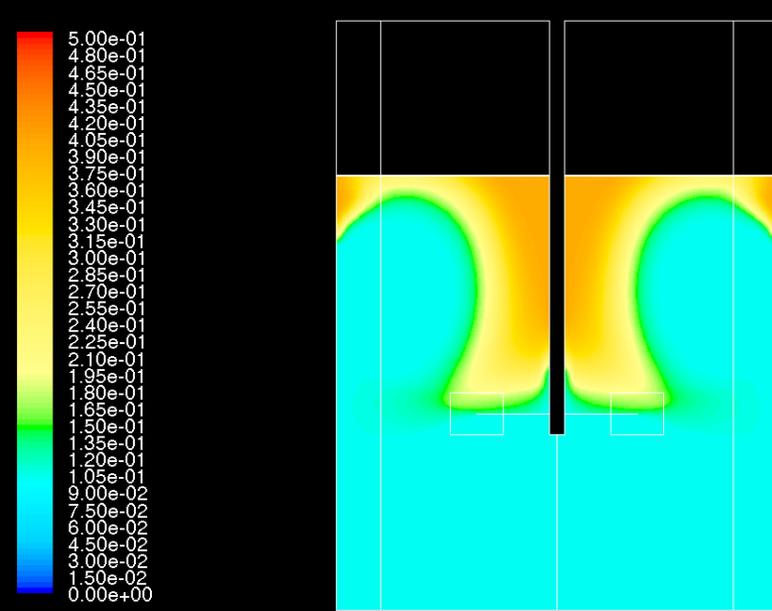


Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

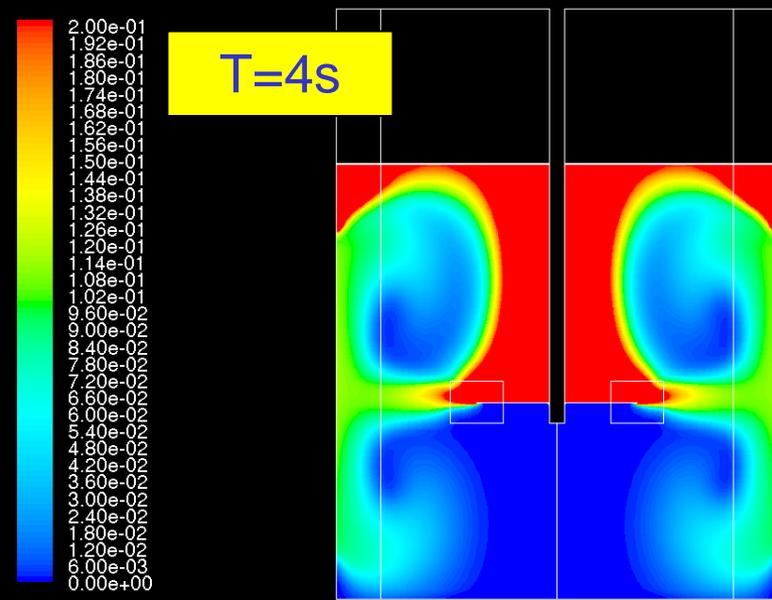
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



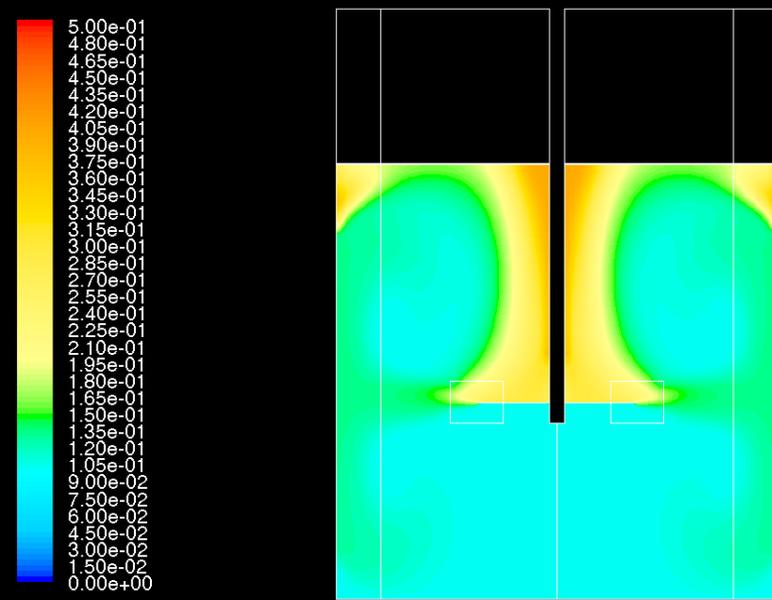
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



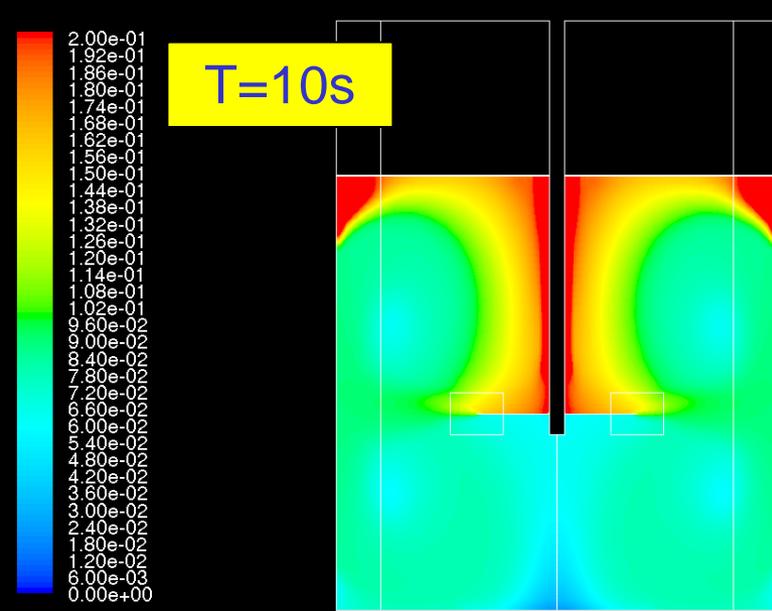
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



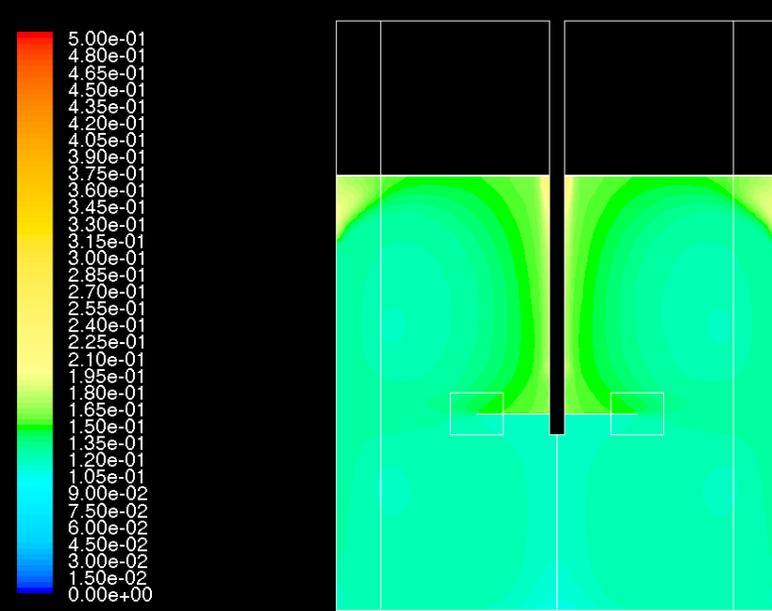
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=4.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



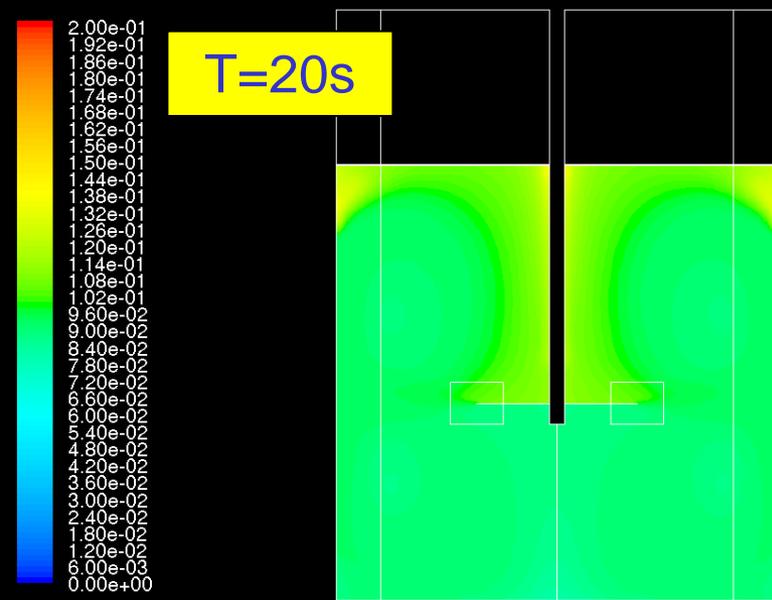
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=4.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



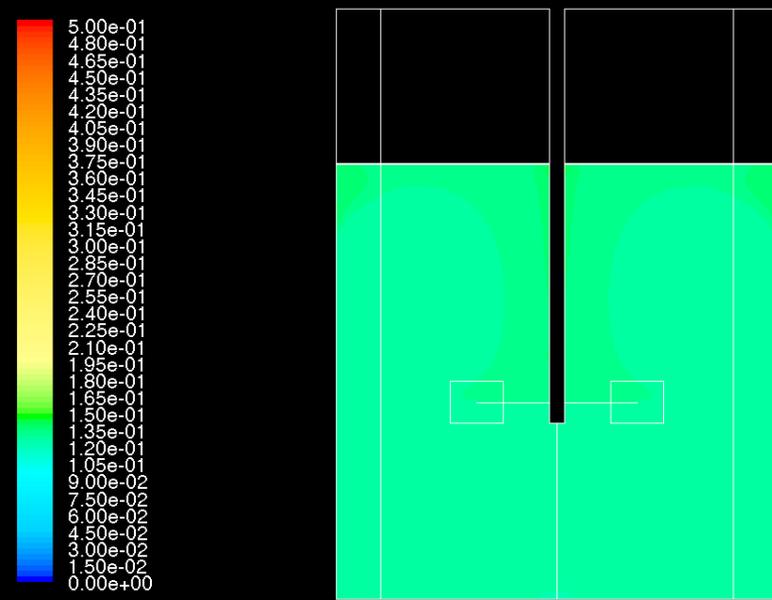
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



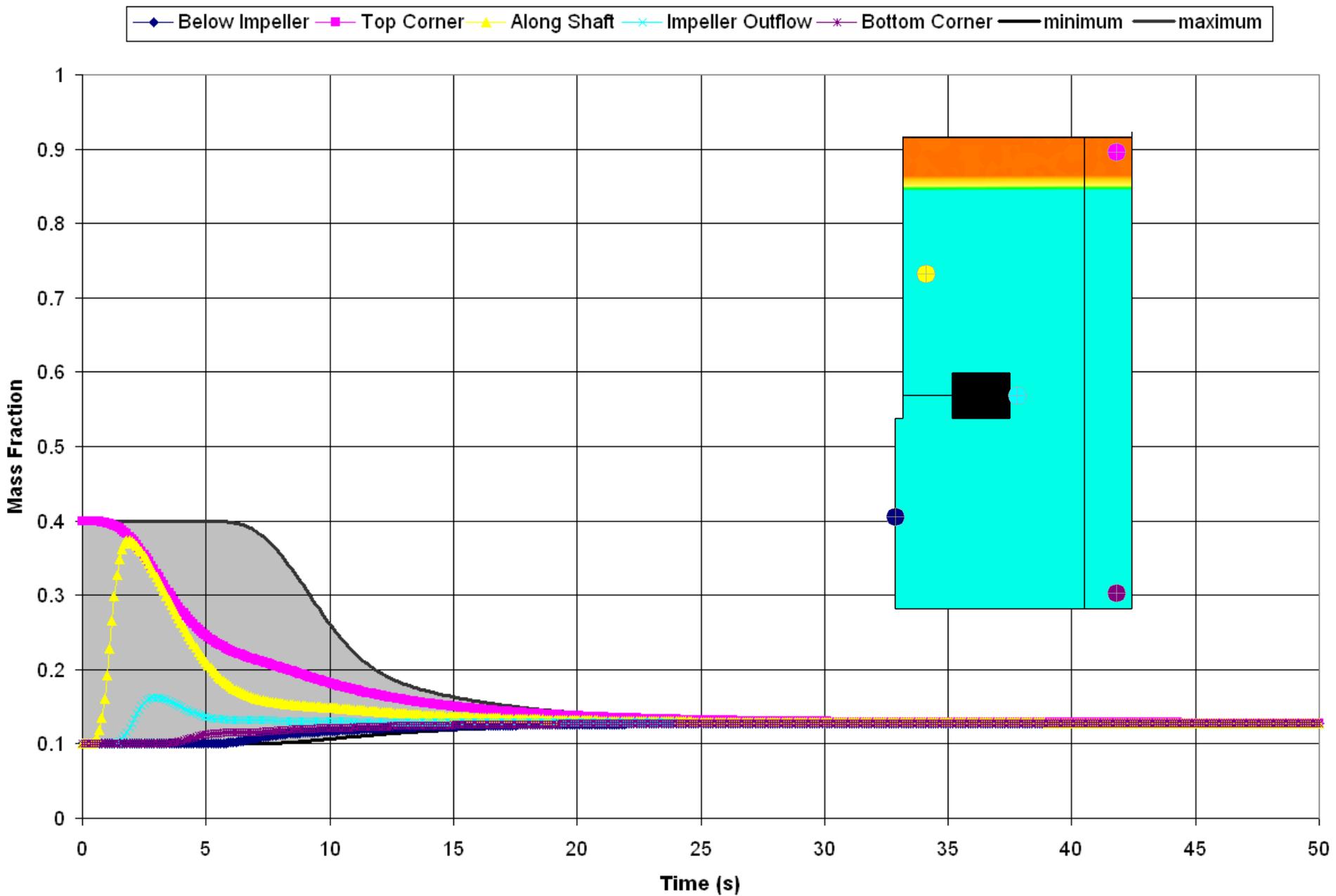
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

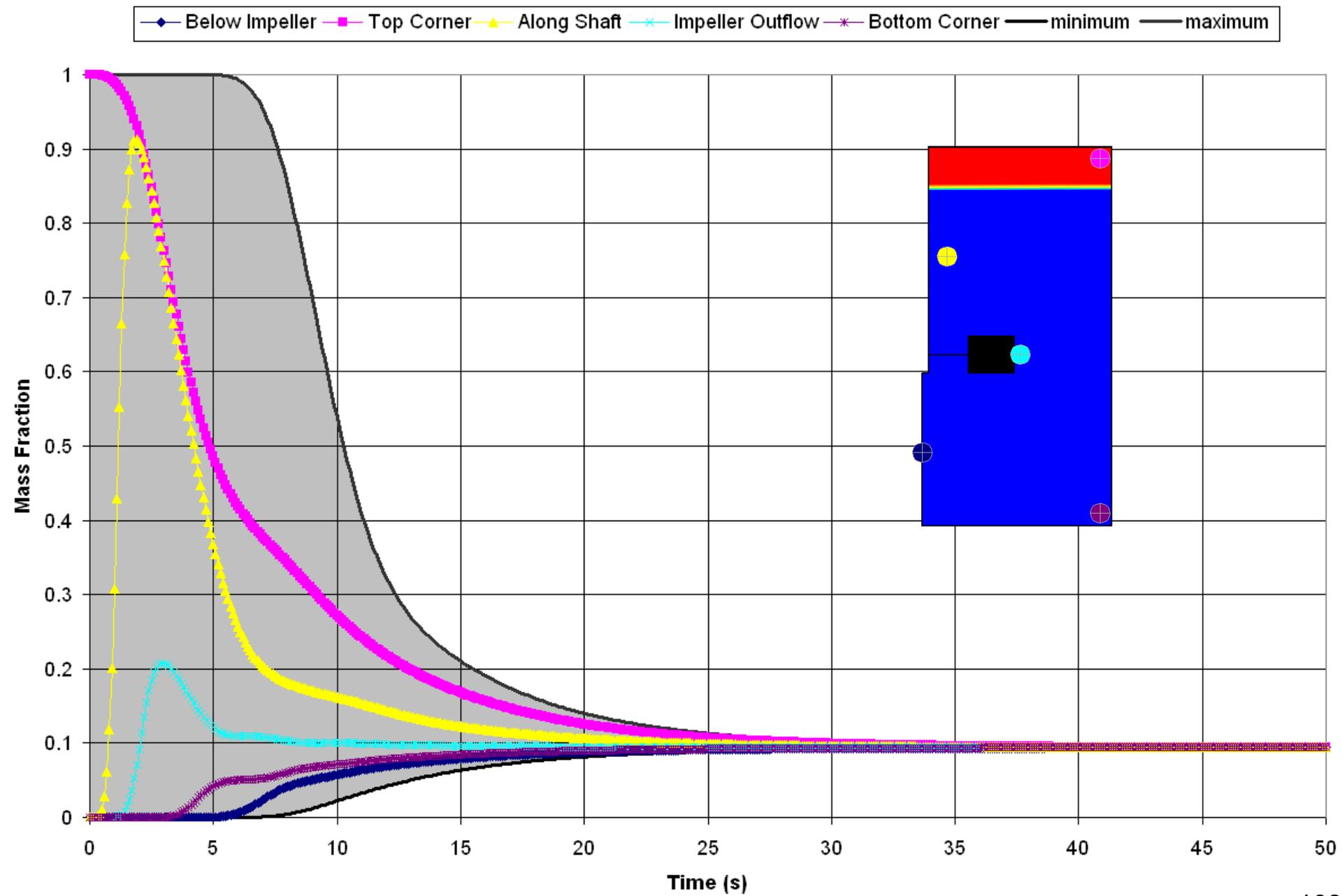


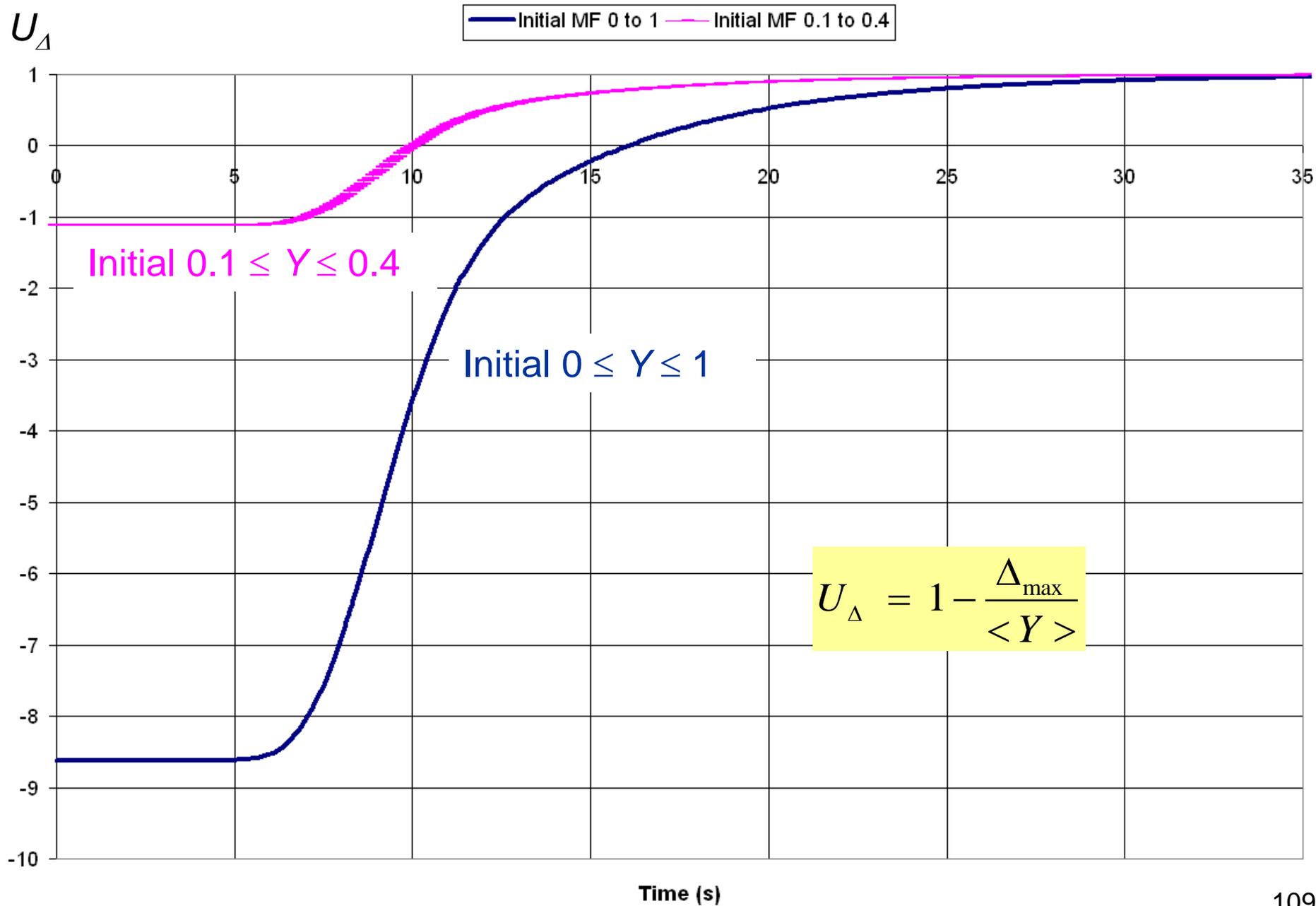
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

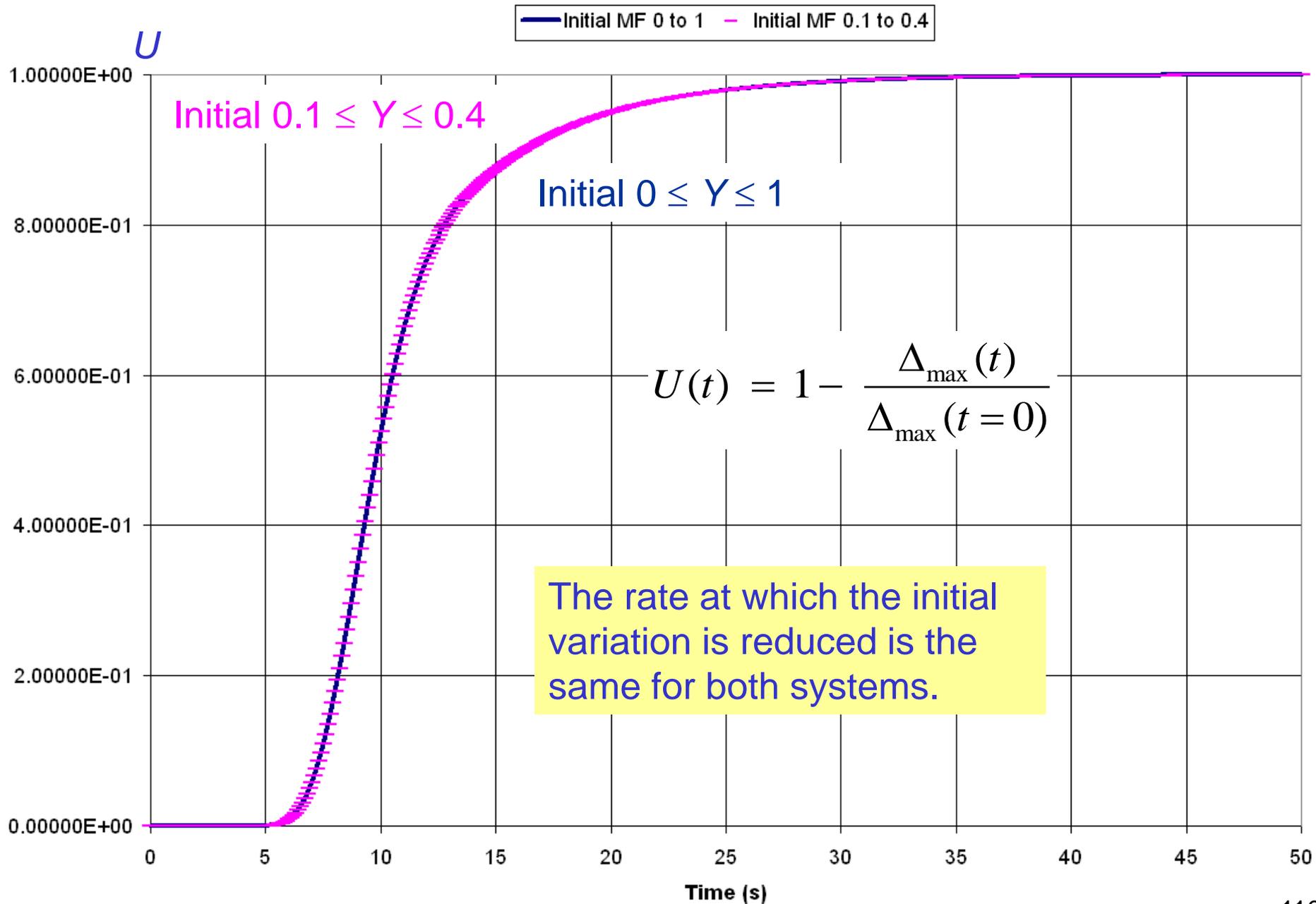


Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF 0.1 - 0.4  
Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



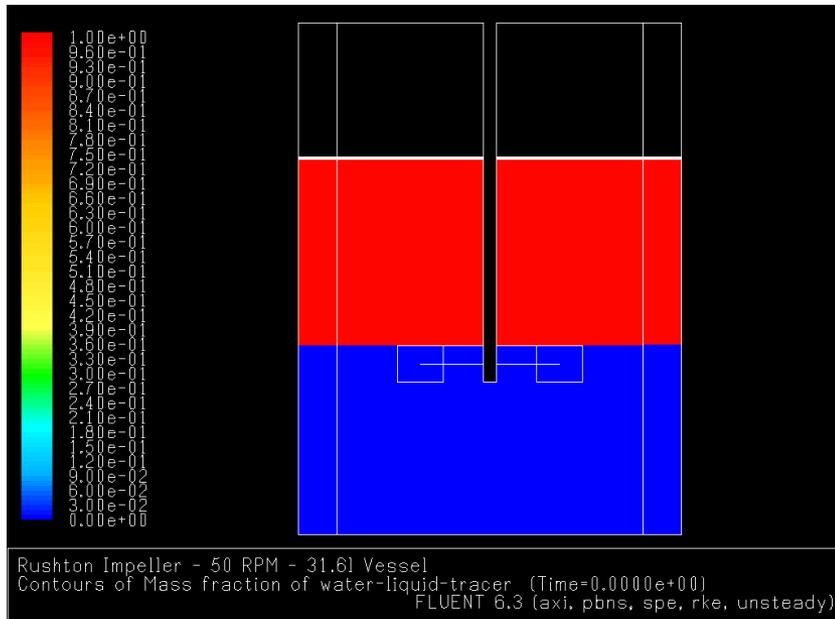




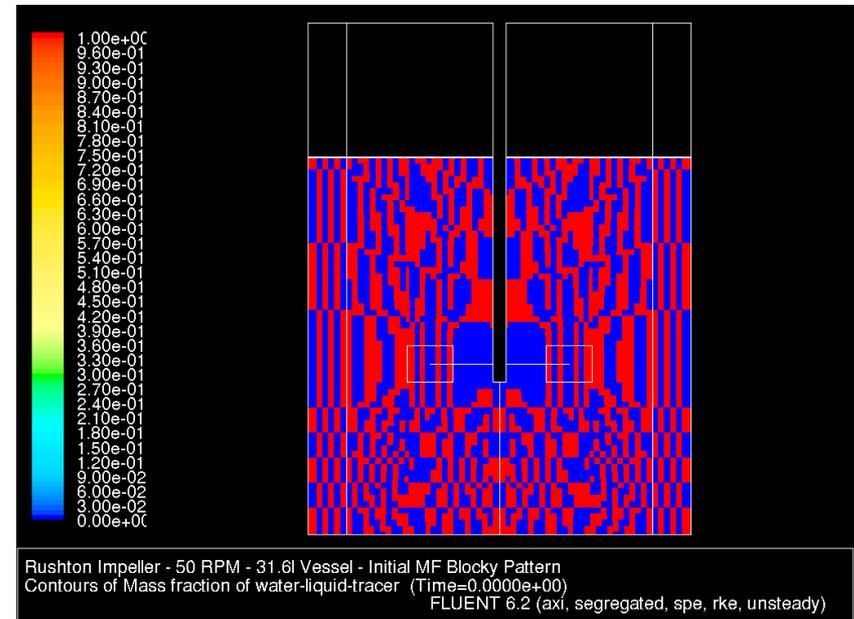


# Compare two more systems

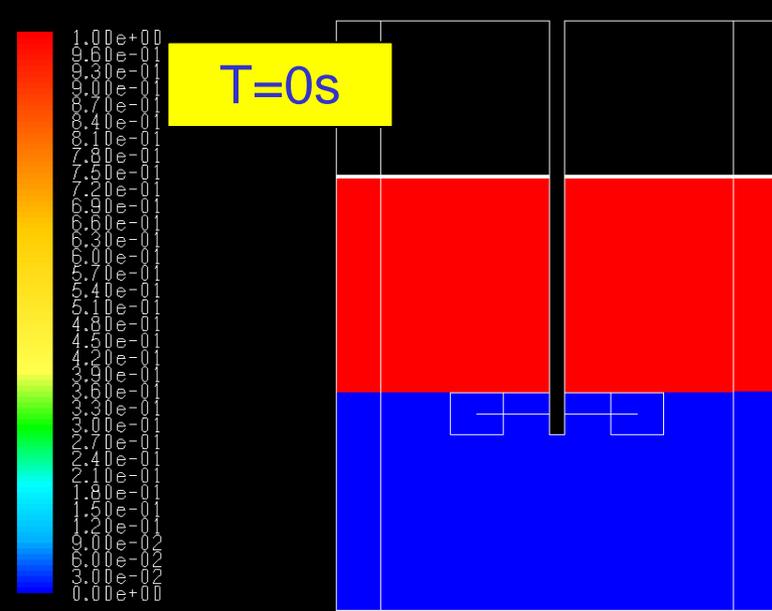
- Two systems with approximately the same average mass fraction of tracer  $\langle Y \rangle \cong 0.5$ .
- The initial distributions are very different: layered vs. blocky pattern.



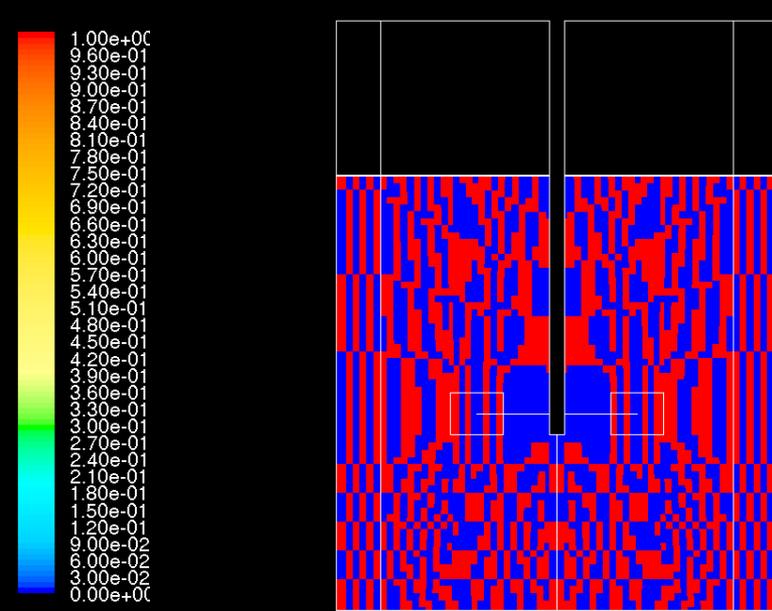
Layer with  $Y_{tracer}=1$  on top of fluid  
with  $Y_{tracer}=0$ .  $\langle Y \rangle = 0.497$ .



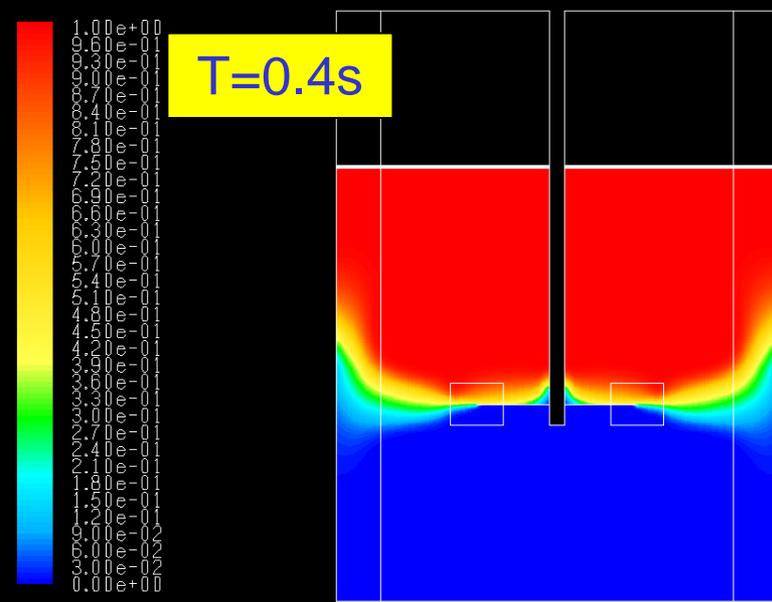
Blocky pattern of fluid with  $Y_{tracer}=0$ .  
and fluid with  $Y_{tracer}=1$ .  $\langle Y \rangle = 0.491$ .



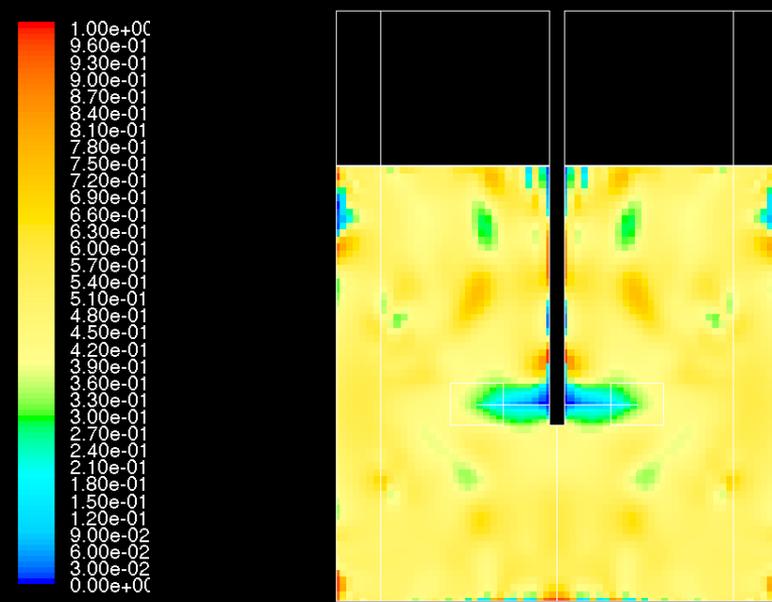
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



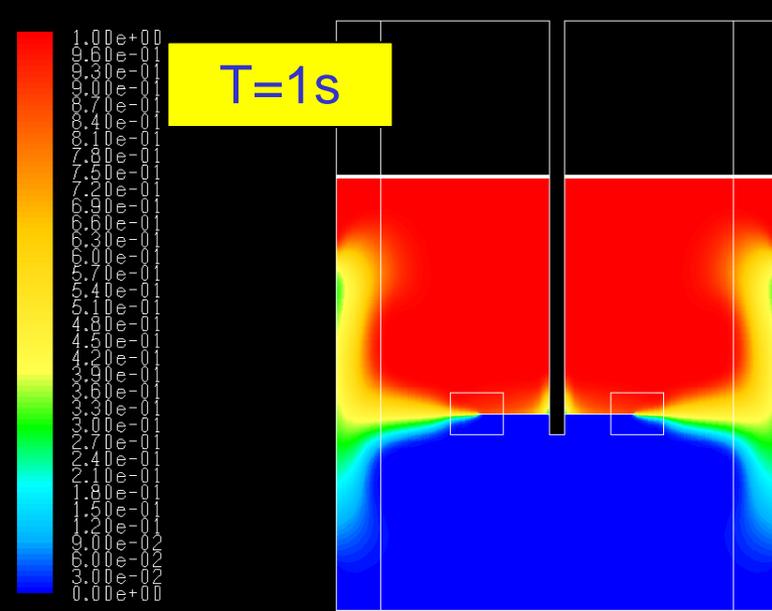
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



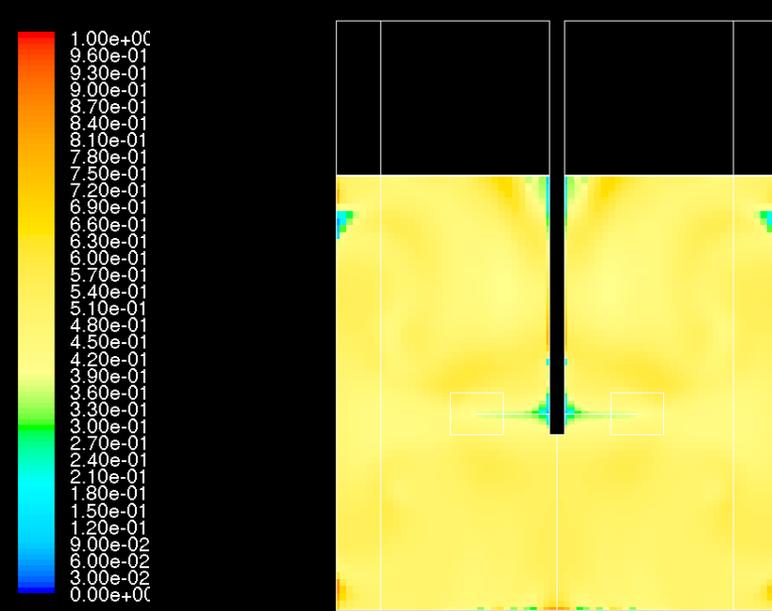
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=4.0000e-01)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



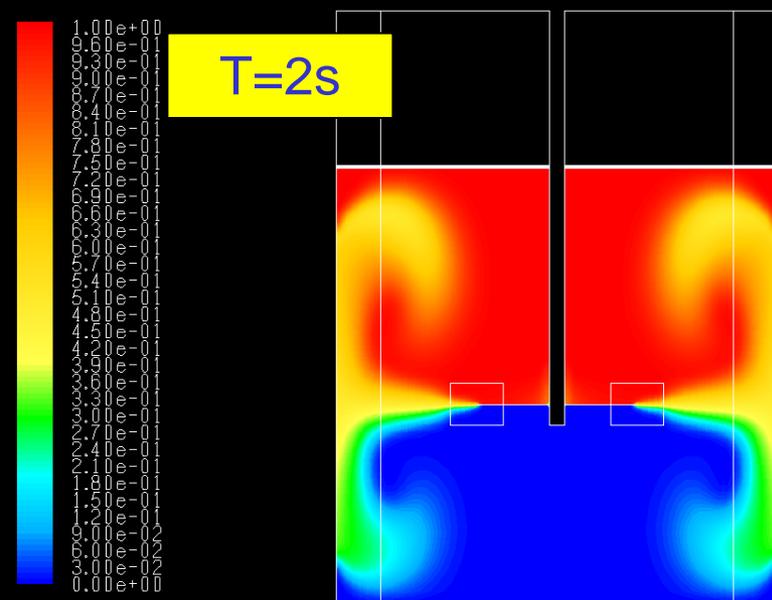
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=4.0000e-01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



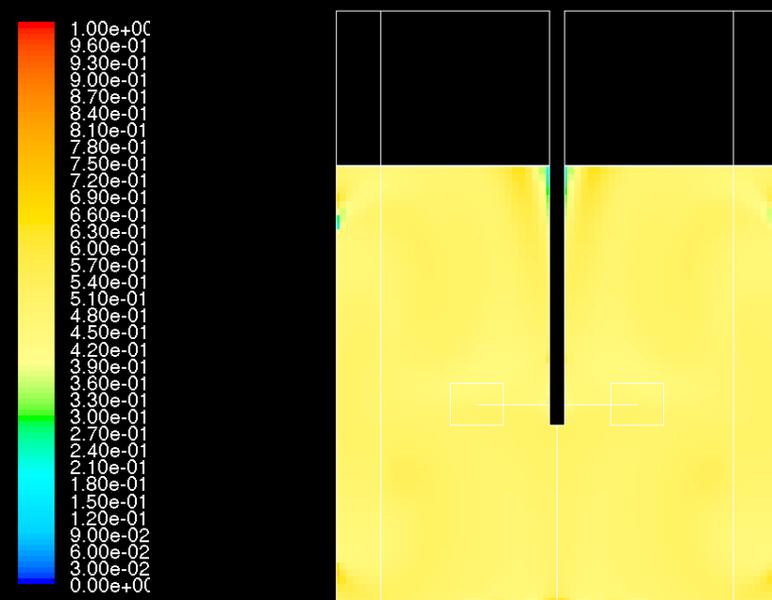
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



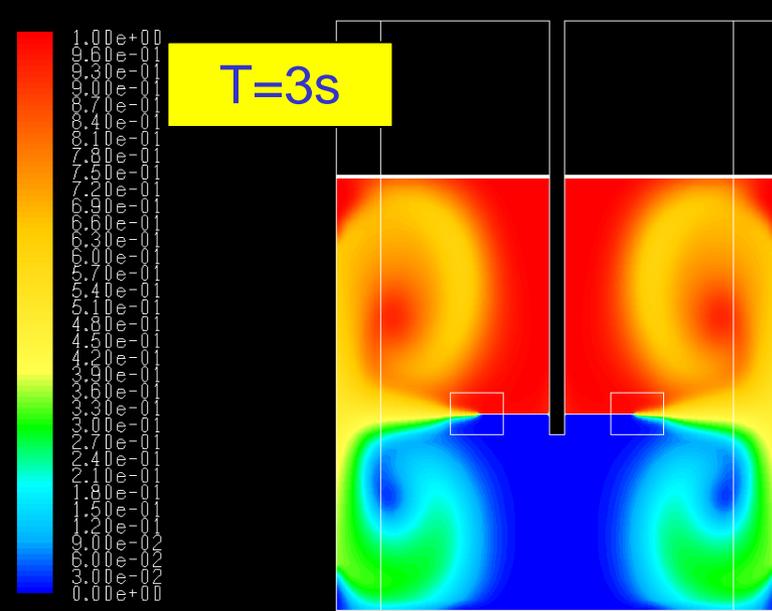
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



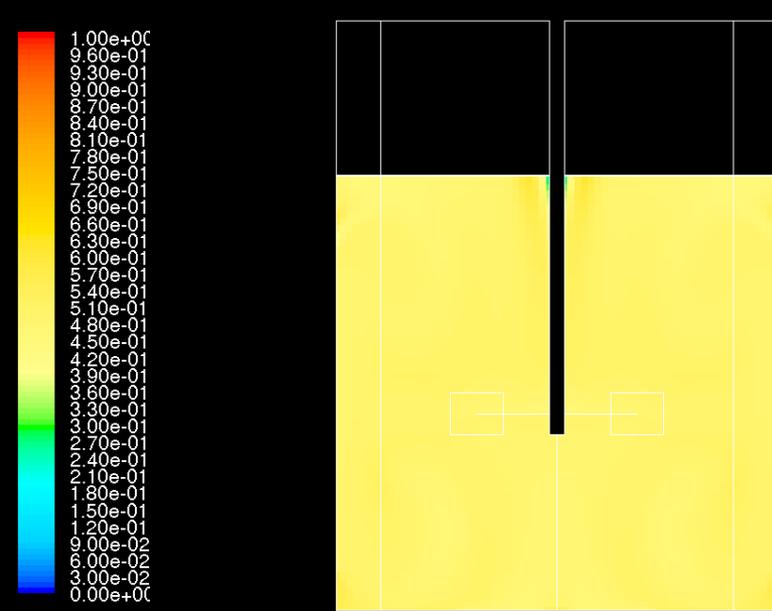
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



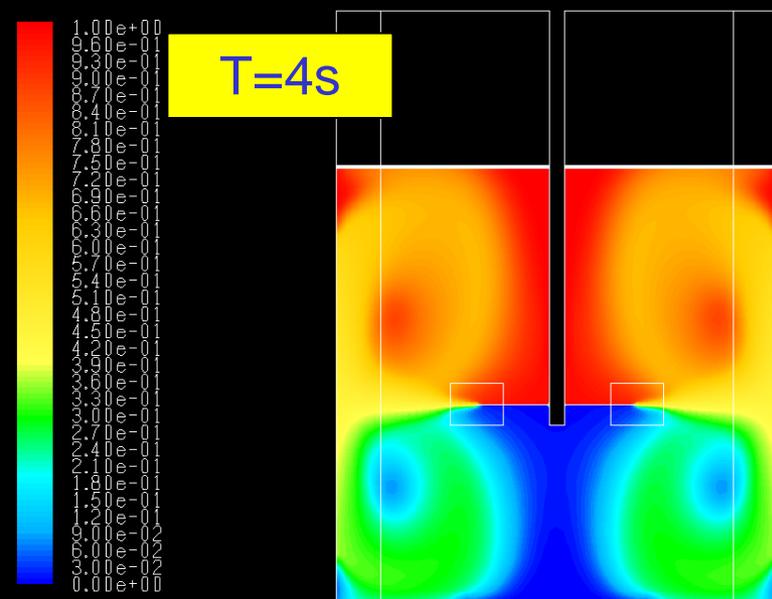
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



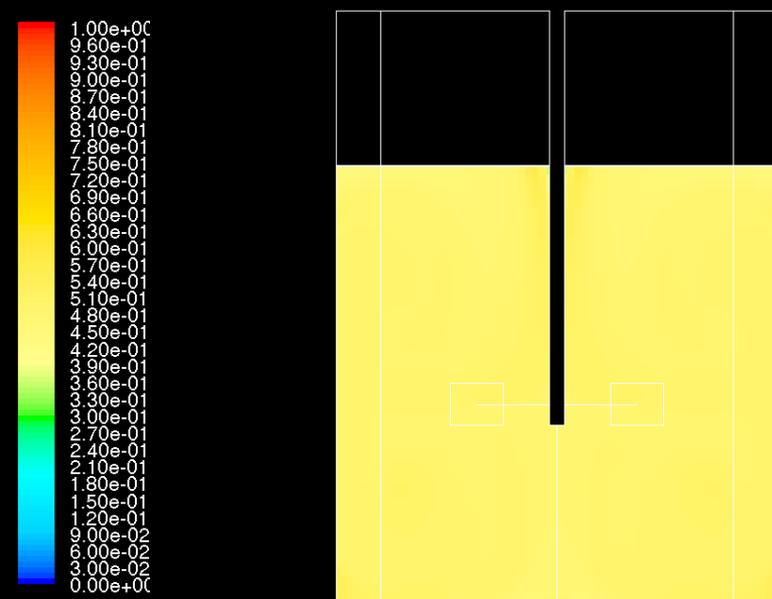
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=3.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



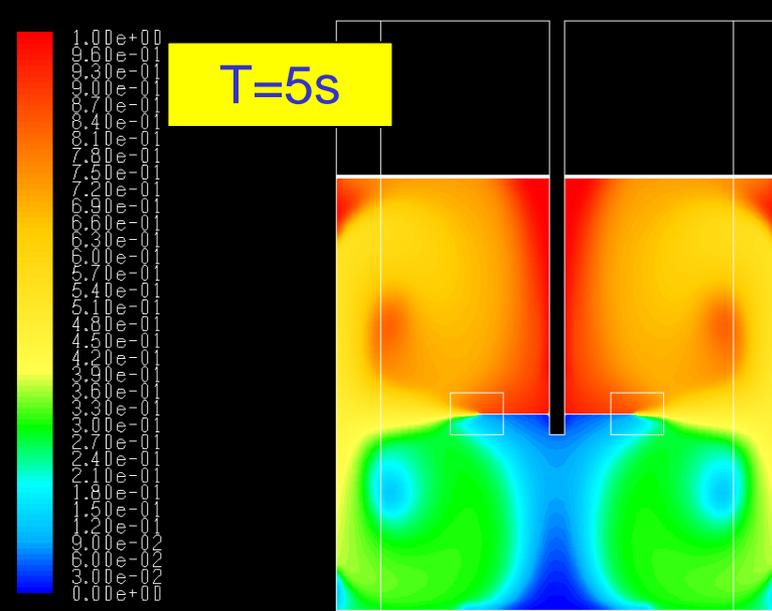
Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=3.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



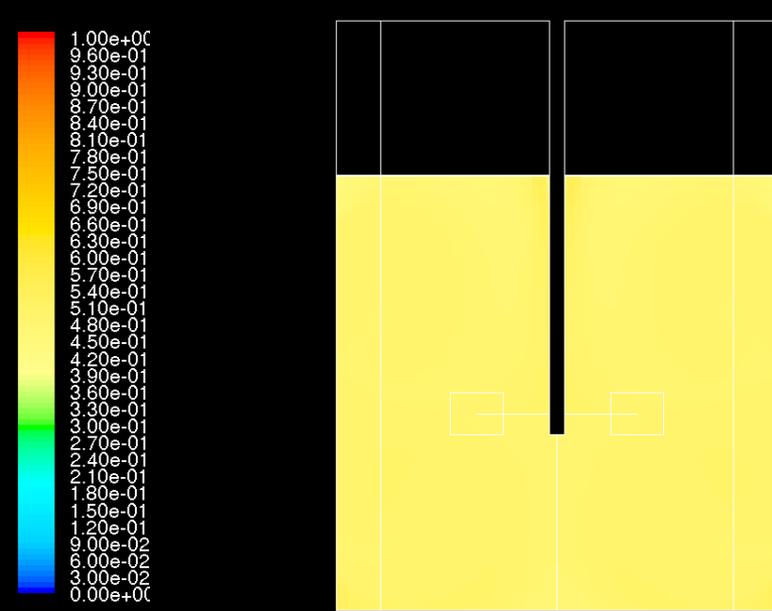
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=4.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=4.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

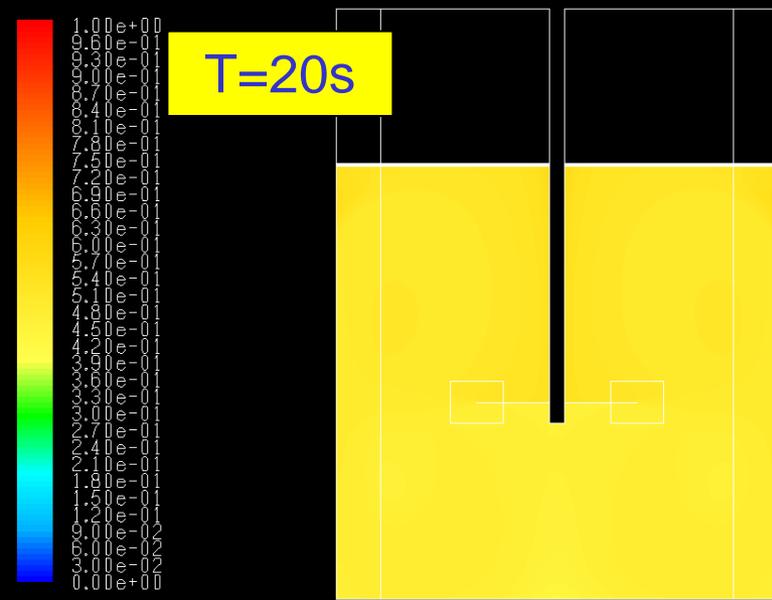


T=5s

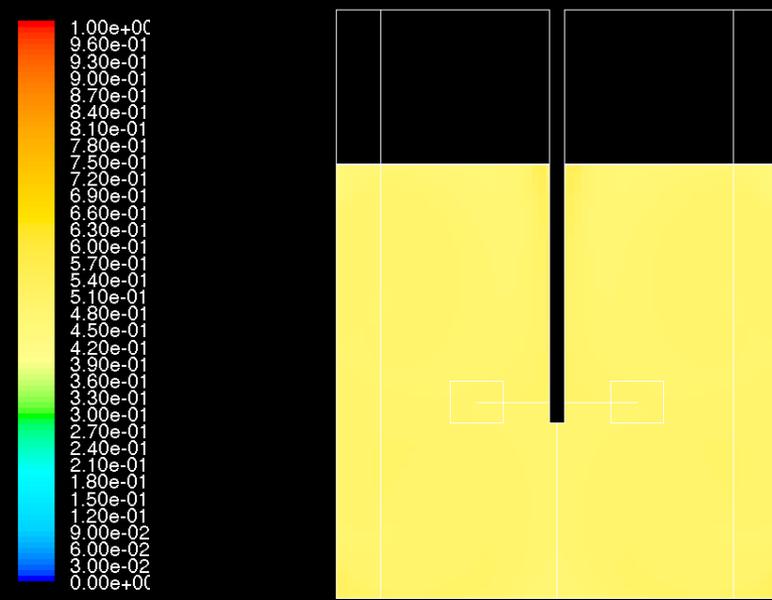


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=5.0000e+00)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer (Time=5.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

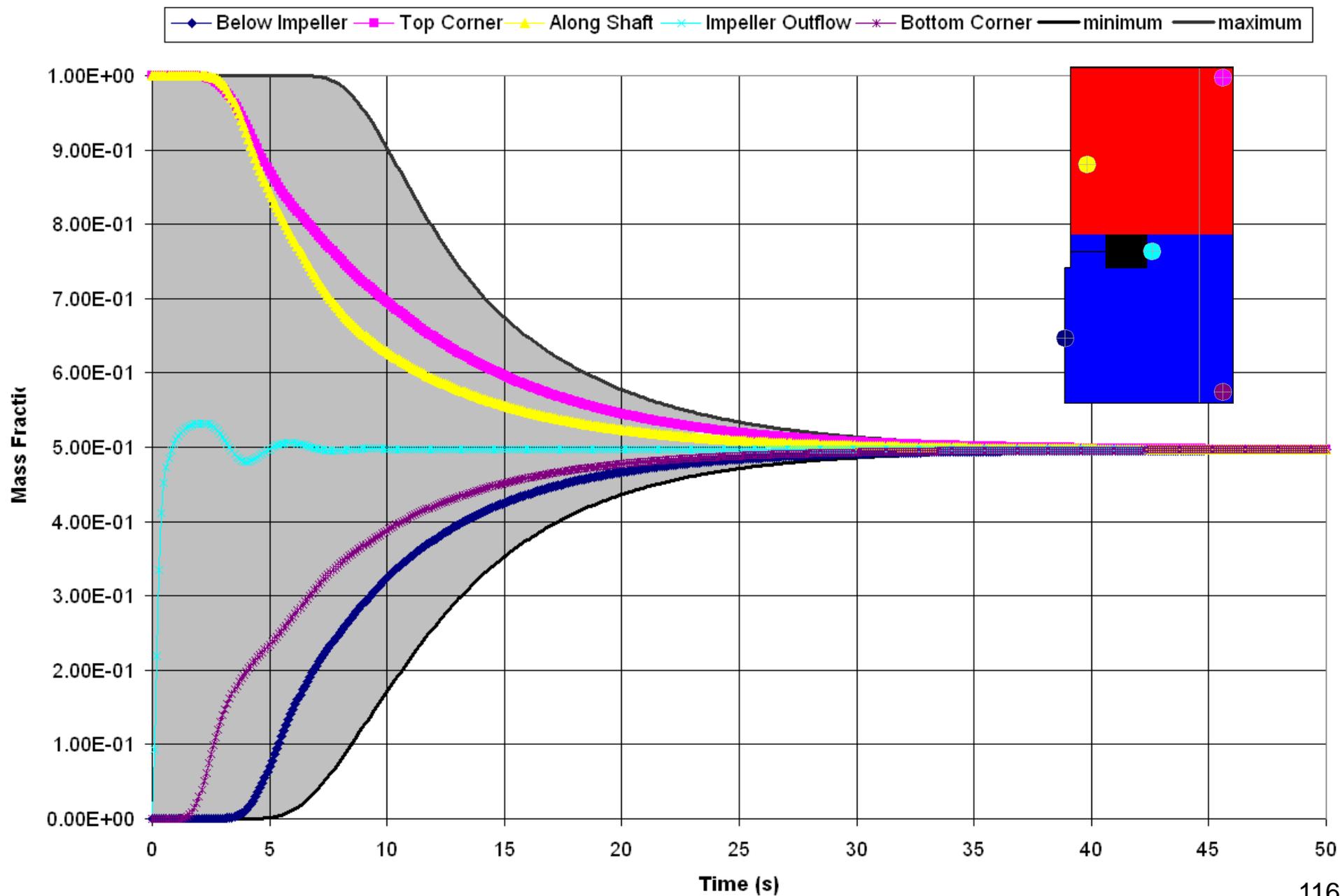


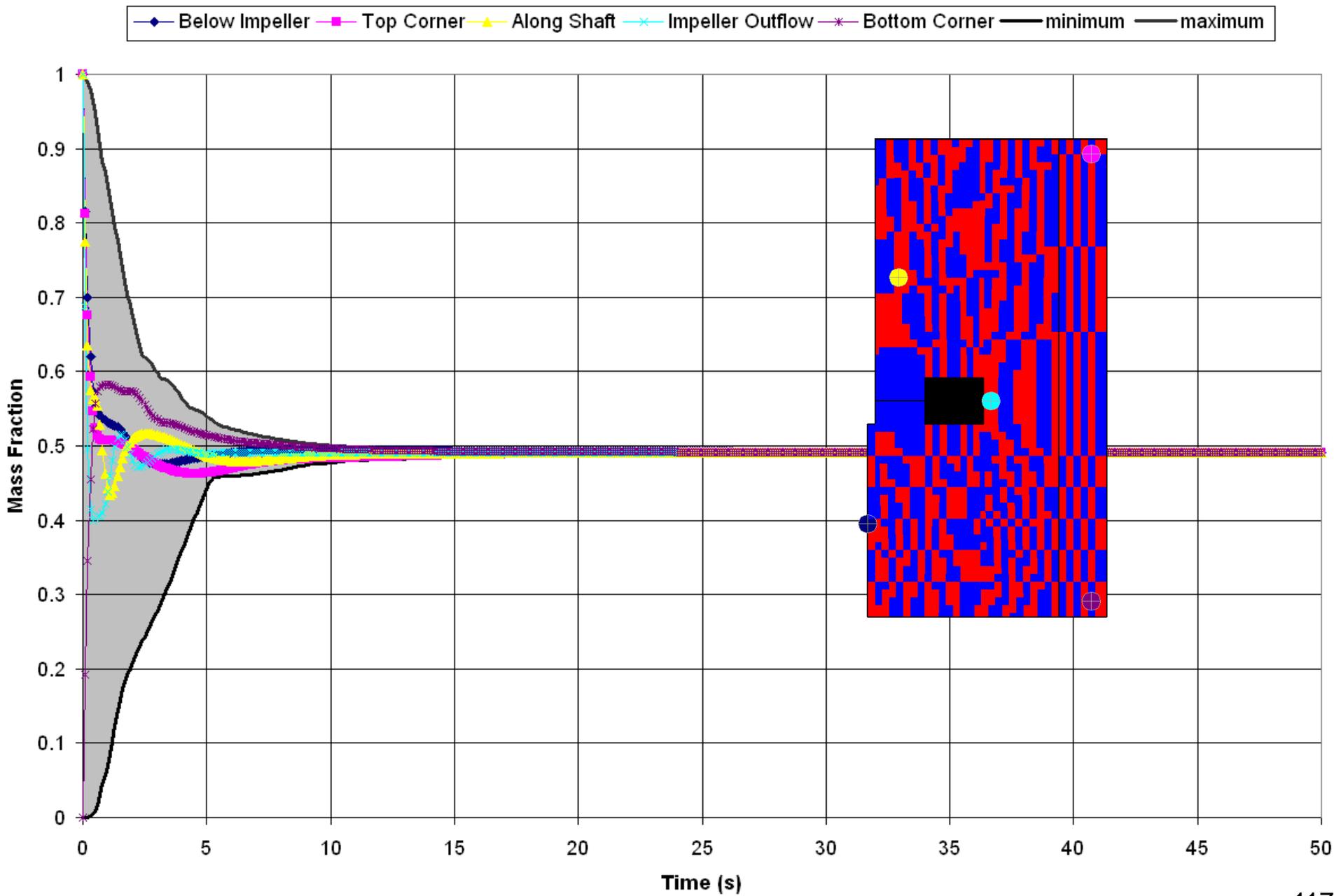
T=20s

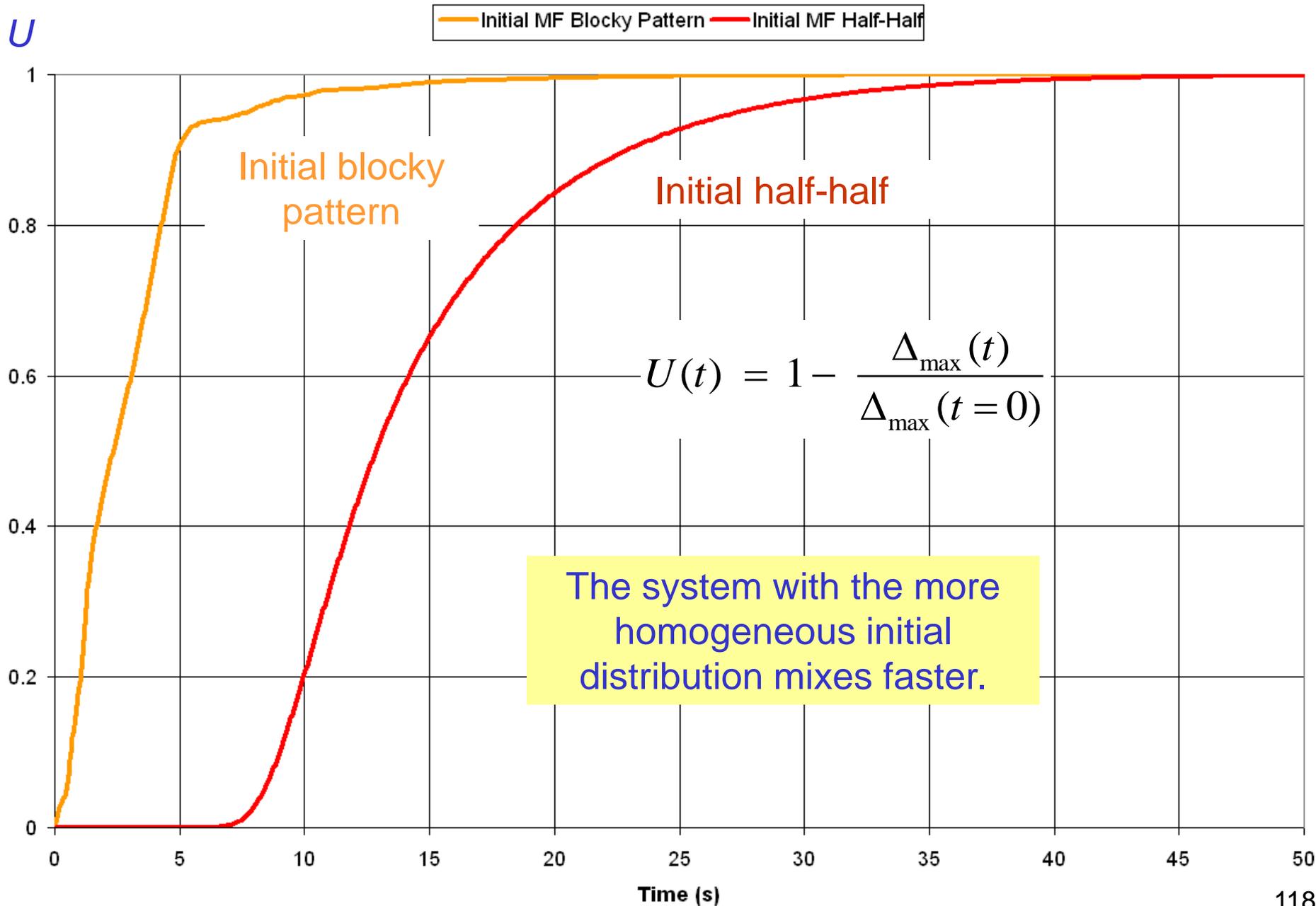


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of water-liquid-tracer (Time=2.0000e+01)  
 FLUENT 6.3 (axi, pbns, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel - Initial MF Blocky Pattern  
 Contours of Mass fraction of water-liquid-tracer  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)







# Compare all four systems

| Initial Y          | U    |
|--------------------|------|
| Layer (0 to 1)     | 20.3 |
| Layer (0.1 to 0.4) | 20.3 |
| Blocky Pattern     | 10.7 |
| Half-Half          | 26.1 |

- Table shows number of impeller revolutions it takes to achieve 99% uniformity for all four systems using the two main criteria:
  - $U$  based on reduction in initial variation.
  - $U_{\Delta}$  based on variation from the average.
- Conclusion: systems with good initial distributions mix faster.
- General recommendation: use  $U$  (reduction in initial variation) to correlate results or to compare with literature blend time correlations.

# Continuous systems

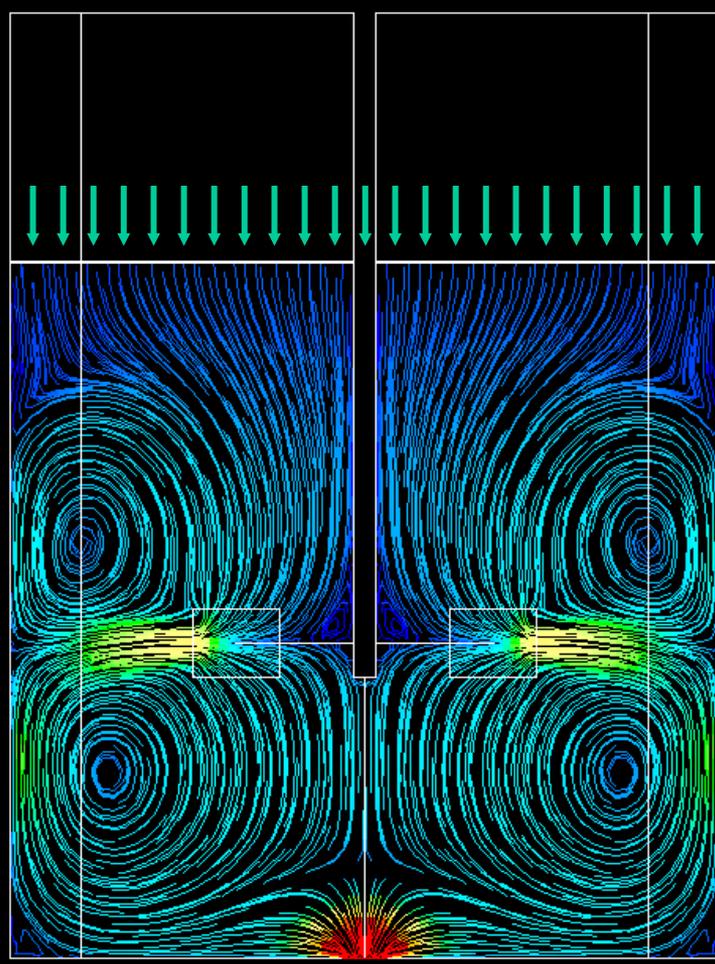
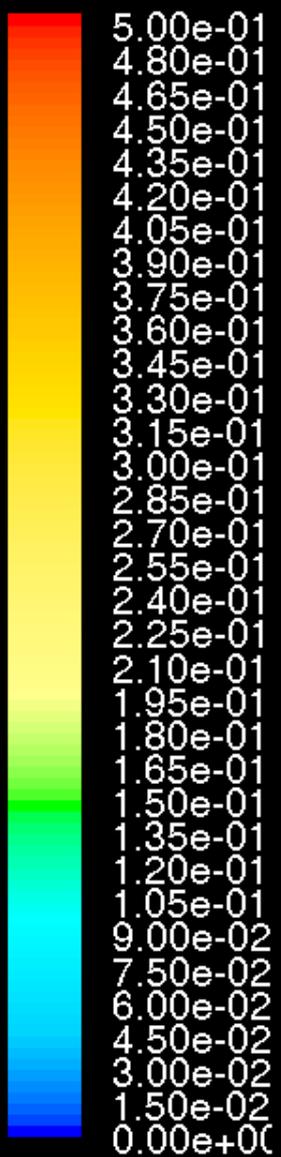
- Methods so far are for batch systems.
- Do these methods work for continuous systems?
  - Requires some modification.
  - Looking at mass fraction extremes does not work, because these may be fixed by the inlet mass fractions.
- Various approaches used:
  - Compare batch blend time with average residence time of the material ( $RT = \text{liquid volume} / \text{volumetric flow rate}$ ). If batch blend time is much smaller than  $RT$ , assume there is no mixing problem.
  - Perform particle tracking simulation, similar to what was shown for static mixers in previous lectures. Analyze residence time distributions.
  - Perform tracer mixing calculation.

# Tracer mixing calculation

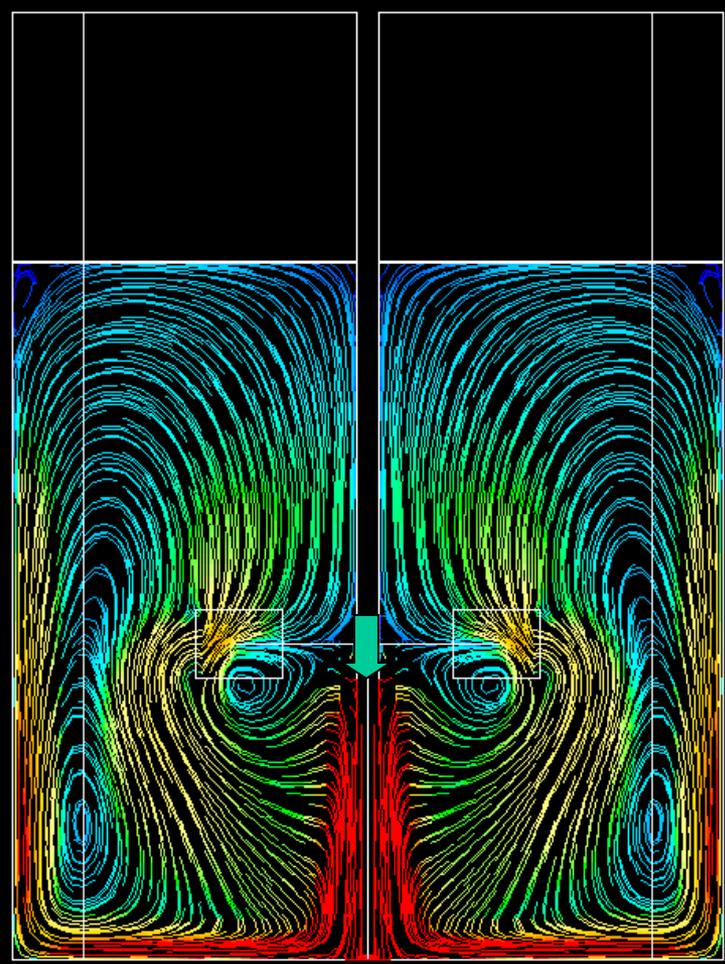
- Calculate continuous, steady state flow field.
- Initial mass fraction of tracer is zero everywhere.
- Perform transient calculation for tracer mixing, with non-zero mass fraction tracer at inlet.
- Monitor:
  - Average mass fraction in domain  $\langle Y \rangle$ .
  - Mass fraction at outlet  $Y_{out}$ .
  - Optional: monitor CoV.
- Definition of perfectly mixed system:  $Y_{out} = \langle Y \rangle$ .
- Mixing time is then the time it takes for the ratio  $Y_{out}/\langle Y \rangle$  to be within a specified tolerance of 1.
- Mixing time can be expressed in number of residence times:  $t/RT$ .

# Compare two systems

- Rushton turbine flow field.
- Continuous system with two different injections:
  - Low velocity feed (0.01 m/s) distributed across liquid surface.
    - Affects flow in upper part of the vessel only.
  - High speed jet feed (9.6 m/s) entering through bottom shaft.
    - Because of the large momentum contained in the jet, it alters the flow field significantly.
- Outflow at center of bottom.
- Average residence time  $RT=30s$ , equivalent to 25 impeller revolutions. The RT is similar to the batch blend time.



Surface inlet,  
 bottom outflow.

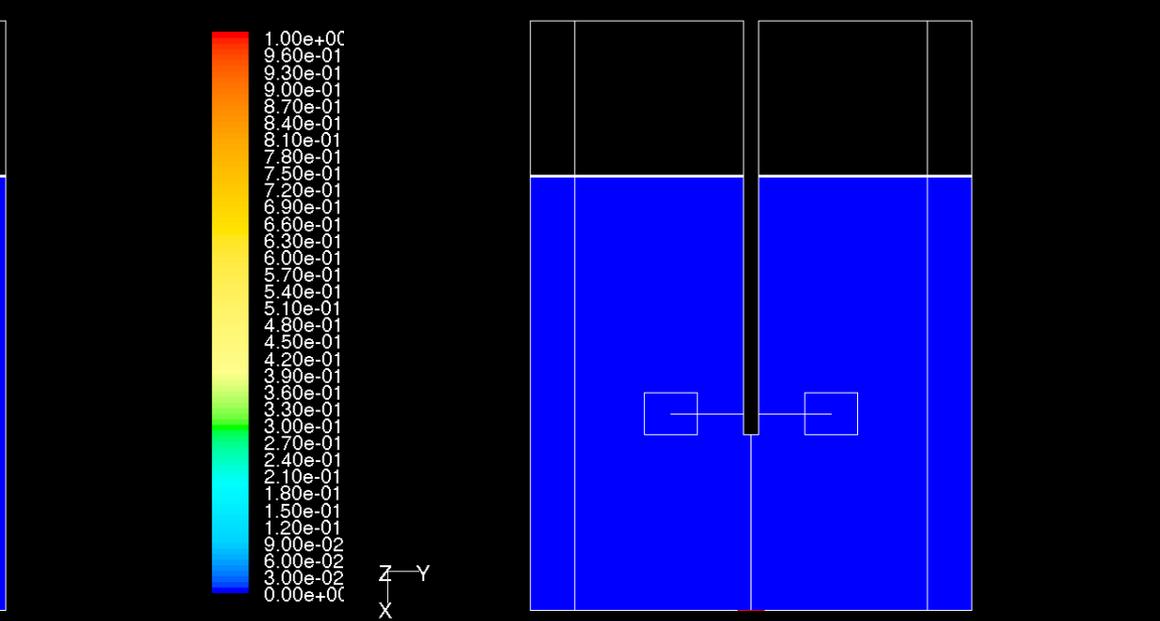
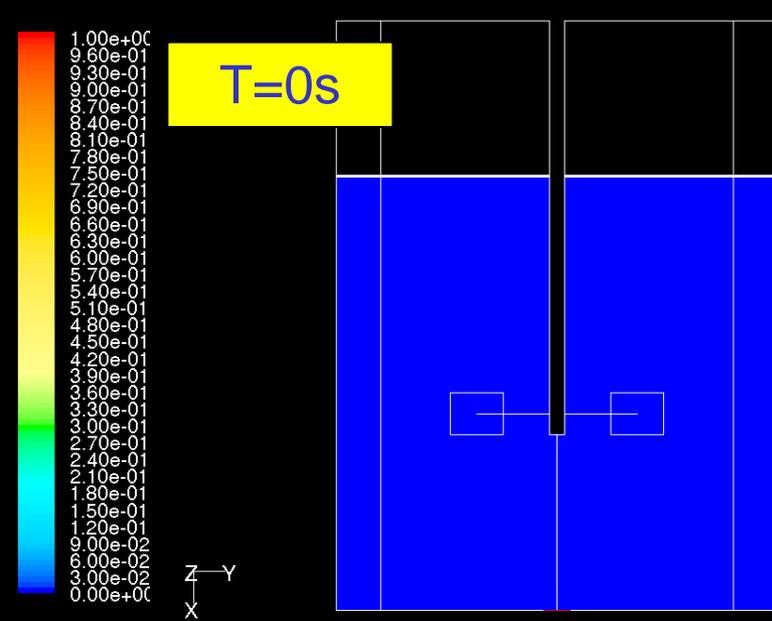


Shaft inlet,  
 bottom outflow.

Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow  
 Path Lines Colored by Velocity Magnitude (m/s)

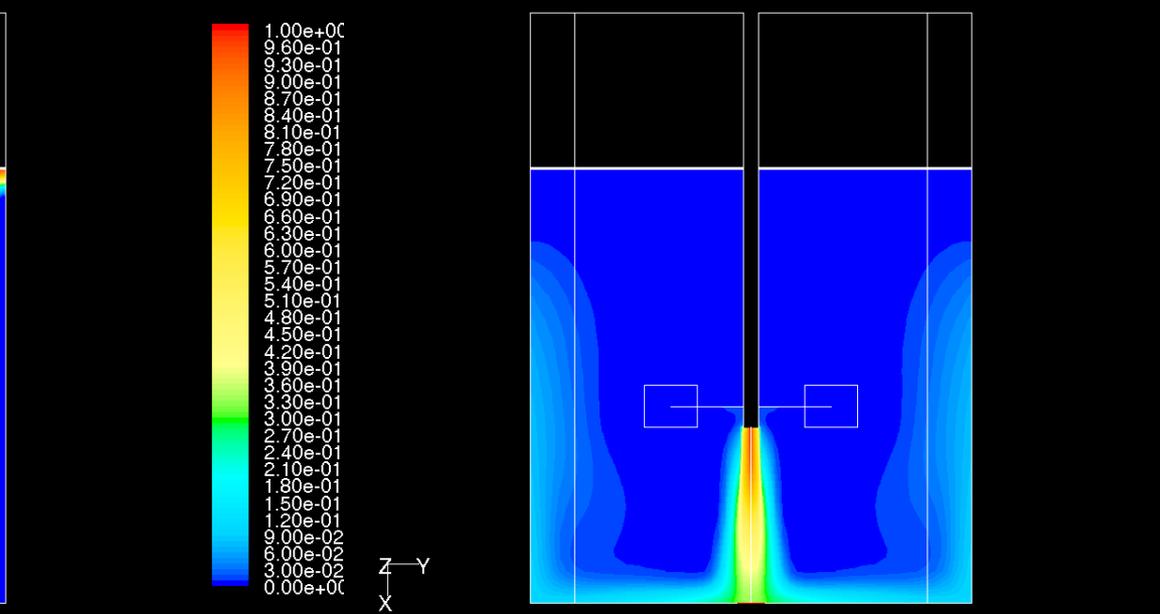
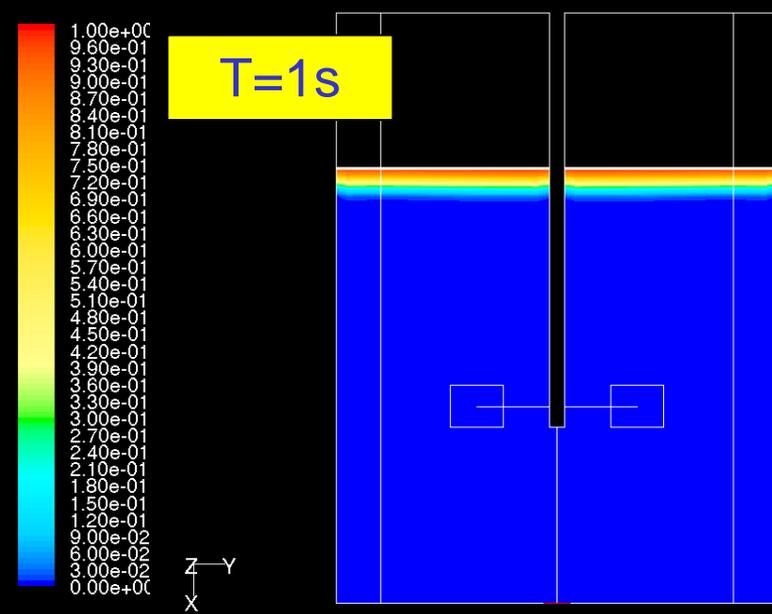
Average residence time  $RT=30s.$

FLUENT 6.2 (axi, segregated, spe, rke)<sub>123</sub>



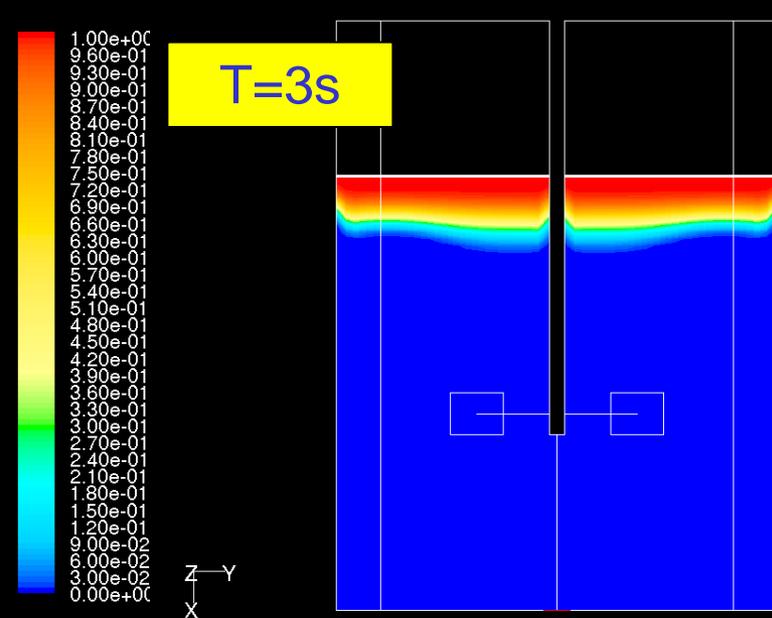
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

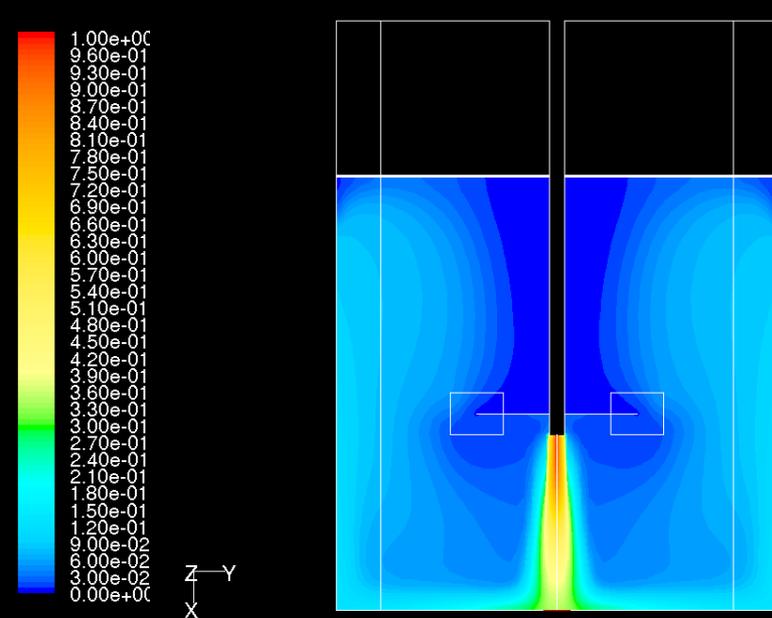


Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

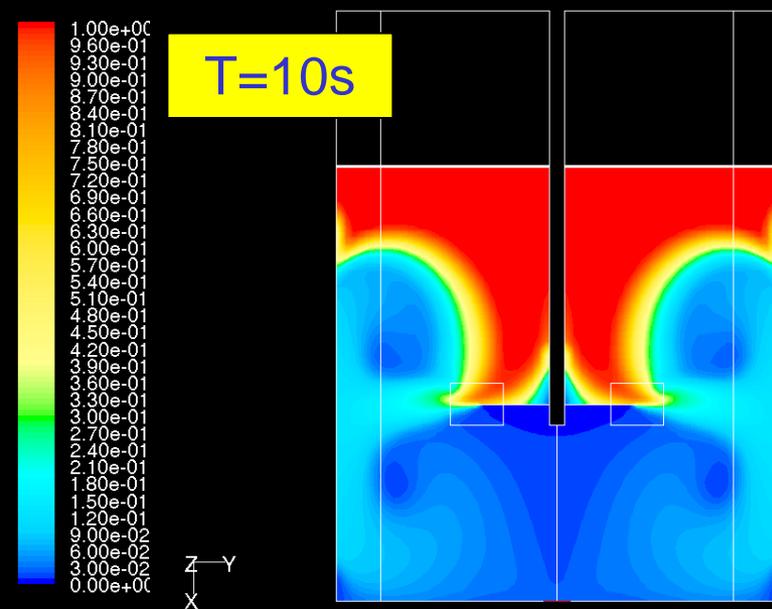
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=1.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



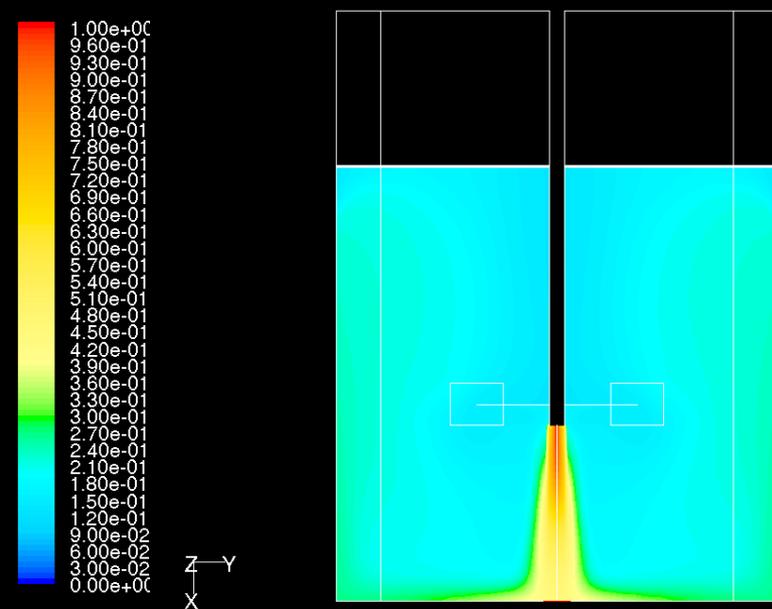
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
Contours of Mass fraction of water-liquid-tracer (Time=3.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



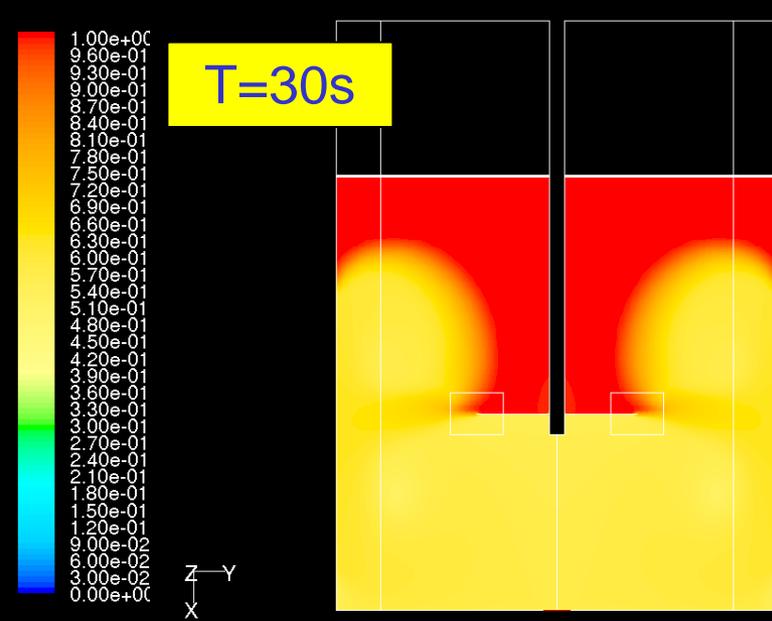
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
Contours of Mass fraction of water-liquid-tracer (Time=3.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



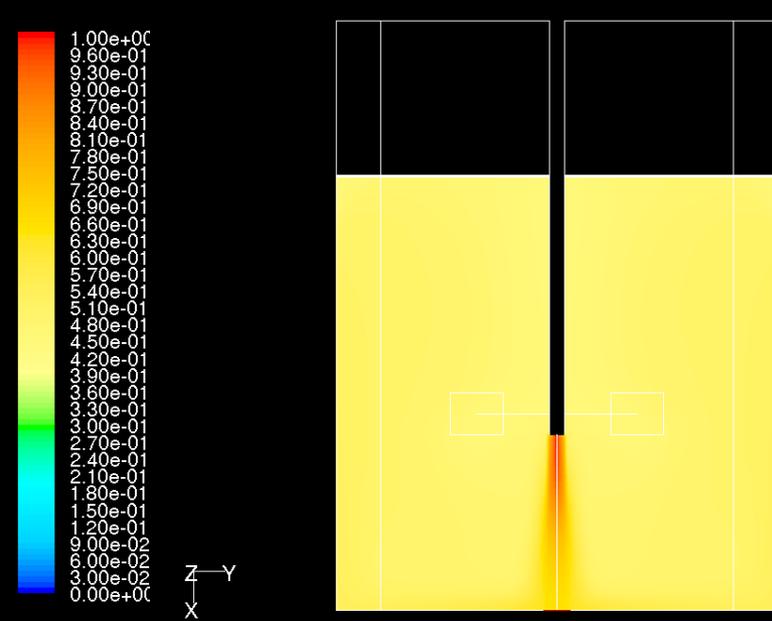
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
Contours of Mass fraction of water-liquid-tracer (Time=1.0200e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



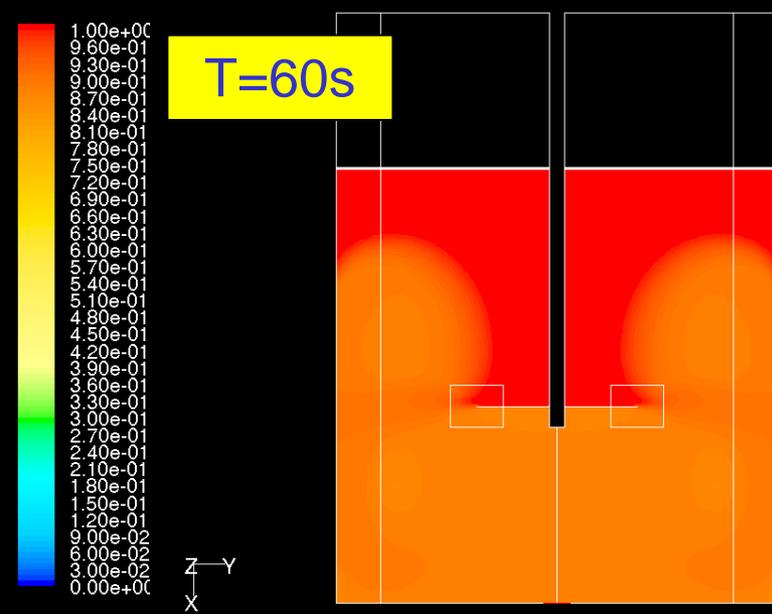
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
Contours of Mass fraction of water-liquid-tracer (Time=1.0200e+01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



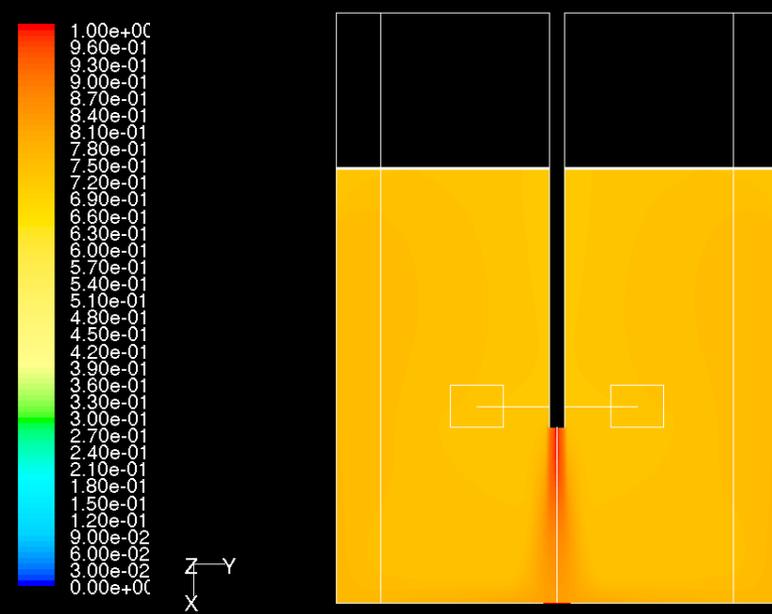
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=3.0200e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



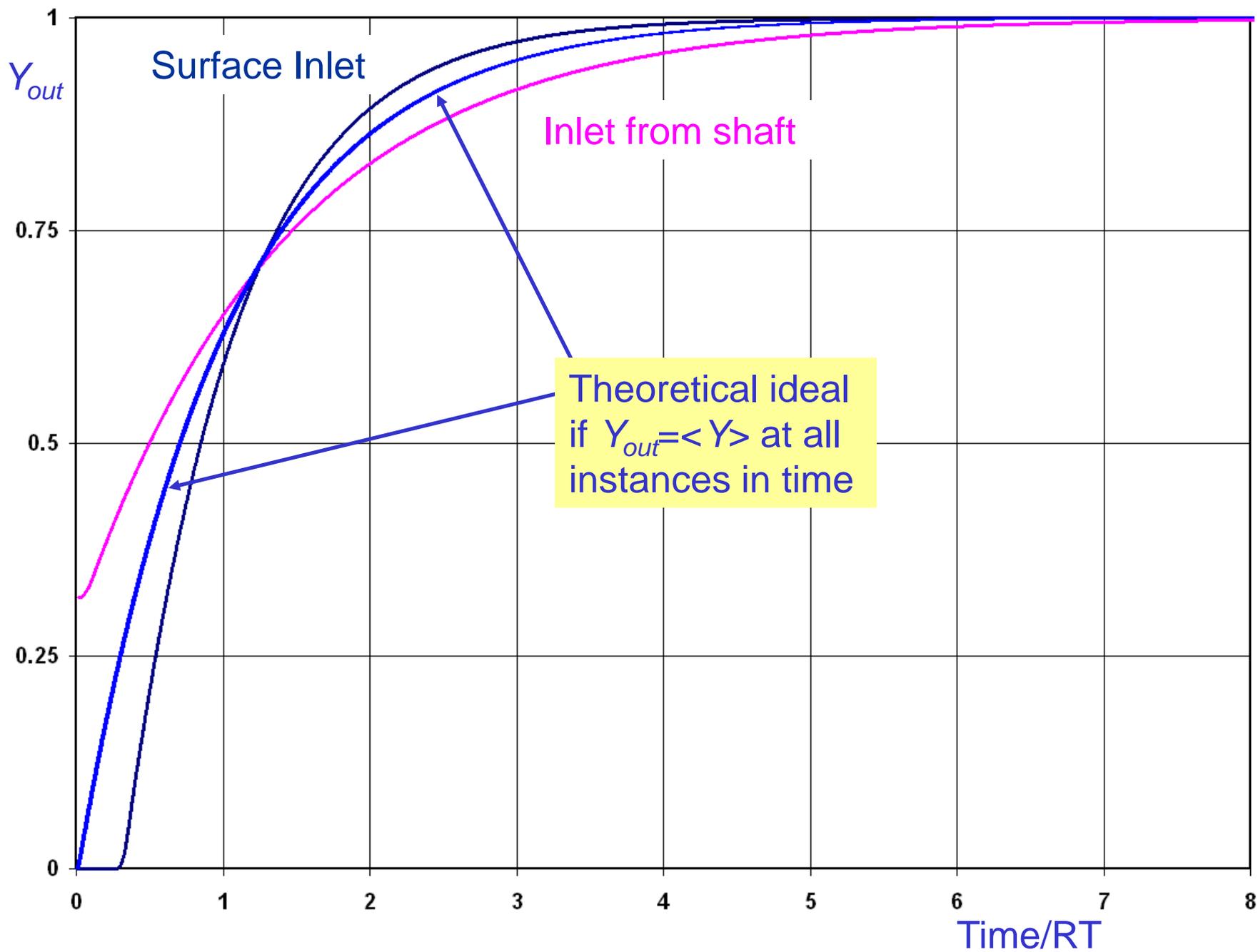
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=3.0200e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



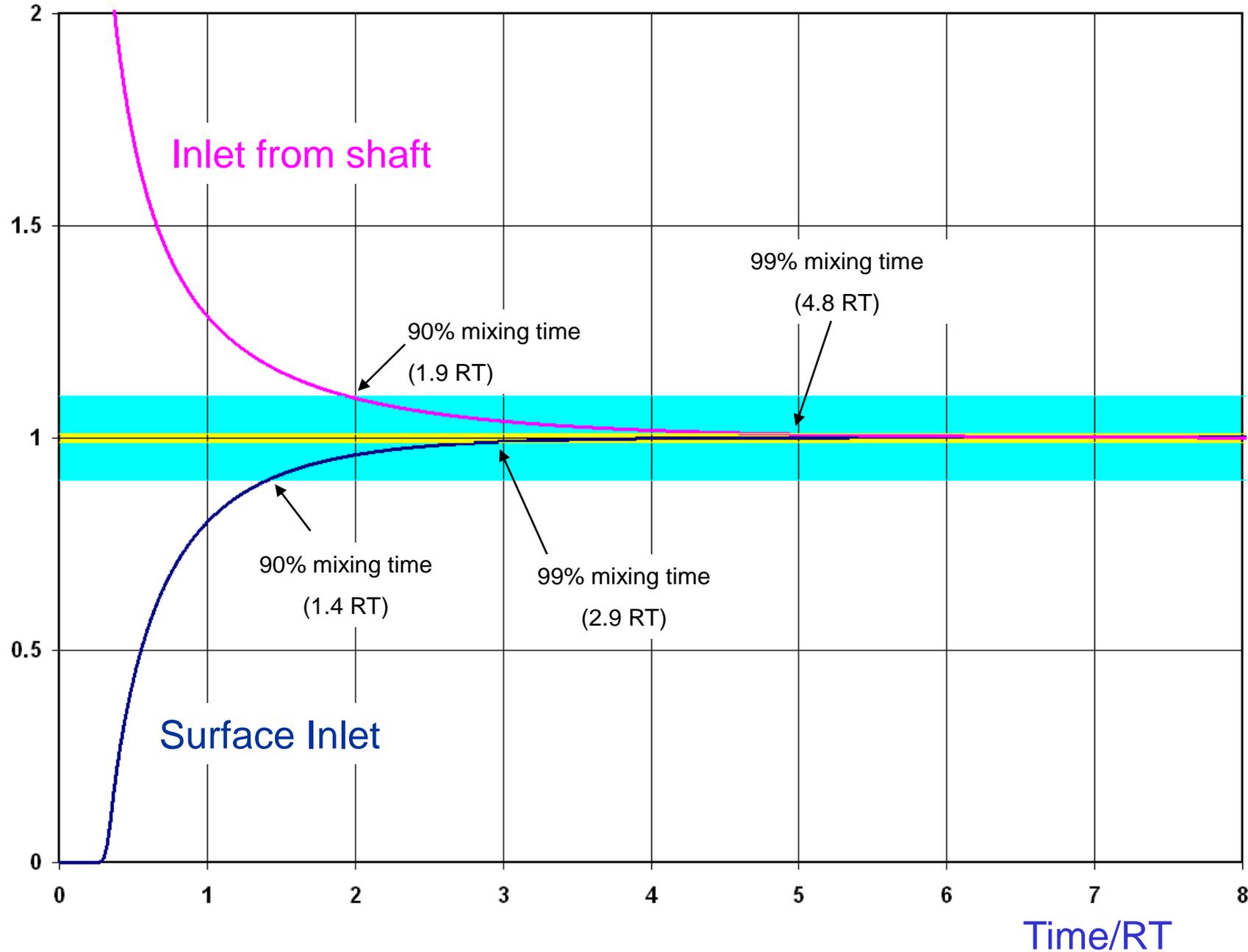
Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Surface Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=6.0200e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel - Continuous flow - Shaft Inlet  
 Contours of Mass fraction of water-liquid-tracer (Time=6.0200e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



$$Y_{out} / \langle Y \rangle$$



# Comments

- The main assumption behind this approach is that the system will eventually reach a steady state where  $Y_{out} = \langle Y \rangle$ .
  - Not all industrial systems may have a steady state operating condition which, in general, is an undesirable situation that would need to be addressed.
- CoV can still be used to compare uniformity of different systems under steady state operating conditions with multiple species.

# Modeling Chemical Reactions with CFD

## Reacting Flows - Lecture IV

André Bakker

# Outline

- Source terms in the species transport equation.
- Chemical kinetics and reaction rates.
- Subgrid scale effects.
- Reaction models and the effects of turbulence.
- Examples:
  - Stirred tank.
  - Catalytic converter.
  - Polymerization reactor.

# Species transport and reaction

- The  $i^{\text{th}}$  species mass fraction transport equation is:

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_j}(\rho u_j Y_i) = \frac{\partial}{\partial x_j} \left( \rho D_i \frac{\partial Y_i}{\partial x_j} \right) + R_i + S_i$$

Rate of change + Net rate of flow (convection) = Rate of change due to diffusion + Rate of change due to reaction sources + Rate of change due to other sources

- The mass fraction of chemical species  $i$  is  $Y_i$ .
- The velocity is  $u_j$ .
- $D_i$  is the diffusion coefficient.
- $R_i$  is the reaction source term. *Chemical reactions are modeled as source terms in the species transport equation.*
- $S_i$  includes all other sources.

# Source of species

- The net source of chemical species  $i$  due to reaction  $R_i$  is computed as the sum of the reaction sources over the  $N_R$  reactions that the species participate in:

$$R_i = M_{w,i} \sum_{r=1}^{N_R} \hat{R}_{i,r}$$

$M_{w,i}$  is the molecular weight of species  $i$

$\hat{R}_{i,r}$  is the molar rate of creation / destruction of species  $i$  in reaction  $r$

- Reaction may occur as a volumetric reaction or be a surface reaction.
- Note: source terms are also added to the energy equation to take heat of reaction effects into account.

# Chemical kinetics

- The  $r^{\text{th}}$  reaction can be written as:
 
$$\sum_{i=1}^N \nu'_{i,r} \mathcal{M}_i \xrightleftharpoons[k_{b,r}]{k_{f,r}} \sum_{i=1}^N \nu''_{i,r} \mathcal{M}_i$$

$\mathcal{M}_i$  = symbol denoting species  $i$

$N$  = number of chemical species in the system

$\nu'_{i,r}$  = stoichiometric coefficient for reactant  $i$  in reaction  $r$

$\nu''_{i,r}$  = stoichiometric coefficient for product  $i$  in reaction  $r$

- Example:



$$M_1 = \text{CH}_4 \quad M_2 = \text{O}_2 \quad M_3 = \text{CO}_2 \quad M_4 = \text{H}_2\text{O}$$

$$\nu'_{1,r} = 1 \quad \nu'_{2,r} = 2 \quad \nu'_{3,r} = 0 \quad \nu'_{4,r} = 0$$

$$\nu''_{1,r} = 0 \quad \nu''_{2,r} = 0 \quad \nu''_{3,r} = 1 \quad \nu''_{4,r} = 2$$

# Chemical kinetics

- The  $r^{\text{th}}$  reaction can be written as:
 
$$\sum_{i=1}^N \nu'_{i,r} \mathcal{M}_i \xrightleftharpoons[k_{b,r}]{k_{f,r}} \sum_{i=1}^N \nu''_{i,r} \mathcal{M}_i$$

- The equation shown is valid for both reversible and non-reversible reactions. Reactions in FLUENT are non-reversible by default. For non-reversible reactions, the backward rate constant  $k_{b,r}$  is simply omitted.
- The summations are for all chemical species in the system, but only species that appear as reactants or products will have non-zero stoichiometric coefficients. Hence, species that are not involved will drop out of the equation.
- Stoichiometry: Quantity relationships between reactants and products in a chemical reaction.
  - Derived from the Greek word stoikheion ("element") and metria ("measure," from metron).
  - Pronounce stoichiometry as "stoy-kee-ah-met-tree" or just "stoyk" if you're in a hurry.

$$\begin{array}{cccc} \nu'_{1,r} = 1 & \nu'_{2,r} = 2 & \nu'_{3,r} = 0 & \nu'_{4,r} = 0 \\ \nu''_{1,r} = 0 & \nu''_{2,r} = 0 & \nu''_{3,r} = 1 & \nu''_{4,r} = 2 \end{array}$$

# Reaction rate

- The molar reaction rate of creation/destruction of species  $i$  in reaction  $r$  is given by:

$$\hat{R}_{i,r} = \Gamma \left( \nu''_{i,r} - \nu'_{i,r} \right) \left( k_{f,r} \prod_{j=1}^{N_r} [C_{j,r}]^{\eta'_{j,r}} - k_{b,r} \prod_{j=1}^{N_r} [C_{j,r}]^{\eta''_{j,r}} \right)$$

$N_r$  = number of chemical species in reaction  $r$

$C_{j,r}$  = molar concentration of each reactant and product species  $j$  in reaction  $r$  (kgmol/m<sup>3</sup>)

$\eta'_{j,r}$  = forward rate exponent for each reactant and product species  $j$  in reaction  $r$

$\eta''_{j,r}$  = backward rate exponent for each reactant and product species  $j$  in reaction  $r$

- $\Gamma$  represents the effect of third bodies (e.g., catalysts) on the reaction rate:

$$\Gamma = \sum_j^{N_r} \gamma_{j,r} C_j$$

Here,  $\gamma_{j,r}$  is the third-body efficiency of the  $j^{\text{th}}$  species in the  $r^{\text{th}}$  reaction.

# Reaction rate constant

- The forward rate constant for reaction  $r$ ,  $k_{f,r}$  is computed using an expanded version of the Arrhenius expression:

$$k_{f,r} = A_r T^{\beta_r} e^{-\frac{E_r}{RT}}$$

$A_r$  = pre-exponential factor

$E_r$  = activation energy

$R$  = universal gas constant = 8313 J/kgmol K

$T$  = temperature

$\beta_r$  = temperature exponent

- If applicable, the backward rate constant for reaction  $r$ ,  $k_{b,r}$  is computed from the forward rate constant using the relationship:  $k_{b,r} = k_{f,r} / K_r$ .
- $K_r$  is the equilibrium constant for reaction  $r$ , which follows from the thermodynamic properties of the materials.

# Reaction rate: the Arrhenius equation

- The Arrhenius equation is a formula for the temperature dependence of a chemical reaction rate. Originally it did not include the term  $T^\beta$ , which was added later by other researchers.

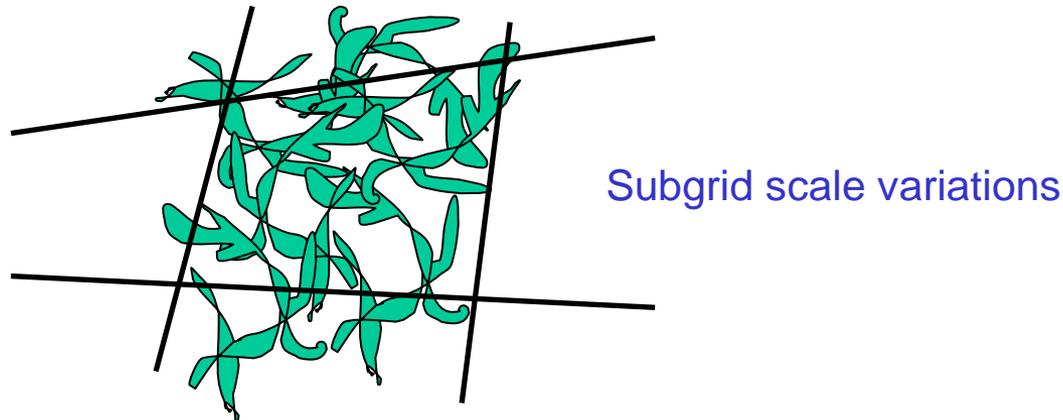
$$R_k \propto e^{-\frac{E}{RT}}$$

- $R_k$  is the Arrhenius reaction rate,  $E$  is the activation energy,  $R$  is the universal gas constant, and  $T$  is the temperature.
- First proposed by the Dutch chemist J. H. van 't Hoff in 1884.
  - Won the 1901 Nobel prize in chemistry for his discovery of the laws of chemical dynamics and osmotic pressure in solutions.
- Five years later (1889), the Swedish chemist Svante Arrhenius provided a physical justification and interpretation for it.
  - Also won the 1903 Nobel prize in chemistry for his electrolytic theory of dissociation and conductivity.
  - He had proposed that theory in his 1884 doctoral dissertation. It had not impressed his advisors who gave him the very lowest passing grade.



# Subgrid effects

- For each grid cell the molecular reaction rate can be calculated using the equations presented.
- What if there are concentration variations smaller than the size of the grid cell?



- Reaction rates calculated at the average concentrations may be overpredicted.
- For turbulent flows, models exist that take turbulent mixing effects at subgrid scales into account.

# Effect of temperature fluctuations

- Temperature may vary in time, and also in space at scales smaller than a grid cell.
- What happens if we model a system as steady state and use average temperatures to predict the reaction rates?
- Reaction rate terms are highly nonlinear:

$$R_k \propto T^{\beta_k} e^{-E_k/RT}$$

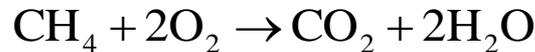
$\Rightarrow$

$$\bar{R}_k \neq R_k(\bar{T})$$

- Cannot neglect the effects of temperature fluctuations on chemical reaction rates.

# Effect of temperature fluctuations - example

- Single step methane reaction ( $A=2E11$ ,  $E=2E8$ ):



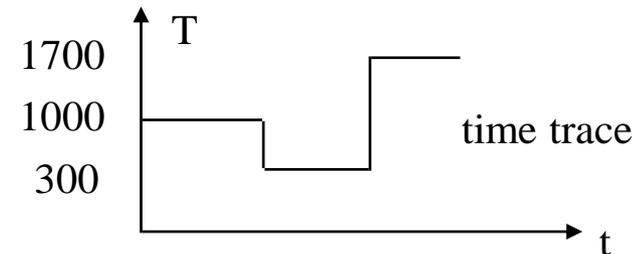
$$R_{\text{CH}_4} = \frac{1}{2}R_{\text{O}_2} = -R_{\text{CO}_2} = -\frac{1}{2}R_{\text{H}_2\text{O}} = -A \exp(-E/RT) [\text{CH}_4]^{0.2} [\text{O}_2]^{0.3}$$

- Assume turbulent fluid at a point has constant species concentration at all times but spends one third its time at  $T=300\text{K}$ ,  $T=1000\text{K}$  and  $T=1700\text{K}$ .
- Calculate the reaction rates:

|                     |                   |      |                   |
|---------------------|-------------------|------|-------------------|
| $\bar{T}(\text{K})$ | 300               | 1000 | 1700              |
| $A \exp(-E/RT)$     | $2.97\text{E}-24$ | 7.12 | $1.43\text{E}+05$ |

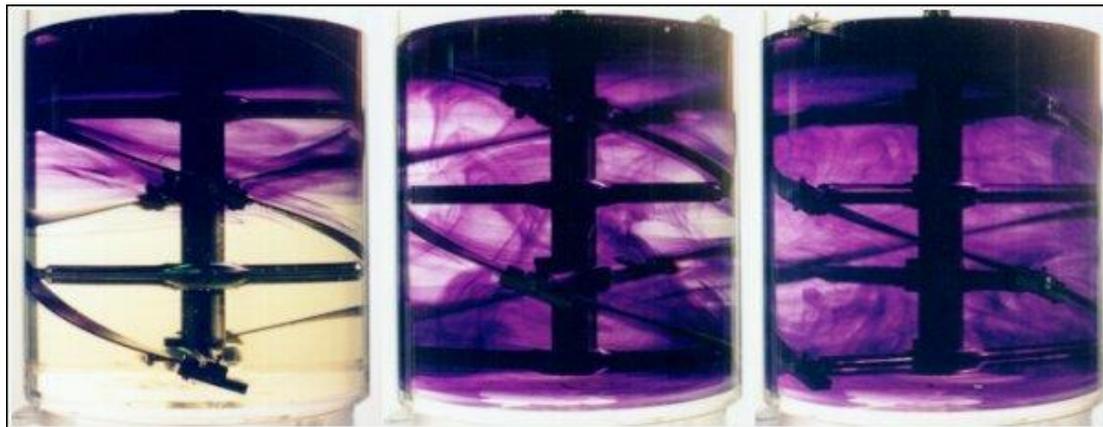
$$\bar{R}_k = 4.8\text{E}4 \neq R_k(\bar{T}) = 7.12$$

- Conclusion: just using the average temperature to calculate reaction rates will give wrong results → special reaction models needed.



# Laminar finite-rate model

- Reaction rates are calculated using the molecular reaction kinetics.
  - Using average species concentration in cell.
  - Using average temperature in cell.
  - No corrections are made for subgrid scale temperature or species concentration variations.
- The mesh and, for transient flows, the timestep should be small enough to properly resolve all spatial and temporal variations.
- This may lead to very fine mesh and timestep requirements.
- If the numerical model is too coarse, species mixing and reaction rates will be overpredicted.



Viscous flow with fine striations

# Effects of turbulence

- In turbulent flows, subgrid and temporal variations in temperature and species concentration are related to the structure of turbulence.
- We already solve for the effect of turbulence on the mean flow using turbulence models.
- This information can then also be used to predict the effects of turbulence on the reaction rate.
  - Usually, subgrid scale non-uniformities in the species concentration (i.e., poor mixing) result in an effective reaction rate that is lower than the molecular rate kinetics based on average concentrations.
- Different reaction models exist for different systems.

# Reaction models in FLUENT

- Surface reactions:
  - Particle surface reactions (e.g., coal combustion).
  - Surface reactions at solid (wall) boundaries (e.g., chemical vapor deposition).
- Combustion or infinitely fast chemistry:
  - Pre-mixed combustion models.
  - Non pre-mixed combustion models.
  - Partially pre-mixed combustion models.
  - Finite-rate kinetics in turbulent flames (composition PDF transport model).
- Finite-rate chemistry based on extended Arrhenius equation:
  - Laminar finite-rate model.
  - Finite-rate/eddy-dissipation.
  - Eddy-dissipation.
  - Eddy-dissipation concept (EDC).

# The eddy-dissipation model

- A model for the mean reaction rate of species  $i$ ,  $R_i$  based on the turbulent mixing rate.
- Assumes that chemical reactions occur much faster than turbulence can mix reactants and heat into the reaction region ( $Da \gg 1$ ).
  - $Da$  is the Damkohler number: characteristic mixing time / reaction time.
- A good assumption for many combustors: most useful fuels are fast burning.
- For fast reactions the reaction rate is limited by the turbulent mixing rate.
- The turbulent mixing rate is assumed to be related to the timescale of turbulent eddies that are present in the flow.
- Concept originally introduced by Spalding (1971) and later generalized by Magnussen and Hjertager (1976).
- The timescale used for this purpose is the so-called eddy lifetime,  $\tau = k/\varepsilon$ , with  $k$  being the turbulent kinetic energy and  $\varepsilon$  the turbulent dissipation rate.
- Chemistry typically described by relatively simple single or two step mechanism.

# The eddy-dissipation model

- The net rate of production of species  $i$  due to reaction  $r$ ,  $R_{i,r}$  is given by the smaller (i.e., limiting value) of the two expressions below.

- Based on mass fraction of reactants: 
$$R_{i,r} = \nu'_{i,r} M_{w,i} A \rho \frac{\epsilon}{k} \min_{\mathcal{R}} \left( \frac{Y_{\mathcal{R}}}{\nu'_{\mathcal{R},r} M_{w,\mathcal{R}}} \right)$$

- Based on mass fraction of products: 
$$R_{i,r} = \nu'_{i,r} M_{w,i} A B \rho \frac{\epsilon}{k} \frac{\sum_P Y_P}{\sum_j^N \nu''_{j,r} M_{w,j}}$$

- Here:

|            |  |
|------------|--|
| $k$        | - turbulence kinetic energy                      |
| $\epsilon$ | - turbulence dissipation rate                    |
| $Y_P, Y_R$ | - mass fraction of species                       |
| $A$        | - Magnussen constant for reactants (default 4.0) |
| $B$        | - Magnussen constant for products (default 0.5)  |
| $M_{w,i}$  | - molecular weight                               |
| $(R), (P)$ | - reactants, products                            |

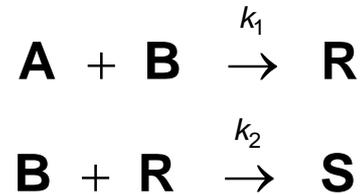
- Note that kinetic rates are not calculated!

# Finite-rate/eddy-dissipation model

- The eddy-dissipation model assumes that reactions are fast and that the system is purely mixing limited.
- When that is not the case, it can be combined with finite-rate chemistry.
- In FLUENT this is called the finite-rate/eddy-dissipation model.
- In that case, the kinetic rate is calculated in addition to the reaction rate predicted by the eddy-dissipation model.
- The slowest reaction rate is then used:
  - If turbulence is low, mixing is slow and this will limit the reaction rate.
  - If turbulence is high, but the kinetic rate is low, this will limit the reaction rate.
- This model can be used for a variety of systems, but with the following caveats:
  - The model constants  $A$  and  $B$  need to be empirically adjusted for each reaction in each system. The default values of 4 and 0.5 respectively were determined for one and two-step combustion processes.
  - The model always requires some product to be present for reactions to proceed. If this is not desirable, initial mass fractions of product of  $1\text{E-}10$  can be patched and a model constant  $B=1\text{E}10$  used.

# Example: parallel competitive reactions

- Stirred tank system with parallel-competitive reactions:



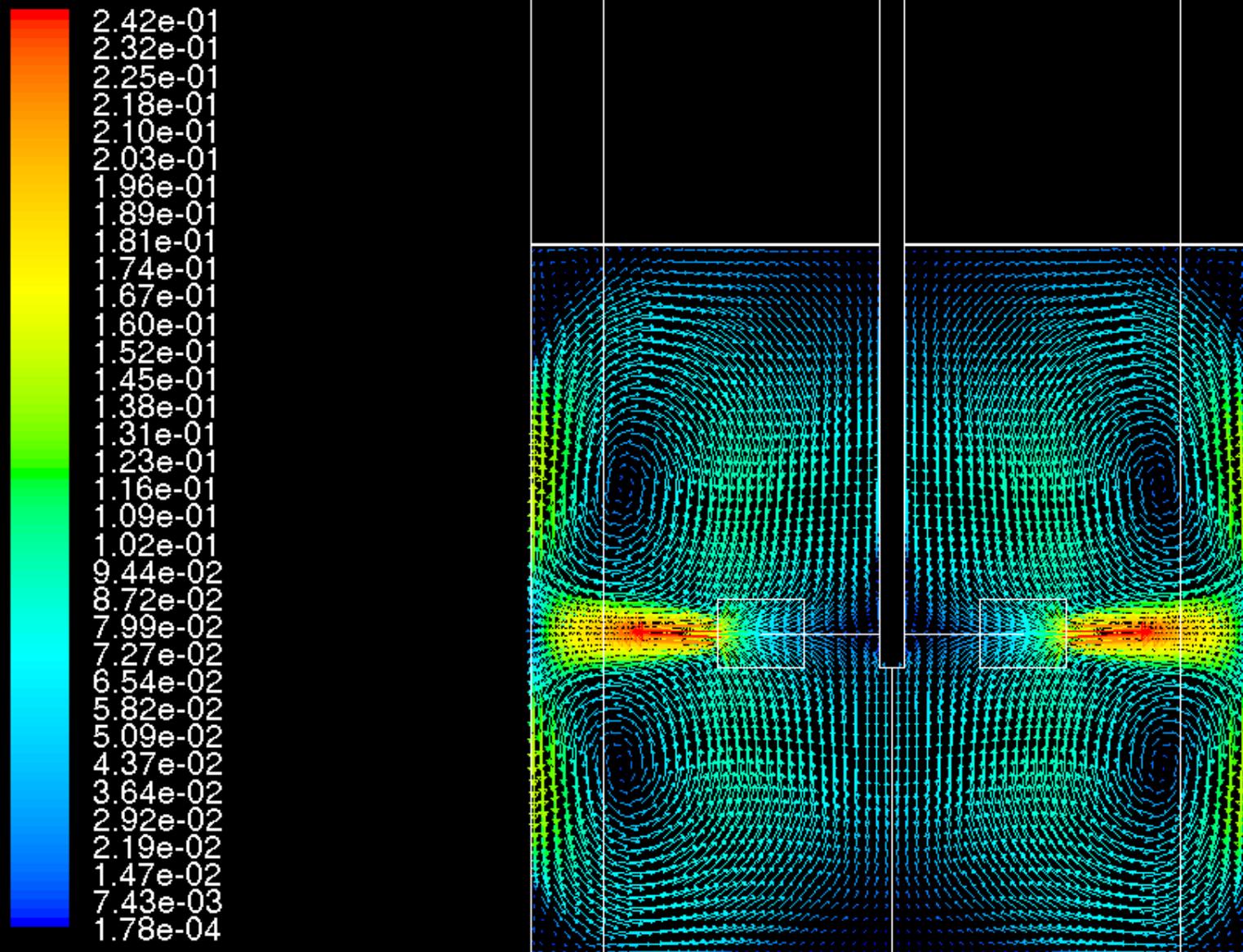
- Reaction 1 is fast ( $k_1=7300 \text{ m}^3/\text{Mole}\cdot\text{s}$ ) and reaction 2 is slow ( $k_2=3.5 \text{ m}^3/\text{Mole}\cdot\text{s}$ ).
- The side-product **S** is only formed in regions with excess **B** and depleted from **A**, i.e., poorly mixed regions.
- The final product is characterized by the product distribution  $X$ :

$$X = \frac{2C_S}{C_R + 2C_S}$$

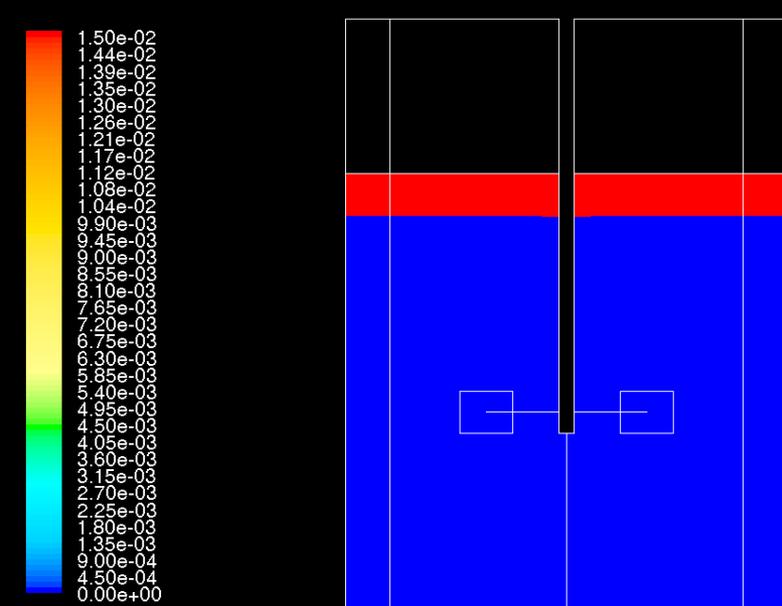
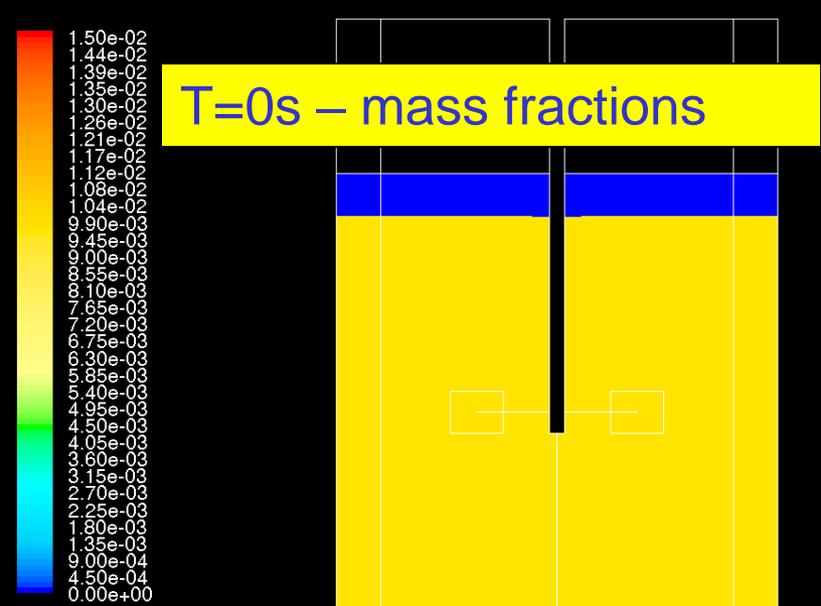
- This indicates which fraction of reactant **B** was used to create side-product. A lower  $X$  indicates less **B** was used to create side-product.

# Using the finite-rate/eddy-dissipation model

- This system was previously investigated.
- The following Magnussen model constants were determined to give good results for this system:
  - Reaction 1: model constant  $A_1=0.08$ .
  - Reaction 2: model constant  $A_2=1E10$ .
  - For both reactions, use model constant  $B=1E10$  and initial product mass fractions of  $1E-10$  to disable the product mass-fraction based reaction rate limiter.
  - The net effect of this set of model constants is that only the first reaction is limited by mixing rate, but not the second reaction.
- The reaction rates were set independent of temperature by specifying zero values for the activation energy and the temperature exponent.

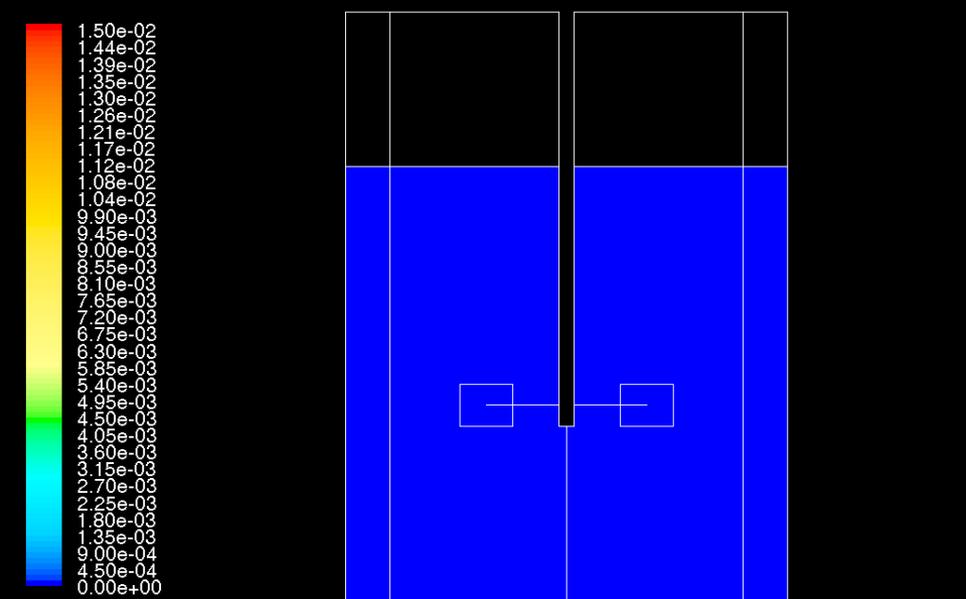
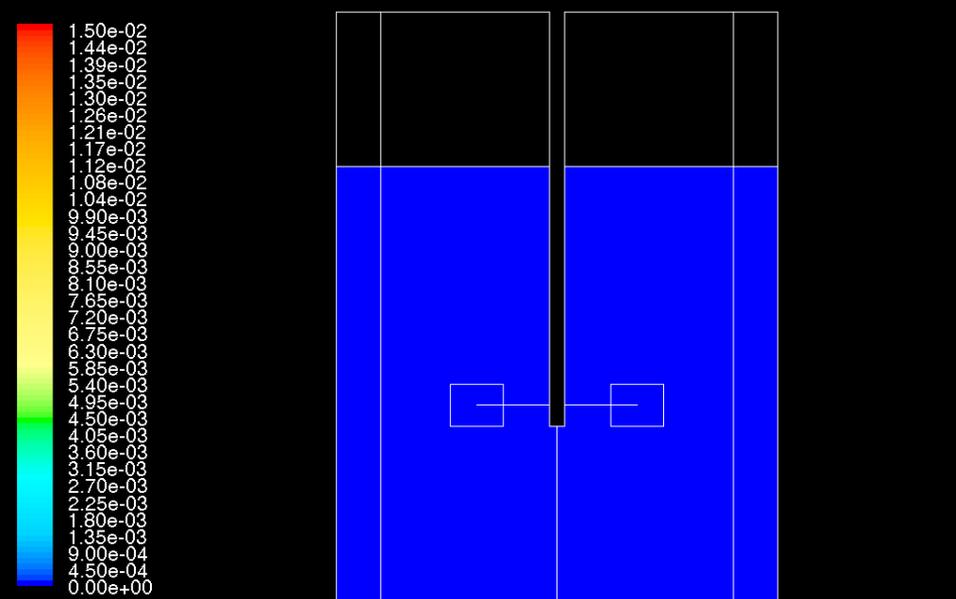


Rushton Impeller - 50 RPM - 31.6l Vessel  
Velocity Vectors Colored By Velocity Magnitude (m/s)



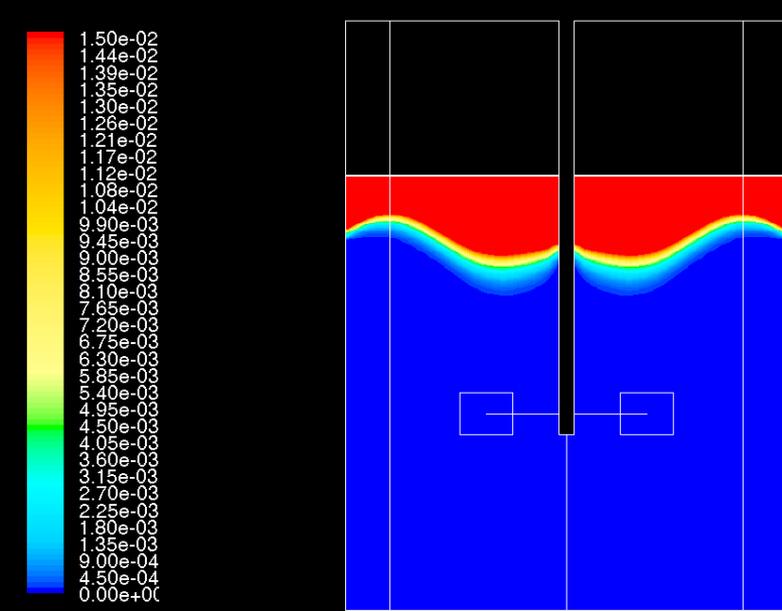
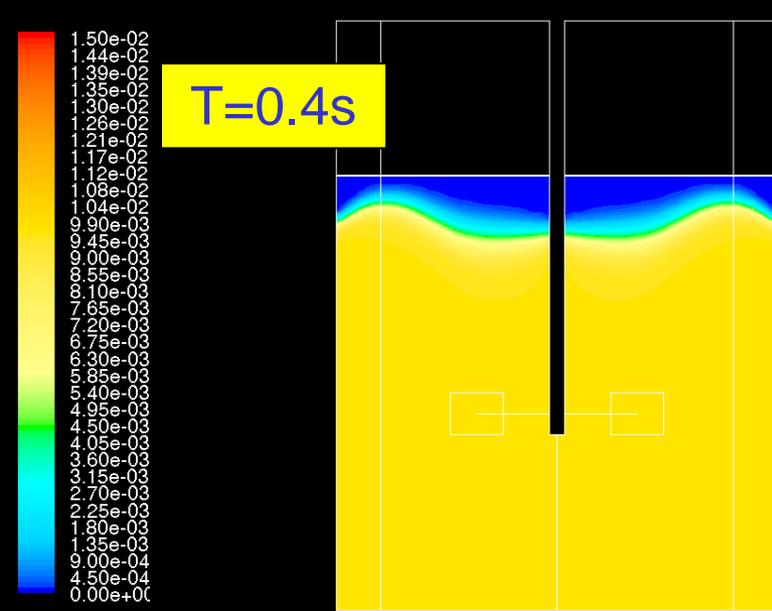
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=0.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

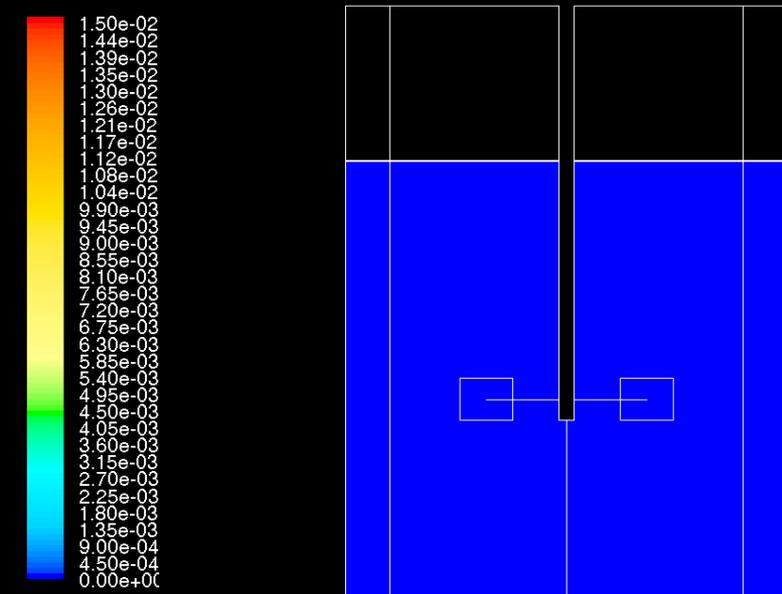
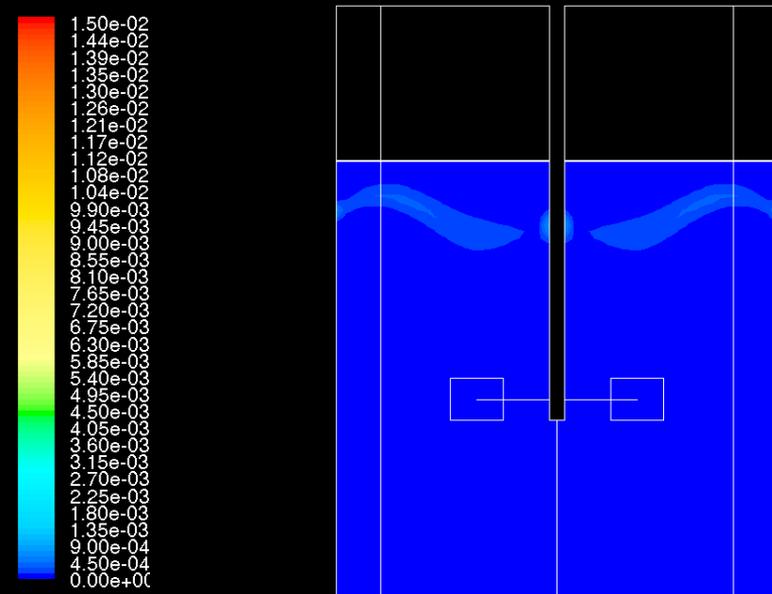


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=4.0000e-01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant A**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=4.0000e-01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant B**

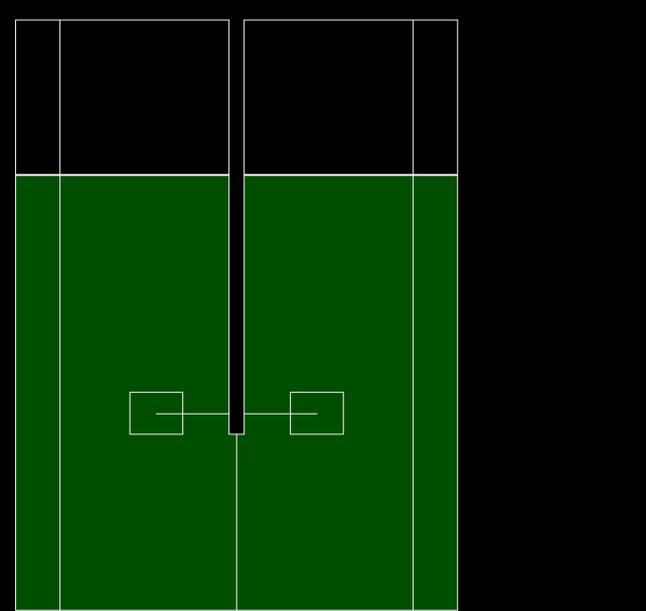
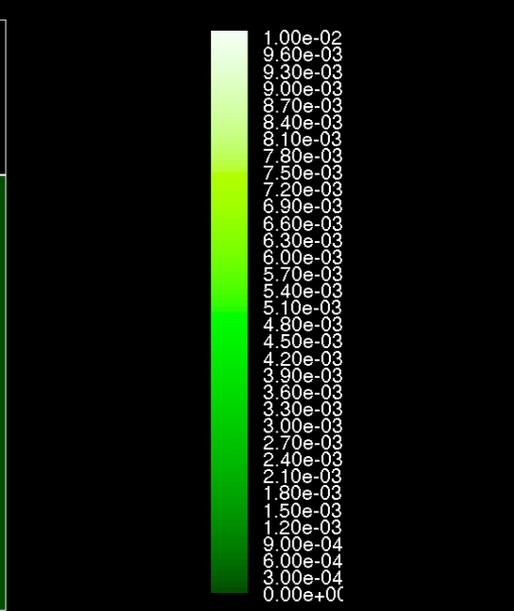


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=4.0000e-01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product R**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=4.0000e-01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product S**



Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Rate of Reaction-1 (kgmol/m3-s)

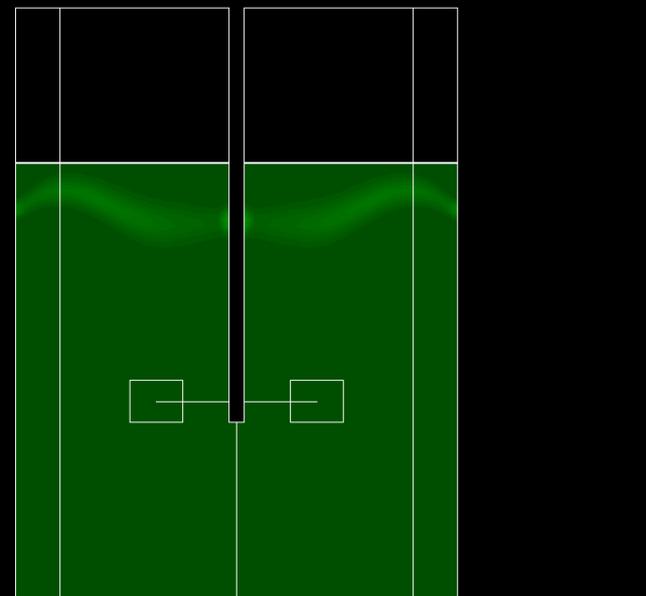
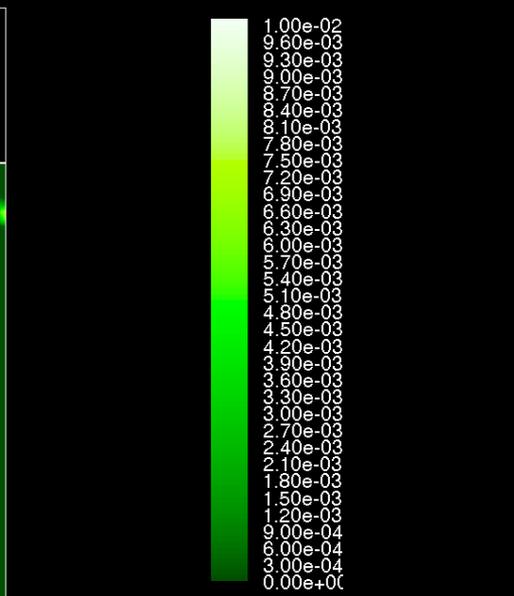
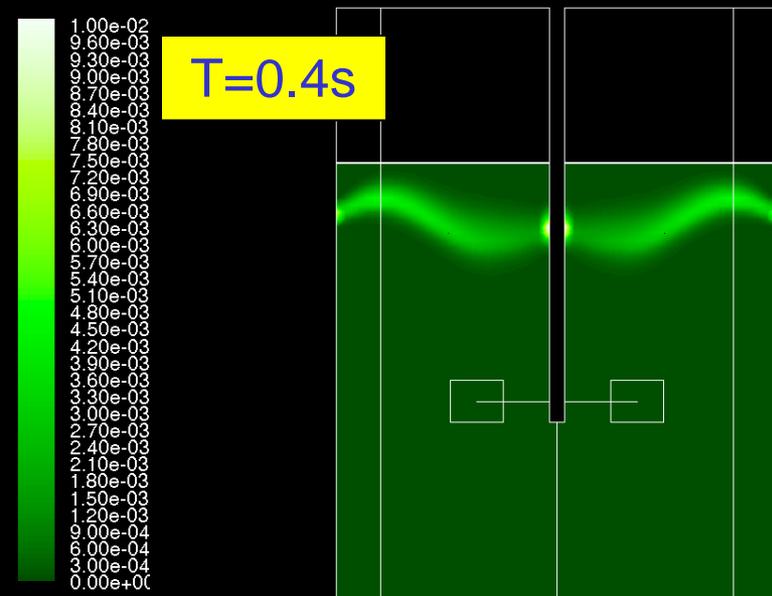
**Reaction rate 1: A + B → R**

FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Rate of Reaction-2 (kgmol/m3-s)

**Reaction rate 2: B + R → S**

FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Rate of Reaction-1 (kgmol/m3-s)

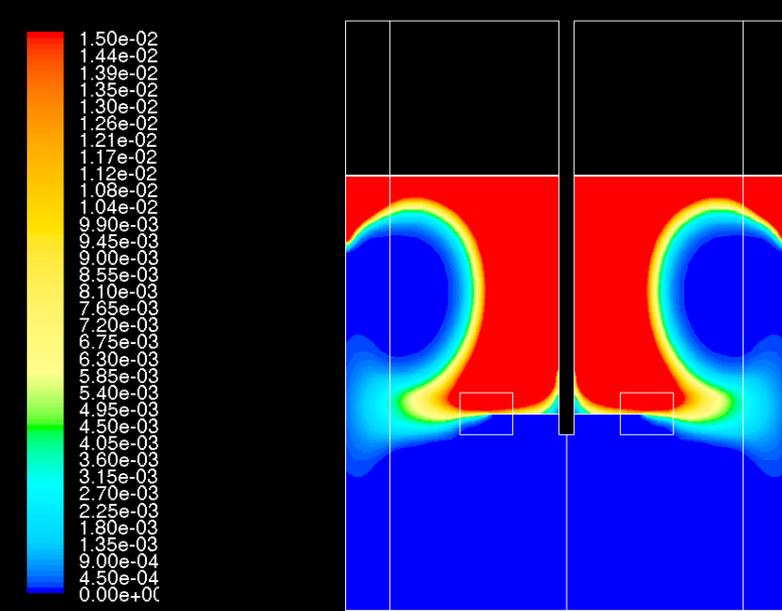
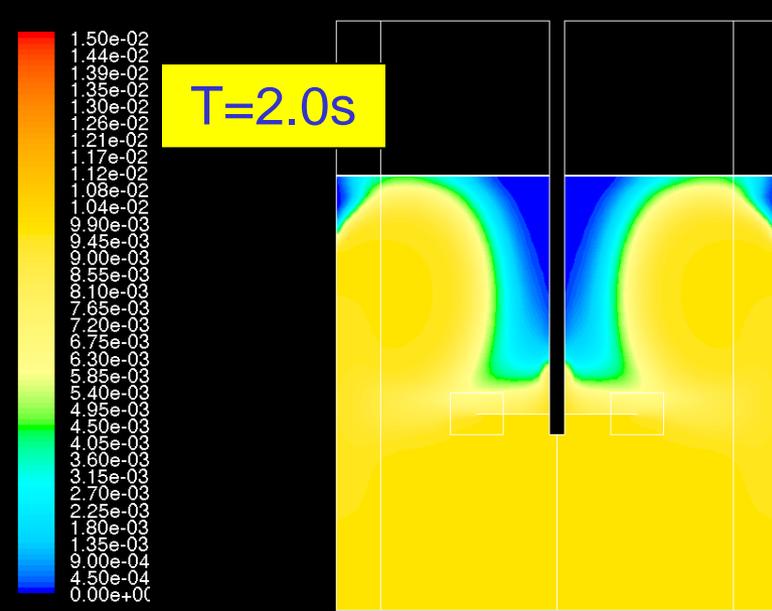
**Reaction rate 1: A + B → R**

(Time=4.0000e-01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Rate of Reaction-2 (kgmol/m3-s)

**Reaction rate 2: B + R → S**

(Time=4.0000e-01)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

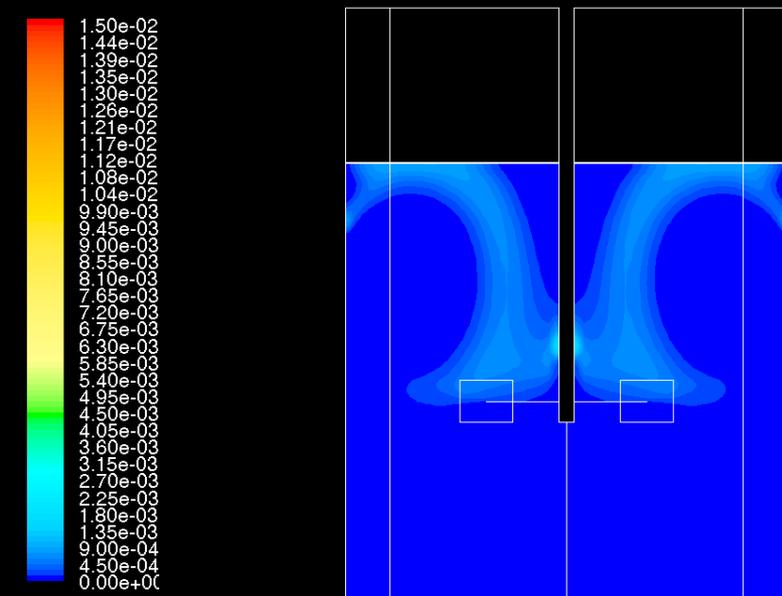
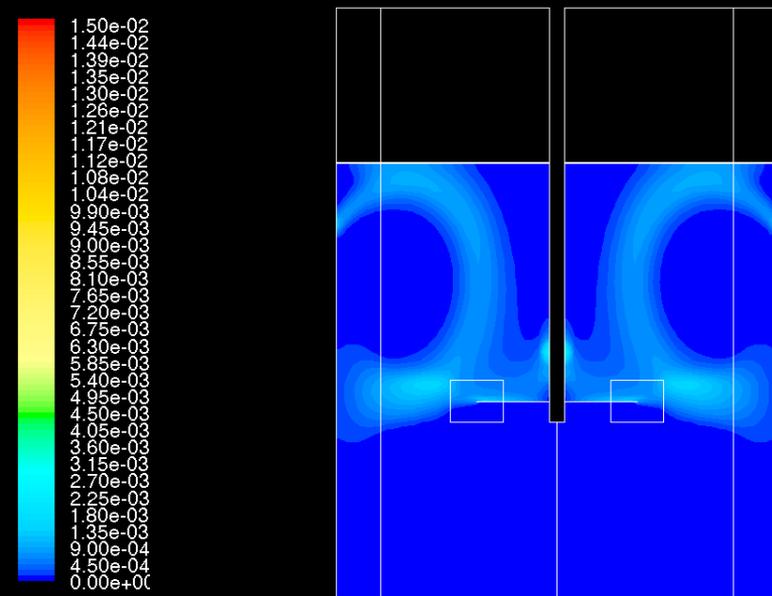


Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of reactant-a (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant A**

Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of reactant-b (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant B**

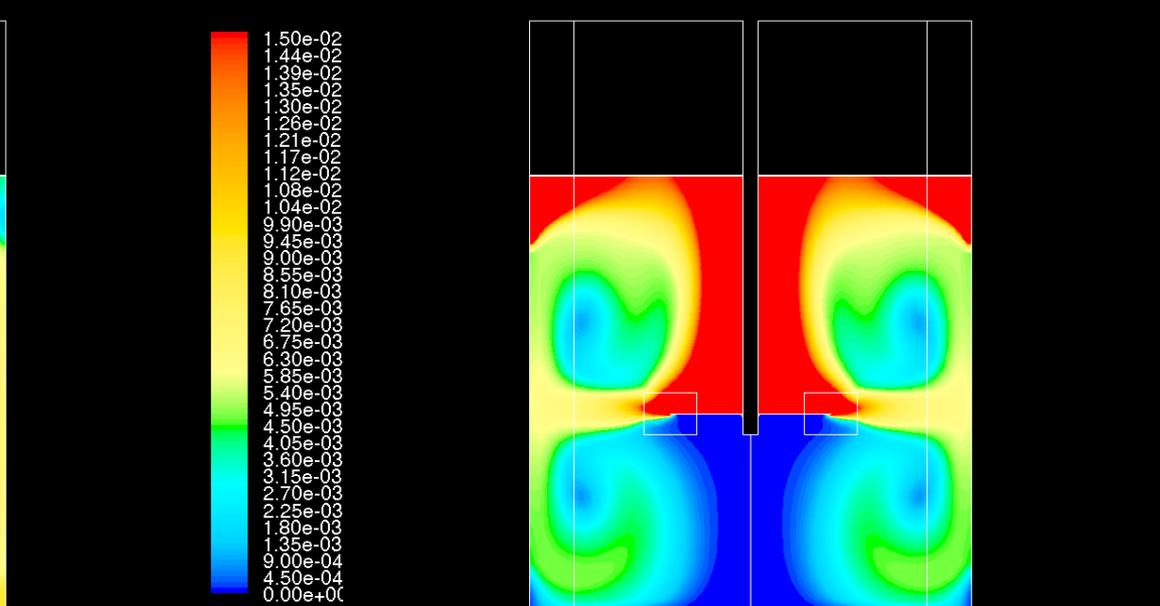
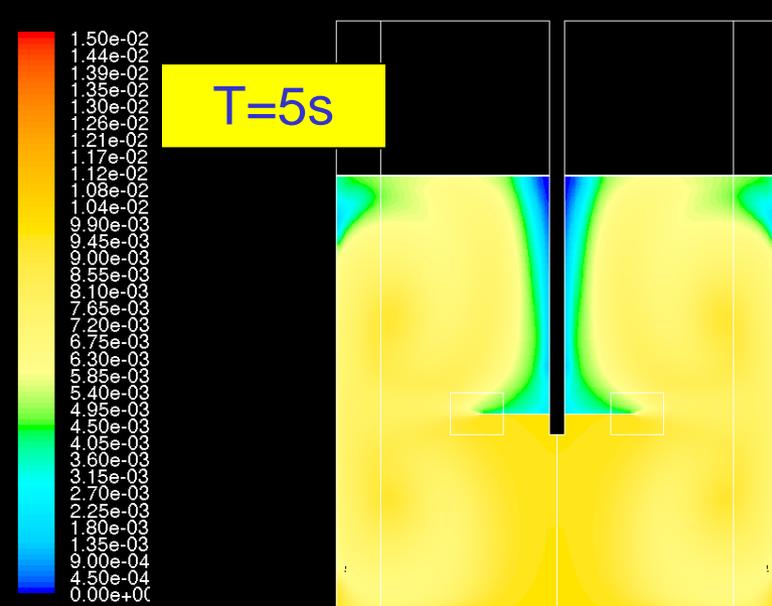


Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of product-r (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product R**

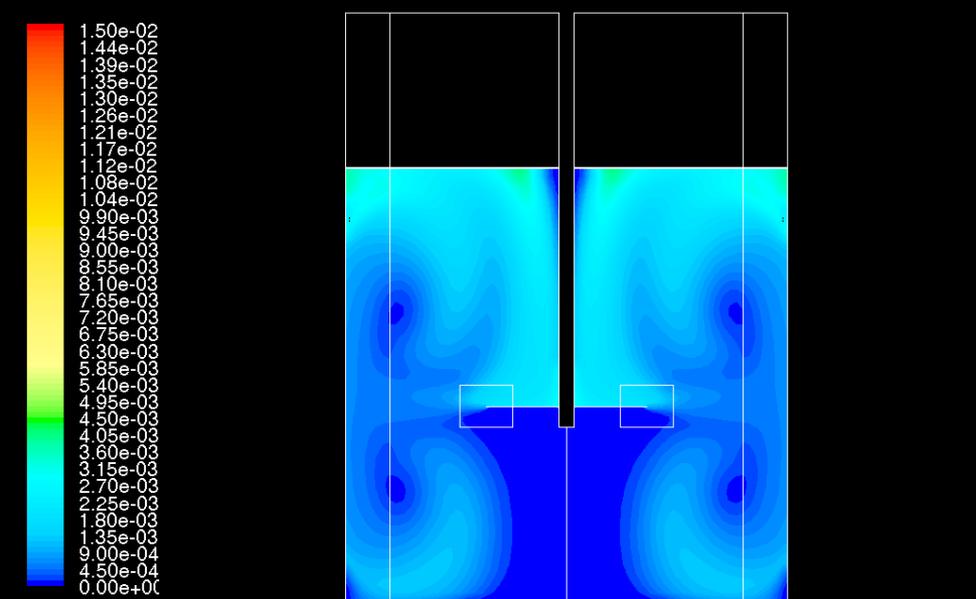
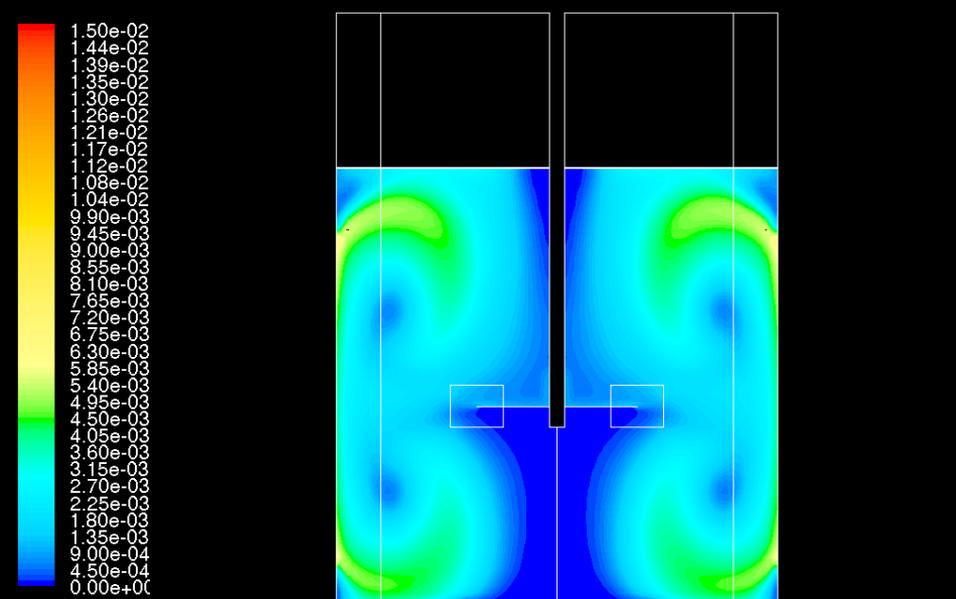
Rushton Impeller - 50 RPM - 31.6l Vessel  
Contours of Mass fraction of product-s (Time=2.0000e+00)  
FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product S**



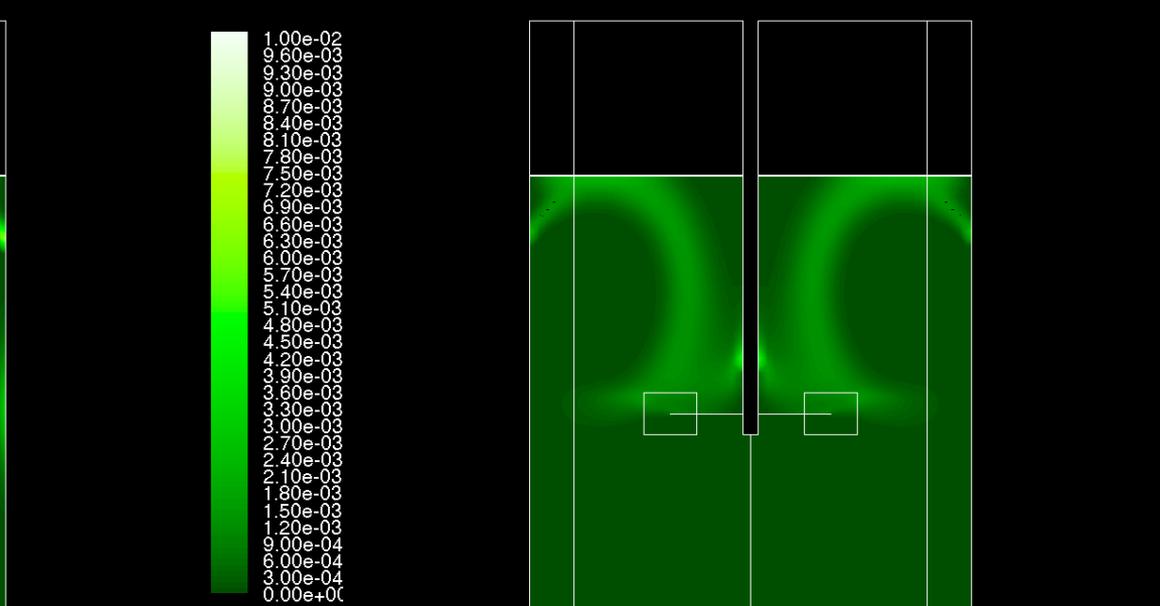
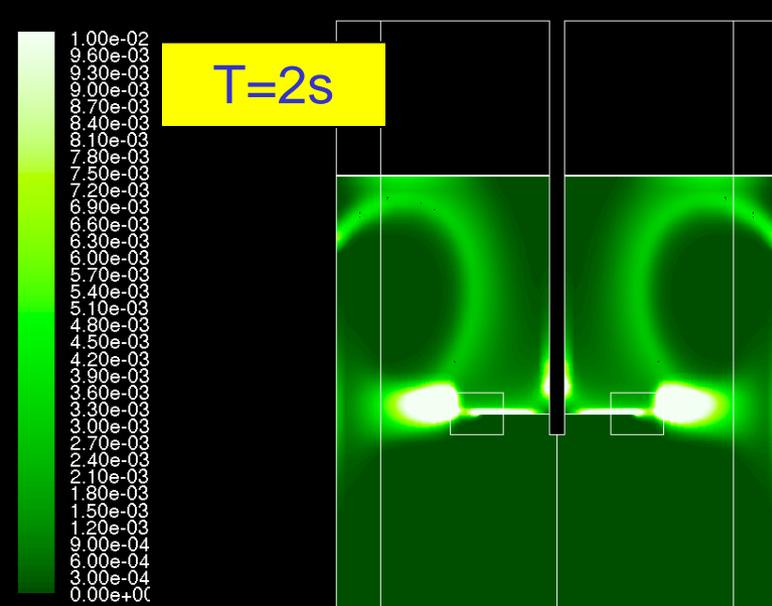
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=5.0000e+00)  
 Mass fraction reactant A  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=5.0000e+00)  
 Mass fraction reactant B  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=5.0000e+00)  
 Mass fraction product R  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=5.0000e+00)  
 Mass fraction product S  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

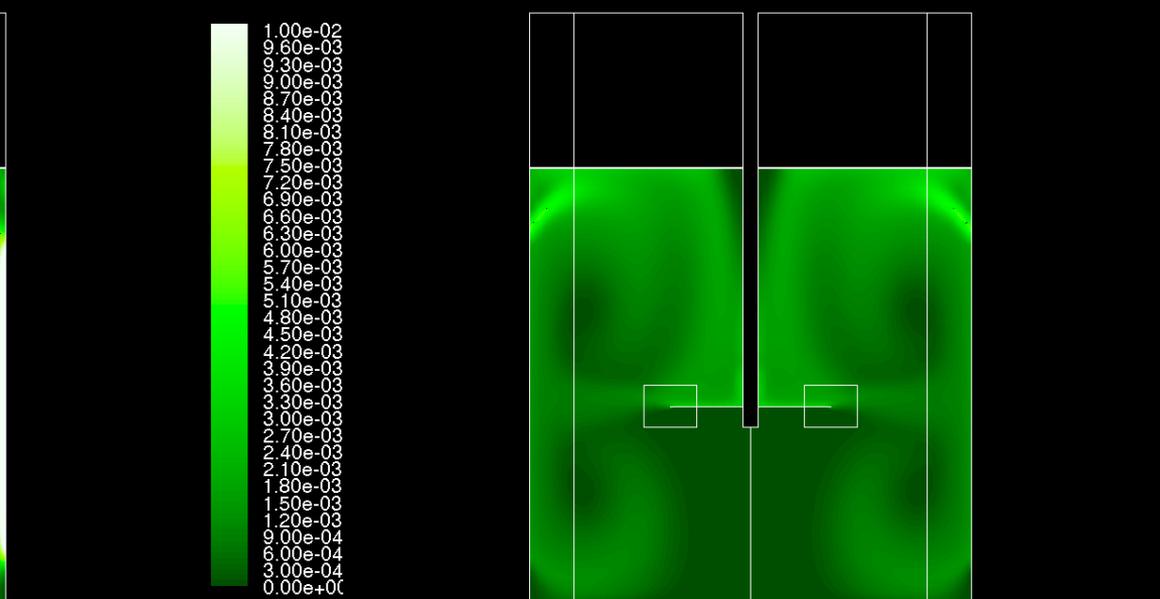
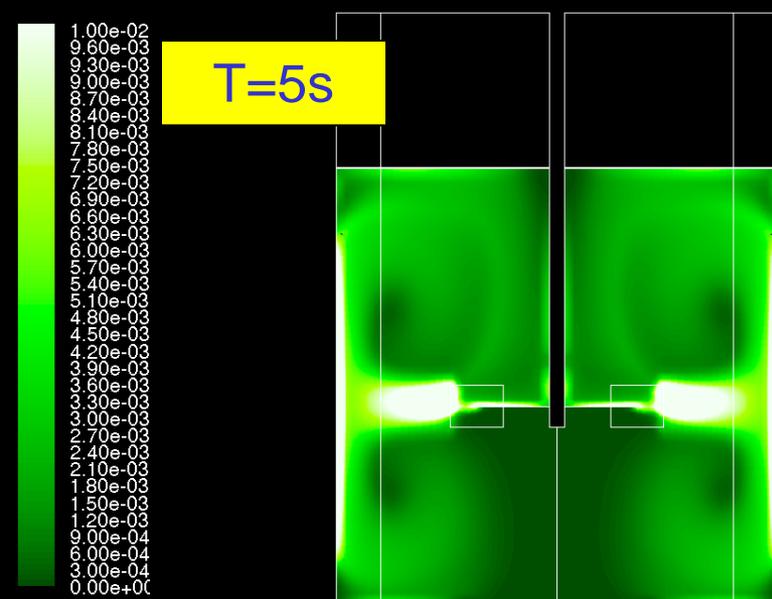


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-1 (kgmol/m3-s) (Time=2.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 1: A + B → R**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-2 (kgmol/m3-s) (Time=2.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 2: B + R → S**

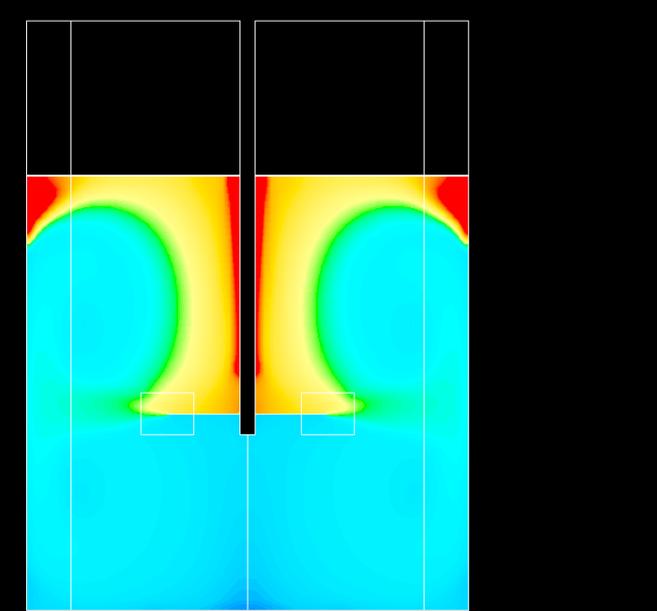
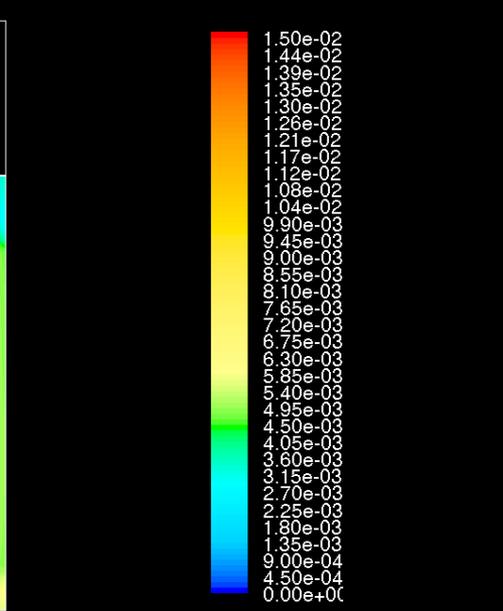
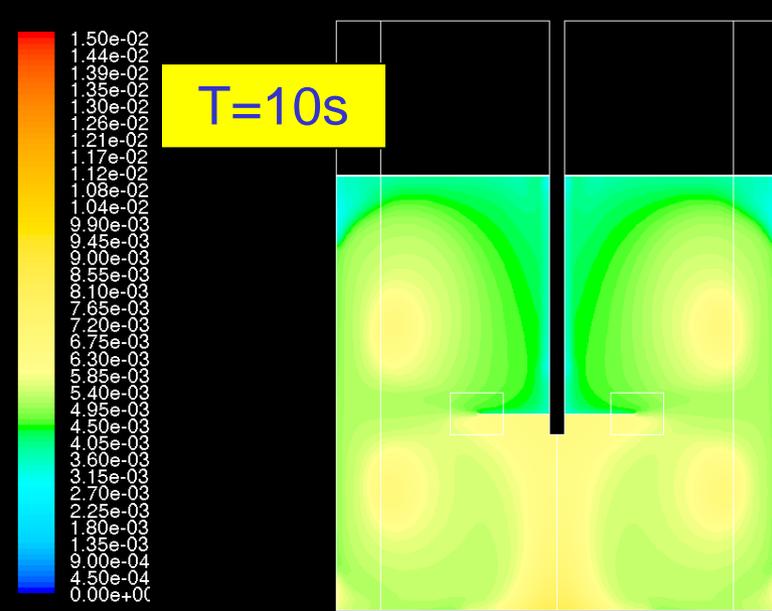


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-1 (kgmol/m3-s) (Time=5.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 1: A + B → R**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-2 (kgmol/m3-s) (Time=5.0000e+00)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 2: B + R → S 156**

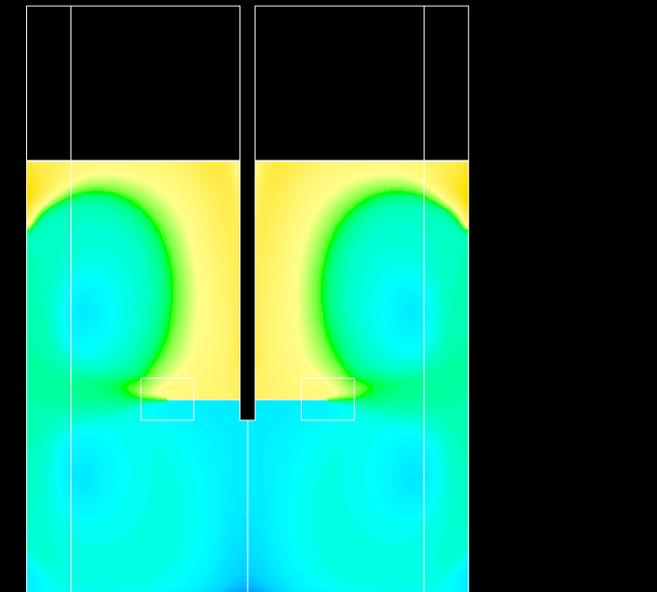
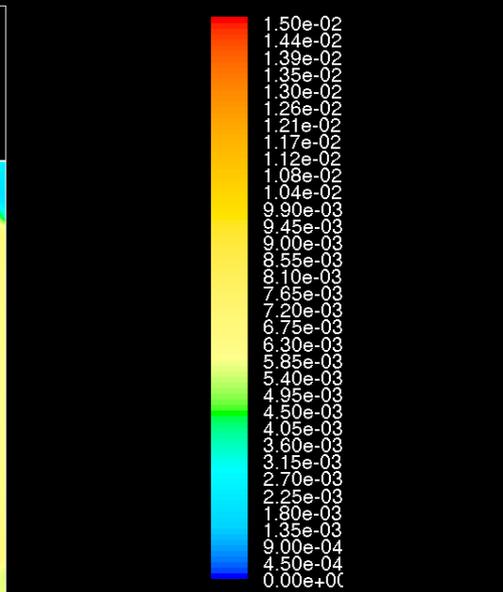
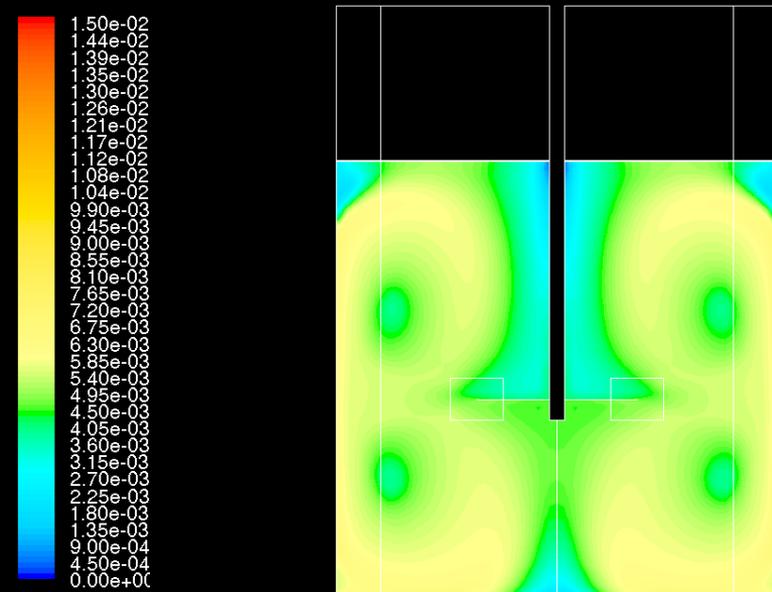


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant A**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant B**

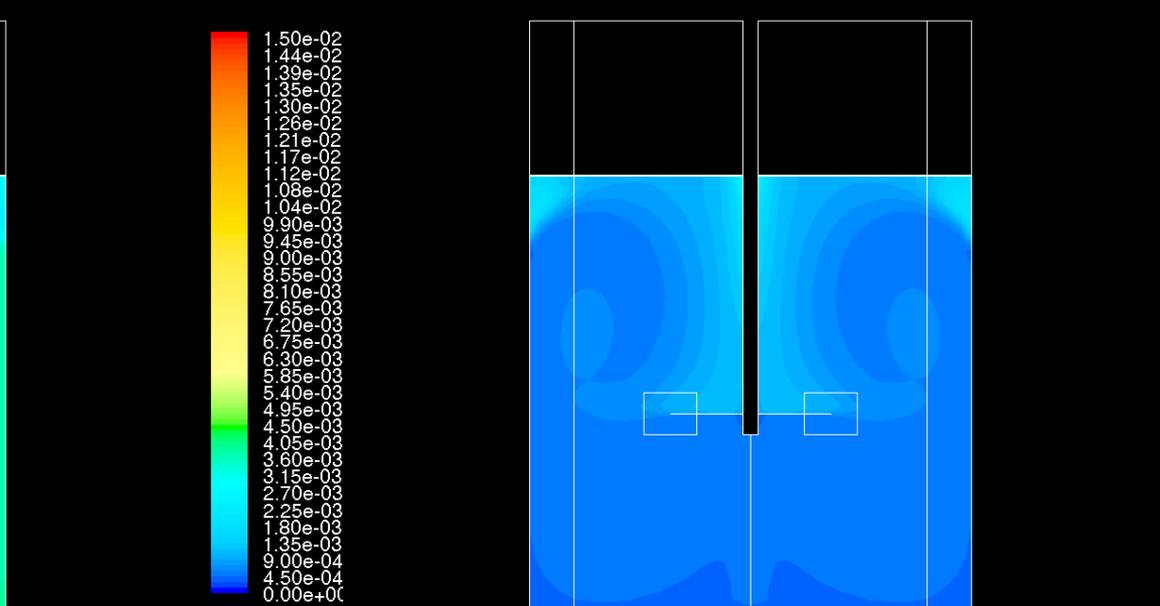
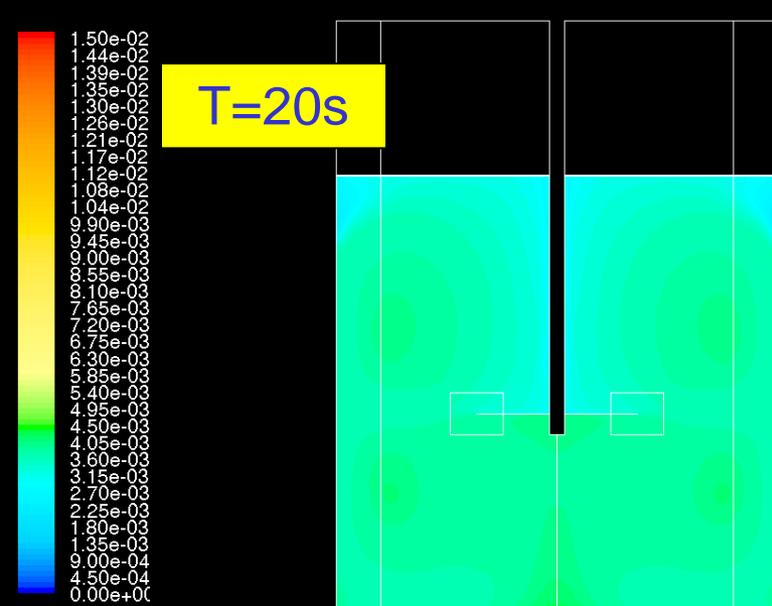


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product R**

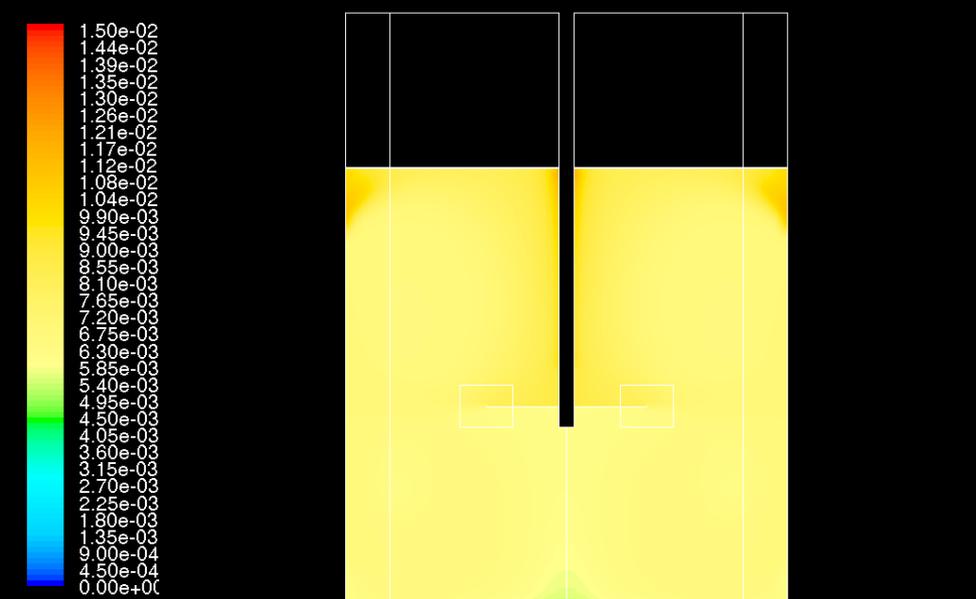
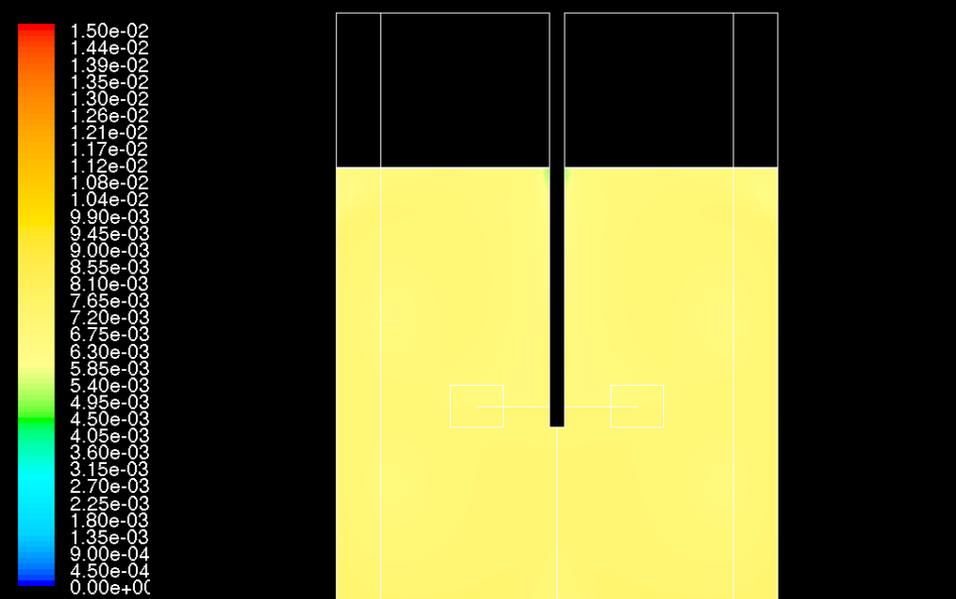
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product S**



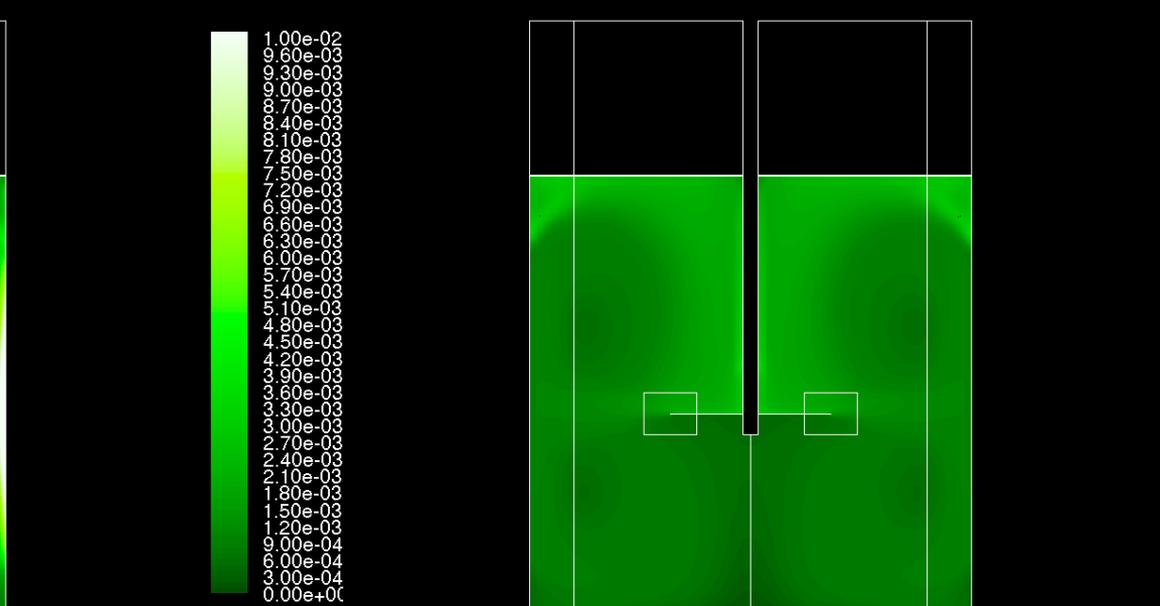
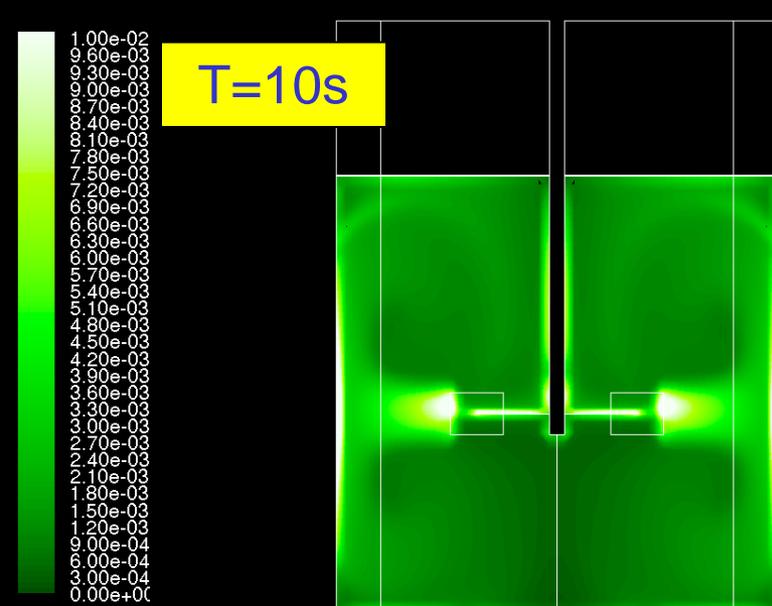
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=2.0000e+01)  
 Mass fraction reactant A  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=2.0000e+01)  
 Mass fraction reactant B  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)



Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=2.0000e+01)  
 Mass fraction product R  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=2.0000e+01)  
 Mass fraction product S  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

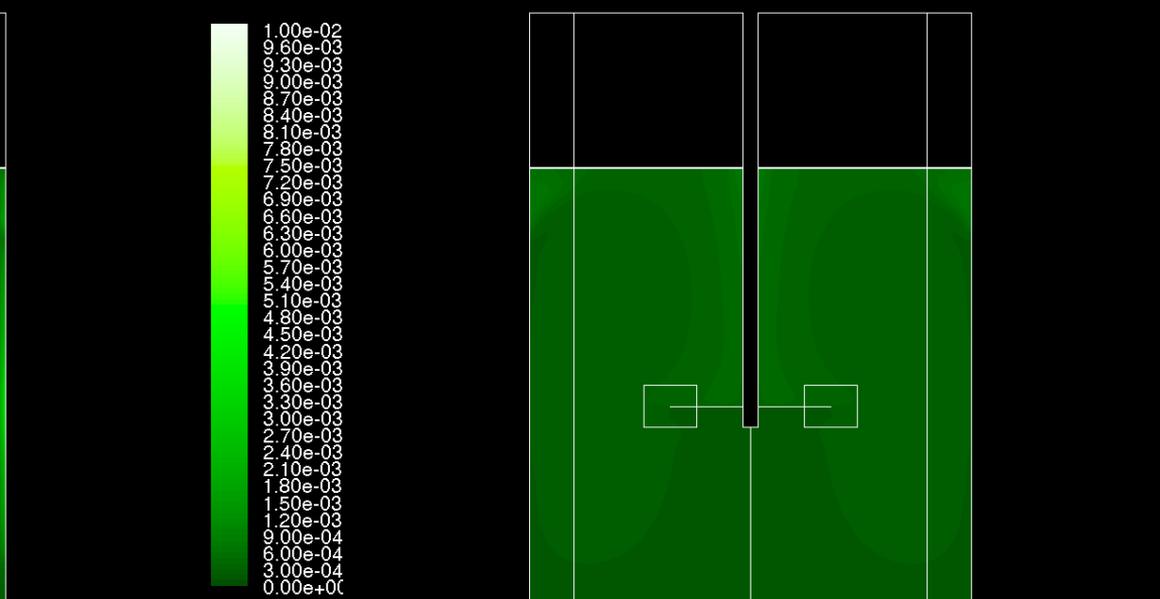
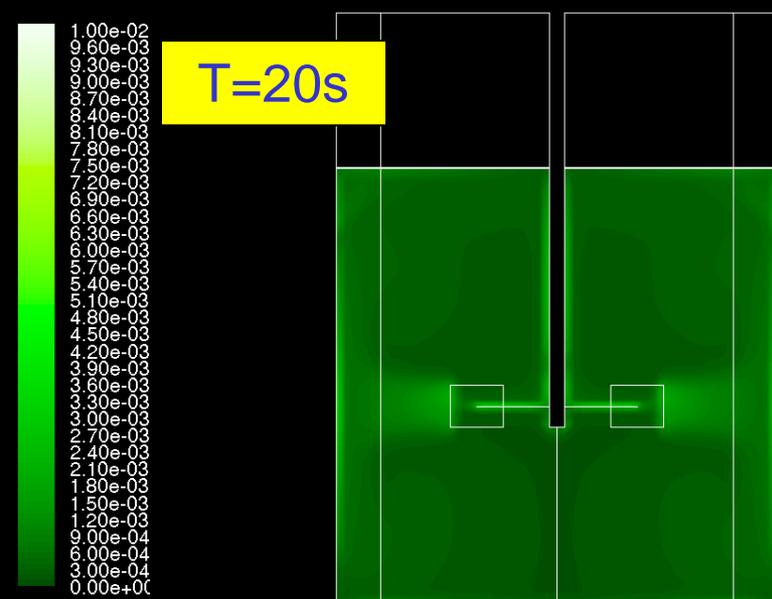


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-1 (kgmol/m3-s) (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 1: A + B → R**

Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-2 (kgmol/m3-s) (Time=1.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 2: B + R → S**

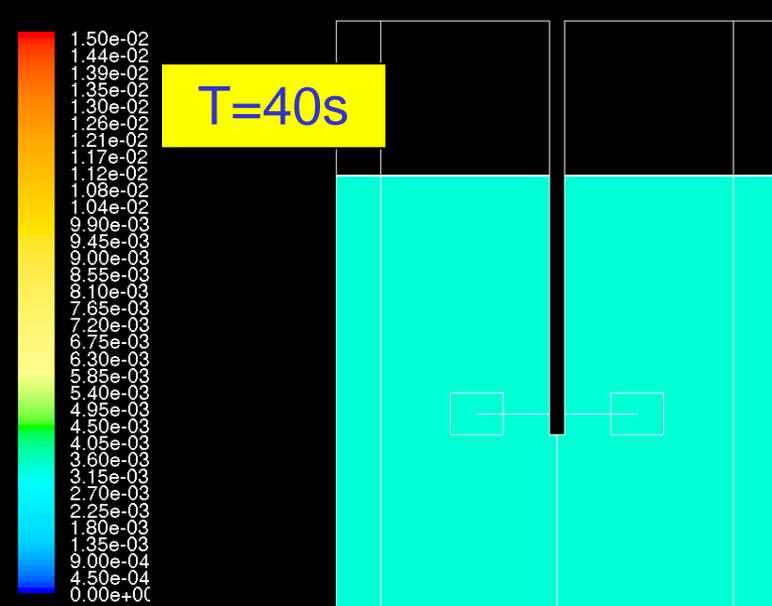


Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-1 (kgmol/m3-s) (Time=2.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 1: A + B → R**

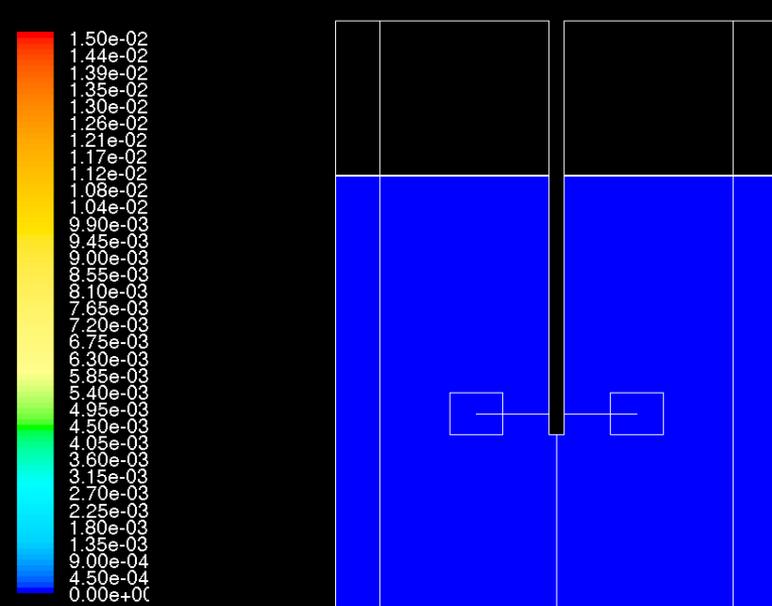
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Rate of Reaction-2 (kgmol/m3-s) (Time=2.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Reaction rate 2: B + R → S 159**



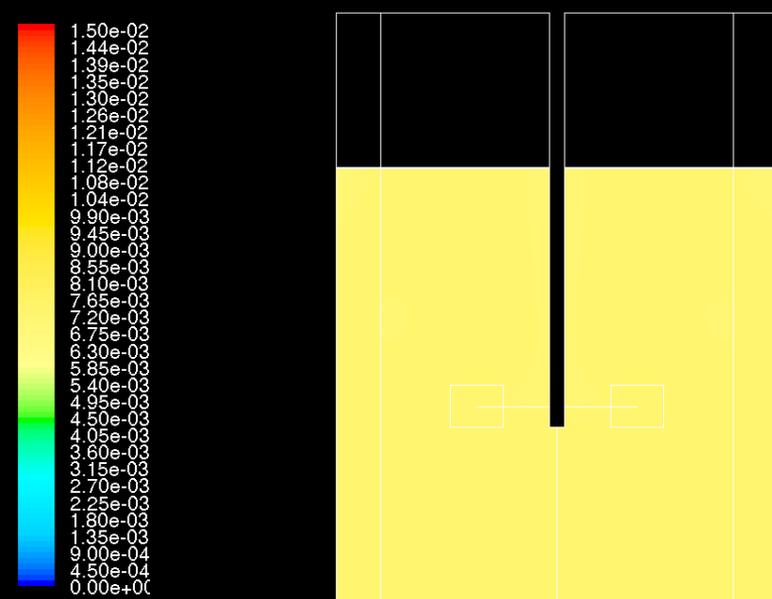
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-a (Time=4.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant A**



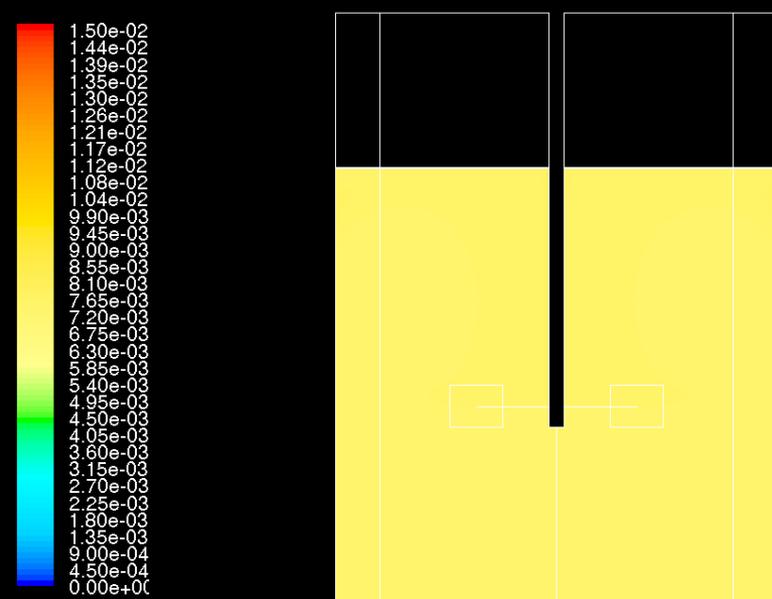
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of reactant-b (Time=4.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction reactant B**



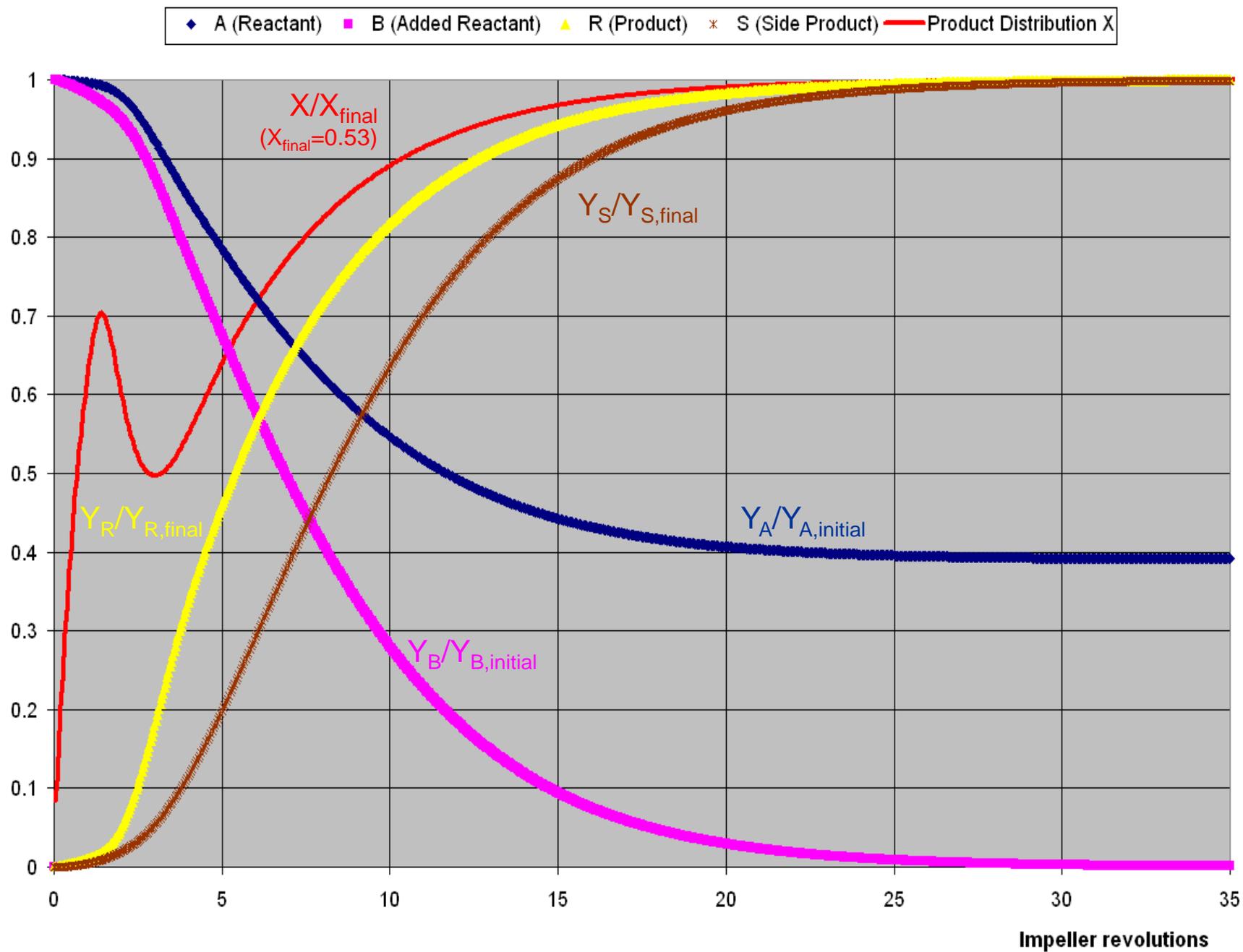
Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-r (Time=4.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product R**



Rushton Impeller - 50 RPM - 31.6l Vessel  
 Contours of Mass fraction of product-s (Time=4.0000e+01)  
 FLUENT 6.2 (axi, segregated, spe, rke, unsteady)

**Mass fraction product S**



# Other models

- The eddy-dissipation-concept (EDC) model.
  - This is an extension of the eddy-dissipation model to finite rate chemistry; proposed by Gran and Magnussen (1996).
  - Equations are very different, however. Assumes reactions occur on small scales and calculates a volume fraction of small-scale eddies in which the reactions occur.
  - It is more suitable for more complex reaction sets than the finite-rate/eddy-dissipation model and requires less user tuning. It is computationally expensive, however.
- Dedicated combustion models:
  - Pre-mixed combustion models.
  - Non pre-mixed combustion models.
  - Partially pre-mixed combustion models.
  - Finite-rate kinetics in turbulent flames (composition PDF transport model).
- Not standard in FLUENT: reactions for which the kinetics cannot practically be described by Arrhenius rate style kinetics. Such kinetics needs to be added through user defined source terms. Examples:
  - Fermentation kinetics.
  - Polymerization.

# Complex reaction sets

- Many real-life systems have complex sets of reactions, often many hundreds.
- Not all reactions may be known in detail, and there may be uncertainty in the rate constants.
- Large differences in time constants may make the reaction set hard (“stiff”) to solve.

⇒ The reaction sets modeled are usually simplifications of what happens in real life.

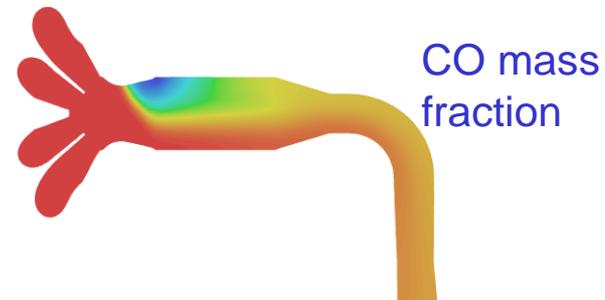
# Example: catalytic converter

- The main component of the catalytic converter is the monolith
- The monolith usually has a honeycomb structure, which is coated with one or more catalysts, known as the washcoat (platinum, rhodium, palladium).

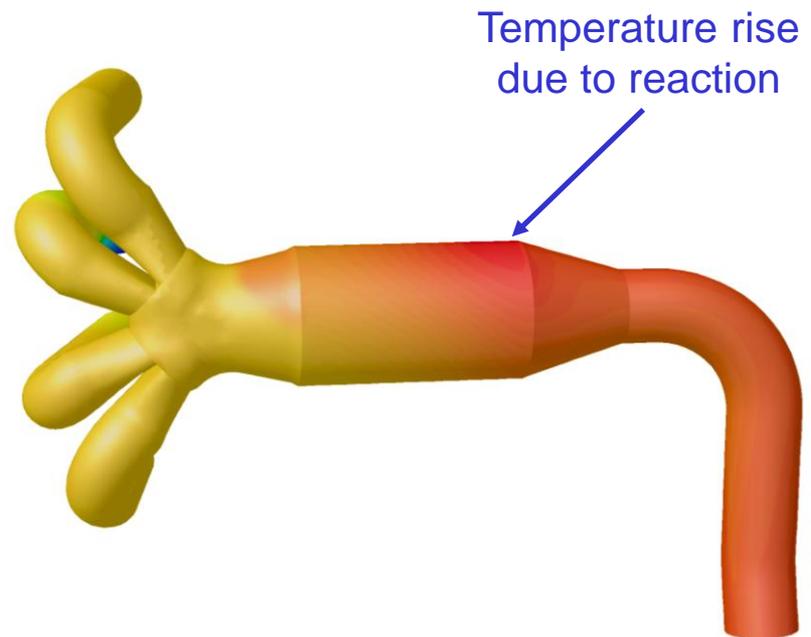


Catalyst Housing

Monolith



CO mass fraction



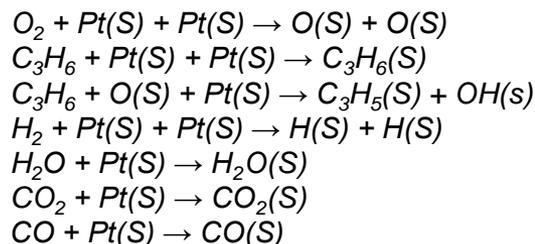
Temperature rise due to reaction

# Reaction mechanism

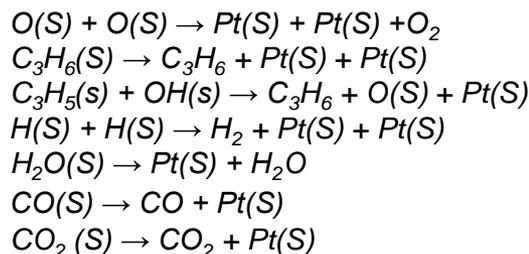
61 surface reactions  
8 gas phase species  
23 surface site species  
2 catalysts

$C_3H_6$  oxidation on Pt

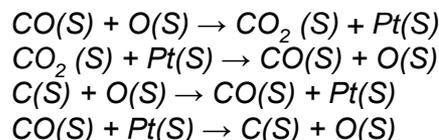
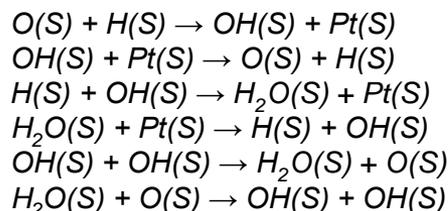
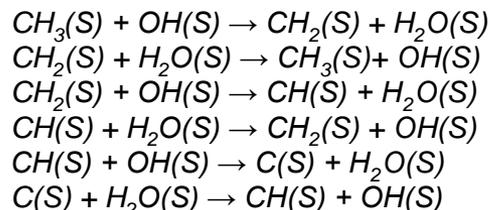
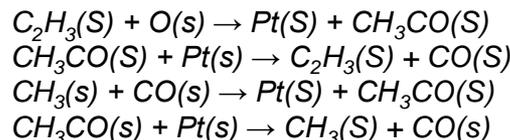
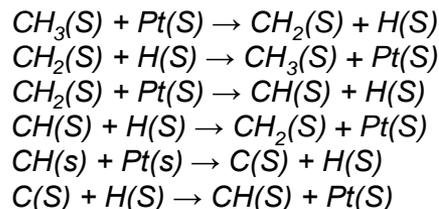
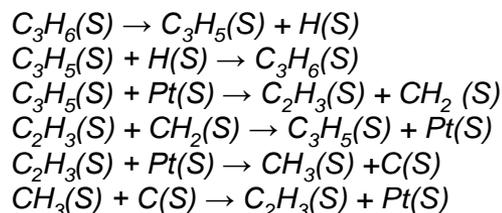
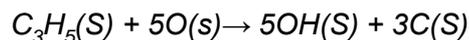
*Adsorption*



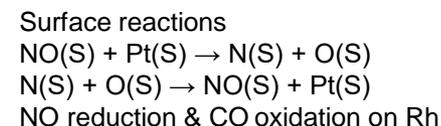
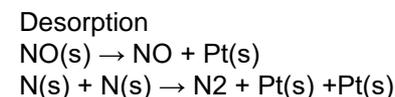
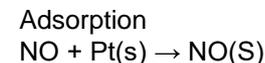
*Desorption*



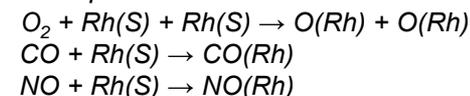
*Surface reactions*



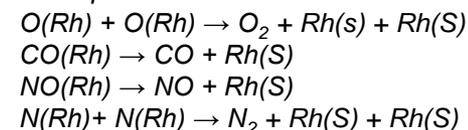
NO reduction on Pt



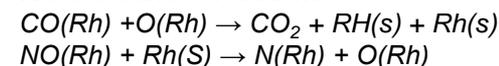
*Adsorption*



*Desorption*

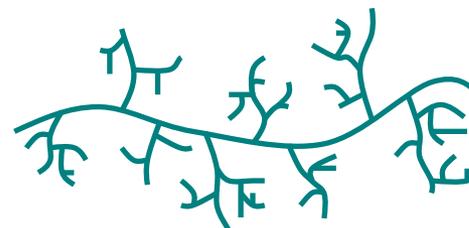


*NO/CO Surface reactions*

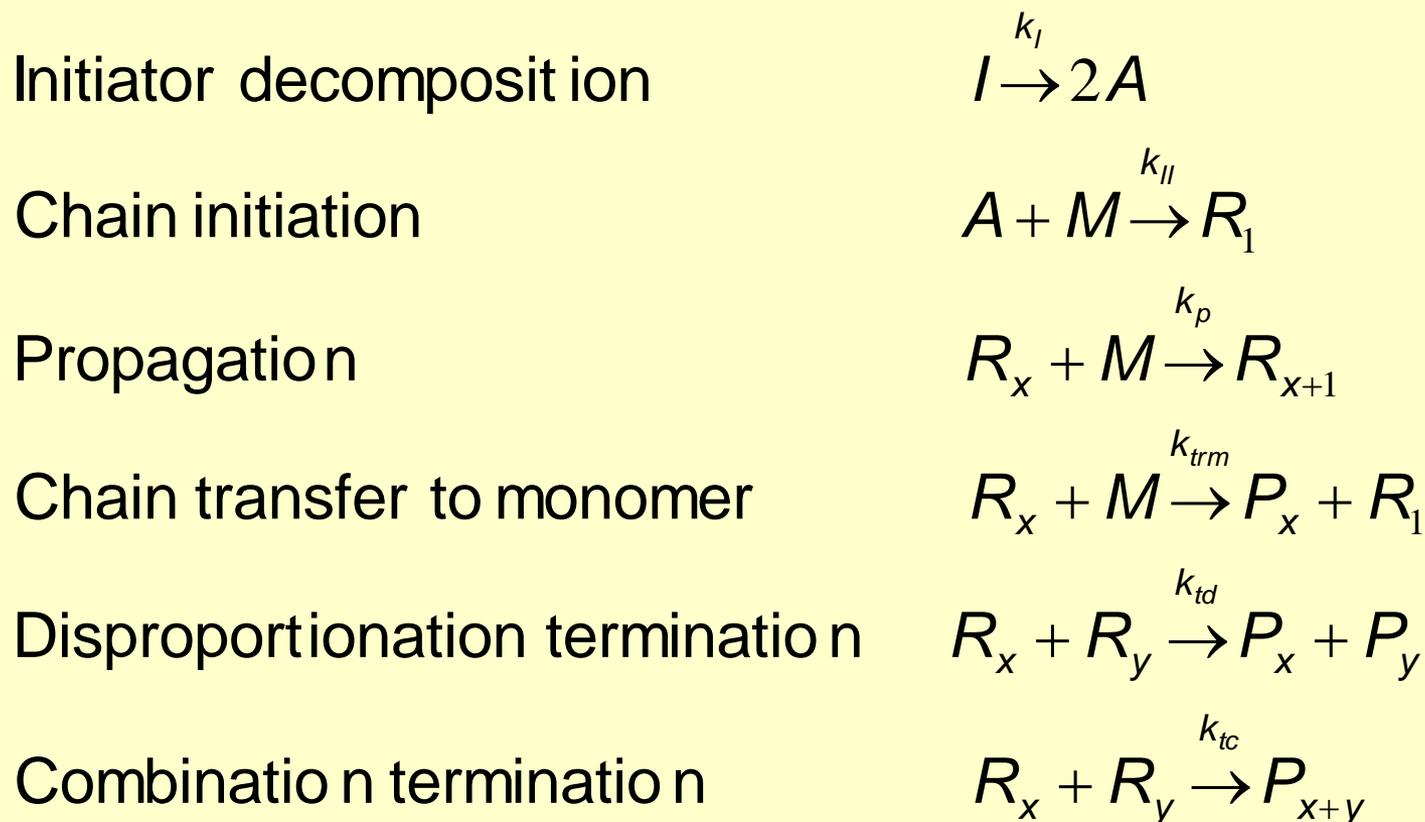


## Example: polymerization

- Polymerization of ethylene  $C_2H_4$  into low-density poly-ethylene (LDPE).
- LDPE is a plastic resin used to make consumer products such as cellophane wrap, diaper liners, and squeeze bottles.
- It is important to be able to predict the properties of the LDPE depending on the precise reaction conditions.
- The low-density polyethylene process is a complex chain of reactions
  - It involves many steps and many radicals of different lengths.
  - It starts with a small amount of initiator mixing with a large amount of monomer (ethylene).
  - The final product is a polymer (polyethylene) of varying length and structure.



# The multi-step polymerization process



$I$  = initiator

$M$  = monomer

$P_x$  = polymer (length  $x$ )

$A$  = initiator radical

$R_x$  = radical (length  $x$ )

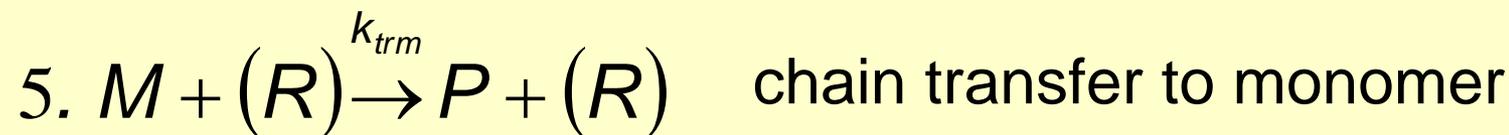
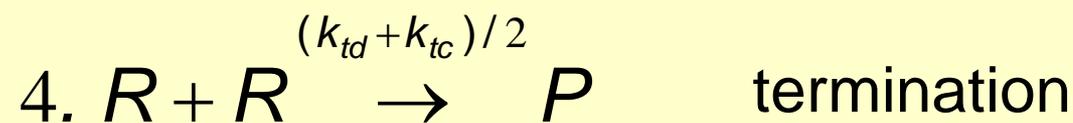
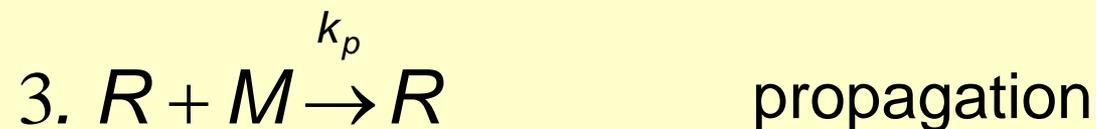
# Solution method

- Instead of solving species equations for every possible radical or polymer length a mathematical method called the “method of moments” is used.
- Introduce moments of radical and dead polymer chains:

$$\begin{array}{lll}
 \lambda_0 = \sum_{x=1 \rightarrow \infty} R_x & \lambda_1 = \sum_{x=1 \rightarrow \infty} xR_x & \lambda_2 = \sum_{x=1 \rightarrow \infty} x^2 R_x \\
 \mu_0 = \sum_{x=1 \rightarrow \infty} P_x & \mu_1 = \sum_{x=1 \rightarrow \infty} xP_x & \mu_2 = \sum_{x=1 \rightarrow \infty} x^2 P_x
 \end{array}$$

- Here  $R_x$  and  $P_x$  are the mole fractions of radical and polymer with length  $x$  (measured in number of monomers per molecule) respectively.
- The moments are used to reduce the reaction set and compute the product characteristics, such as molecular weight distribution.
- Energy sources are added to represent the heat of the propagation reaction.
- The method of moments is used to derive the molecular weight distribution and polydispersity.
- Six additional scalar transport equations are solved for the moments of radicals and polymers.

# Simplified polymerization process



# Obtaining the product characteristics

- Molecular weight:

- Number averaged:

$$NWD = MW_m \frac{\mu_1}{\mu_0}$$

- Mass averaged:

$$MWD = MW_m \frac{\mu_2}{\mu_1}$$

- Here  $MW_m$  is the molecular weight of the monomer.

- Polydispersity  $Z_p$ : this is the ratio of the mass average molecular weight to the number average molecular weight. It indicates the distribution of individual molecular weights in a batch of polymers.

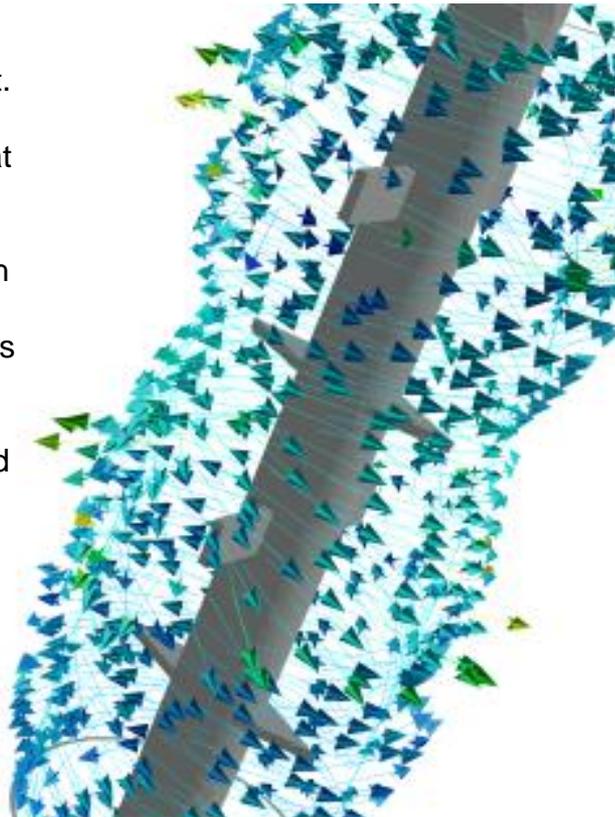
$$Z_p = \frac{\mu_0 \mu_2}{\mu_1^2}$$

- Monomer conversion  $X$ . Here  $Y_M$  and  $Y_{0,M}$  are the final and initial monomer mass fractions respectively.

$$X = 1 - \frac{Y_M}{Y_{0,M}}$$

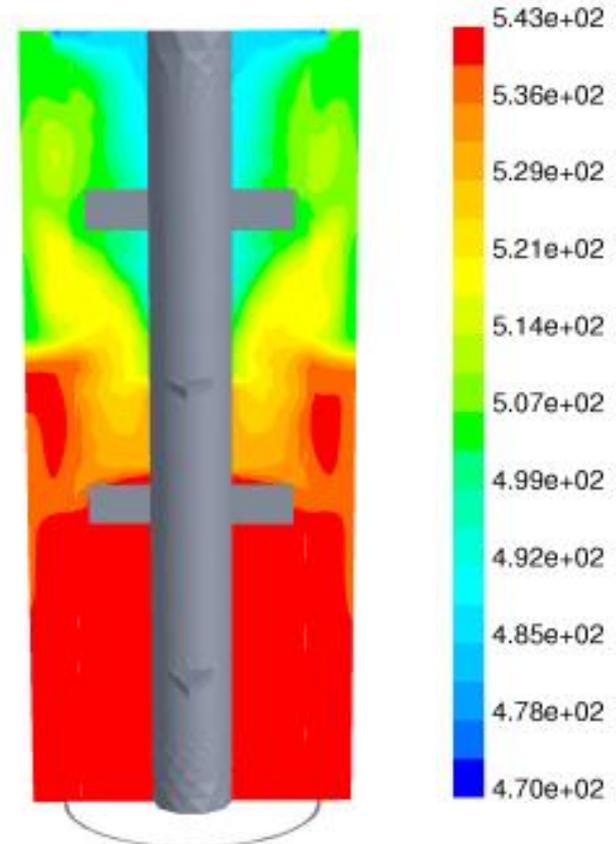
# Autoclave reactor results

- An autoclave reactor is a closed vessel for conducting chemical reactions under high pressure and temperature.
- Flow is from top inlet to bottom outlet.
- Energy sources are added to the energy equation to represent the heat of the propagation reaction.
- The reaction is exothermic, and the heat of reaction is often removed with cooling jackets.
- But in this model, the reactor wall was modeled as adiabatic.
- The temperature ceiling is  $\sim 610$  K, above which ethylene is decomposed via a number of highly exothermic reactions causing thermal runaway.



Velocity vectors

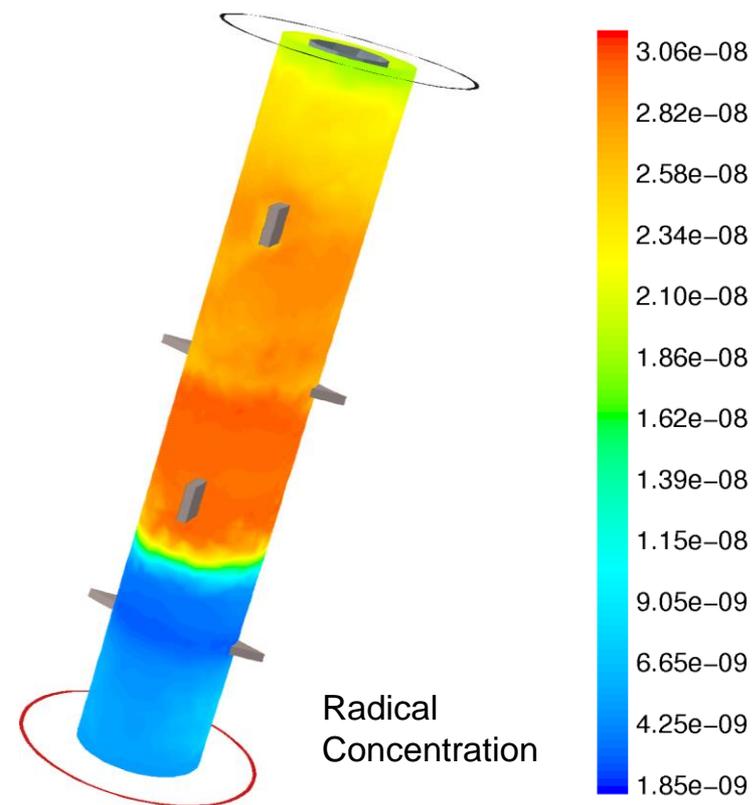
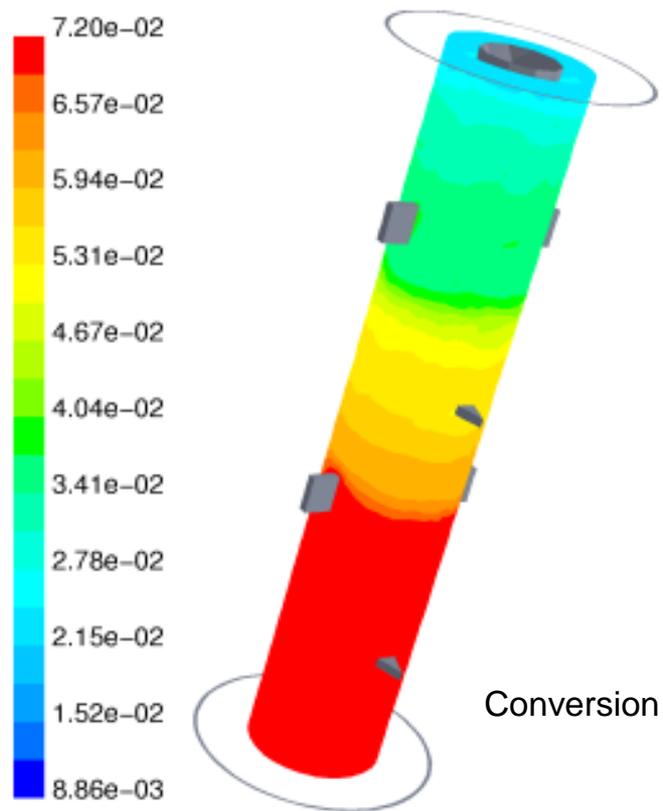
- ✓ Strong swirling due to the lack of baffles



Temperature (K)

- ✓ Maximum temperatures above 610K would cause ethylene decomposition and thermal runaway

# Autoclave reactor results

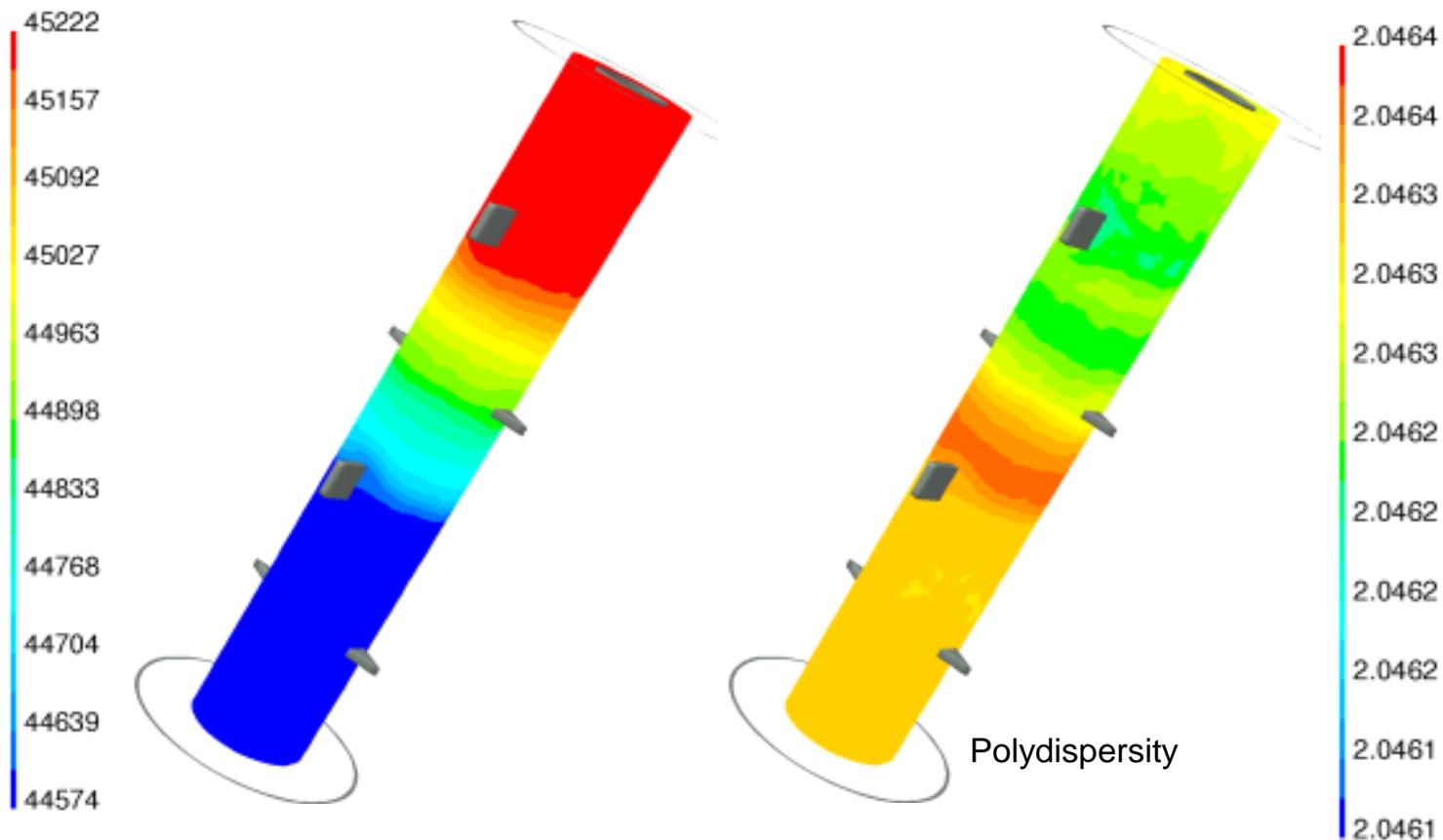


- ✓ A 7.2% conversion achieved
- ✓ Conversion strongly depends on the inlet initiator concentration and inlet temperature
- ✓ For the conversion, a literature reference stated 8% and our results are in good agreement.

- ✓ Radicals are formed in the middle of the reactor by the initiation reaction and consumed to form polymer by the termination reaction

# Autoclave reactor results

- Polymers formed at the top (inlet) of the reactor have larger molecular weights, consistent with literature.
- This is thought to be caused by greater temperature non-uniformity in that region.
- Note that the fact that the molecular weight in the bottom of the reactor is slightly lower does not mean that there is less polymer there.
- The mass fraction of polymer is higher than at the top of the reactor (after all, more material has been converted) just the length is slightly shorter.



✓ Mass averaged molecular weights are from 44574 - 45222

✓ Polydispersity is about 2.046

✓ A uniform distribution indicates a high-quality production of polymers

# Conclusion

- Modeling chemical reaction requires the definition of source terms.
- Reaction kinetics can usually be defined, but not in all systems does the reaction proceed at the kinetic rate.
- Mixing effects can be incorporated into using a variety of models, developed and optimized for particular systems.
- In many cases, one of the following will be necessary:
  - Simplification of the reaction set.
  - Determination of model constants.
  - Implementation of custom source terms or models.

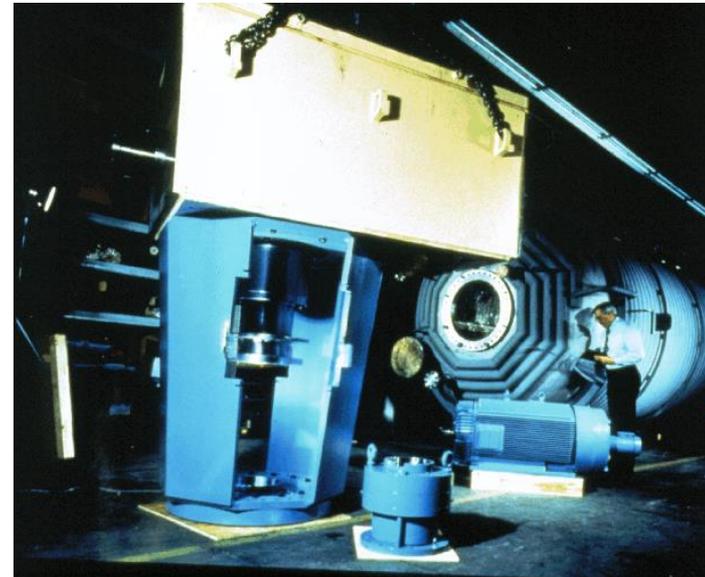
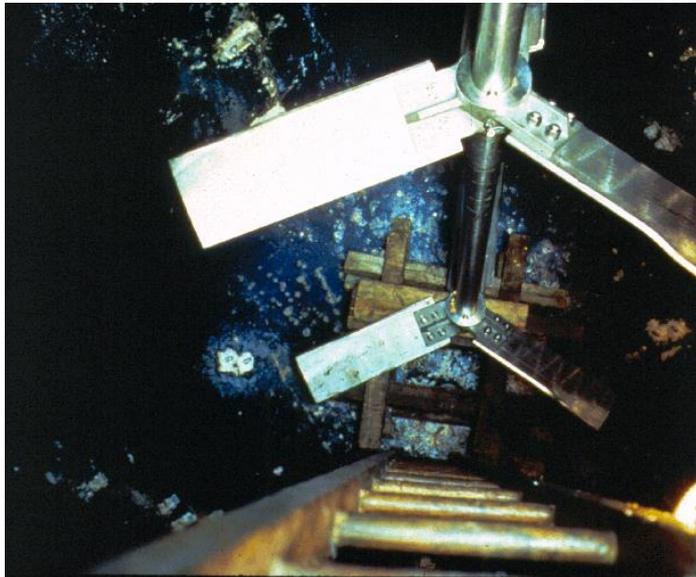
# Fermenter Specific Modeling Topics

## Reacting Flows - Lecture V

André Bakker

# Industrial fermenters

- Industrial fermenters usually consist of stirred vessels with one or more impellers.
- Gas is usually sparged from the bottom (aerobic reactors), and therefore the design of the bottom impeller differs from the upper impellers.
- Cooling coils may be used for temperature control.



# Mixing related design issues

- Agitator selection. Power draw and torque calculations. Mechanical design.
- Blending performance (scale of agitation, turnovers-per-minute, blend time).
- Scale-up and reaction performance (productivity, selectivity).
  - Mixture homogeneity affects selectivity, which determines product composition.
  - High degree of homogeneity required for single-product processes (e.g., most pharmaceuticals, industrial alcohol). High degree of homogeneity not necessarily desirable for products that consist of a complex mixture of chemicals, e.g., flavor dependent food products such as wine and beer).
- Heat removal, temperature field, possible heat damage.
- Solid-liquid mixing (just-suspended speed, settled solids fraction, cloud height).
- Gas-liquid mixing (mass transfer, gas holdup, power factors).
- Surface motion, solids and gas drawdown.
- Shear rates, impact velocities, possible shear damage.
- Optimum feed locations.
- Substrate concentration field, nutrient starvation.
- Oxygen starvation or poisoning (local or global).
- CO<sub>2</sub> or other product poisoning (local or global).
- pH control.



# Empirical mixer design - liquid only

- Typical parameters used are:
  - Power input per unit volume.
  - Power draw is calculated as  $P(W) = P_o \rho(\text{kg/m}^3) N(1/\text{s})^3 D(\text{m})^5$ . Literature correlations for the power number  $P_o$  are available for a variety of impeller styles.
  - Mixing time. For turbulent flow mixing time is inversely proportional to the impeller speed. Correlations for the proportionality constant are available.
  - Reynolds number  $\rho ND^2/\mu$  to determine the flow regime: laminar vs. turbulent.
- Geometrically similar scale-up:
  - Froude number  $N^2D/g$  to scale up at equal surface motion.
  - Constant impeller tip speed  $\pi ND$  to scale up at equal liquid velocities.
  - Constant impeller speed  $N$  to scale up at equal average shear rate.
- Scale-up with non-geometric similarity: keep most important hydrodynamic and process conditions similar. Need to be able to determine what those are. Shear rates? Turbulence?

# Empirical mixing design - multiphase

- Liquid-solid systems:
  - Correlations for just-suspended speed. Large variability. Often necessary to determine model constants for given system empirically.
  - Minimal data for solids distribution.
- Gas-liquid systems:
  - Correlations for gassed power draw, mass transfer rates, flow regime (dispersing or flooded), for the most commonly used impeller styles.
- Liquid-liquid:
  - Some power draw and impeller speed-based correlations for droplet size available.

# Fermenter models

- Single node models.
  - Typically, the reactor performance is predicted by solving a set of ODE's for one node.
  - Model may assume perfect mixing or take some hydrodynamics into account.
- Networks of zones models.
  - The reactor is divided into a relatively small number of zones with user-defined exchange flows, the effect of which is added to the ODE's.
- CFD models.
  - Hydrodynamics only.
  - Full modeling.

# Fermenter modeling issues

- Anaerobic fermenters:
  - Flow field: laminar vs. turbulent, and Newtonian vs. non-Newtonian.
  - Rotating impellers.
  - Batch vs. continuous.
  - Liquid phase blending.
  - Reaction modeling.
  - Multiphase flow: solid suspension and CO<sub>2</sub>.
- Aerobic fermenters have the following additional modeling issues:
  - Multiphase flow: gas-liquid, or three-phase.
  - Mass transfer between the phases.
  - Degassing.

# CFD models of fermenters

- In principle, full fermenter models can be created:
  - Flow and turbulence.
  - Multiphase flow and mass transfer.
  - Fermentation kinetics and species concentrations.
  - ... and more ... anything for which equations are known can be included in the CFD model!
- In practice, the following hurdles are encountered:
  - Full models require long calculation times.
  - Not all equations and interactions are fully described.

# Anaerobic fermenters

- Anaerobic fermenters have single-phase flow, or possibly suspended solids.
- Single-phase fermentation:
  - Modeling is relatively straightforward.
  - Flow field, impeller motion, species transport all modeled as other reacting flow problems.
  - Main difference: formulation of reaction kinetics.
  - Molecular reaction rates usually formulated as:

$$\hat{R}_{i,r} \propto \prod_{j=1}^{N_r} [C_{j,r}]^{\eta'_{j,r}}$$

- Fermentation kinetics are usually formulated differently.

# Fermentation kinetics example

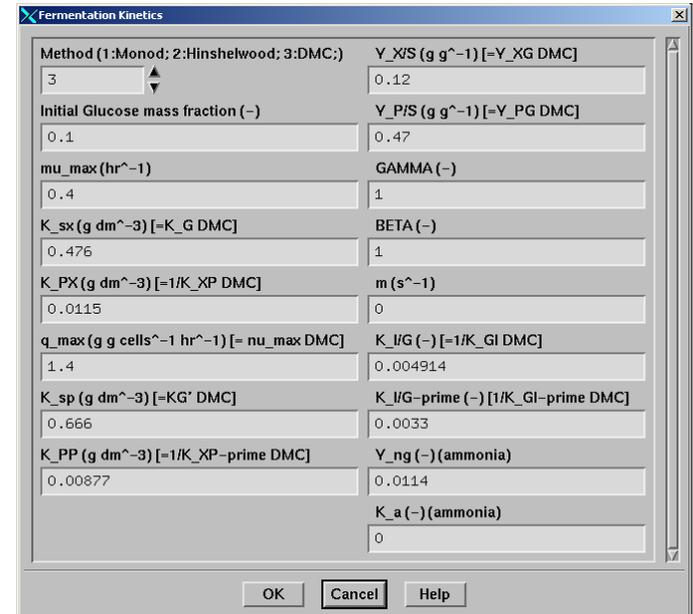
- Anaerobic yeast fermentations to produce ethanol.
  - Widely studied and reasonably well defined.
- Equations for substrate, product, cell density:

$$r_X = \frac{Xc \times \mu_{\max} \times G}{K_G + G + \frac{G^2}{K_{G/I}}} \times \left\{ 1 - \left( \frac{P}{K_{X/P}} \right)^\beta \right\}$$

$$r_p = \frac{Xc \times v_{\max} \times G}{K_G' + G + \frac{G^2}{K_{G/I}'}} \times \left\{ 1 - \left( \frac{P}{K_{X/P}'} \right)^\gamma \right\}$$

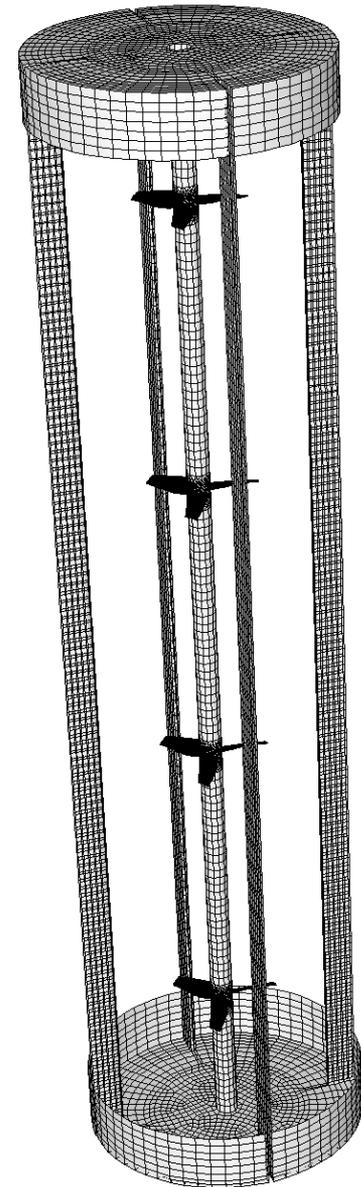
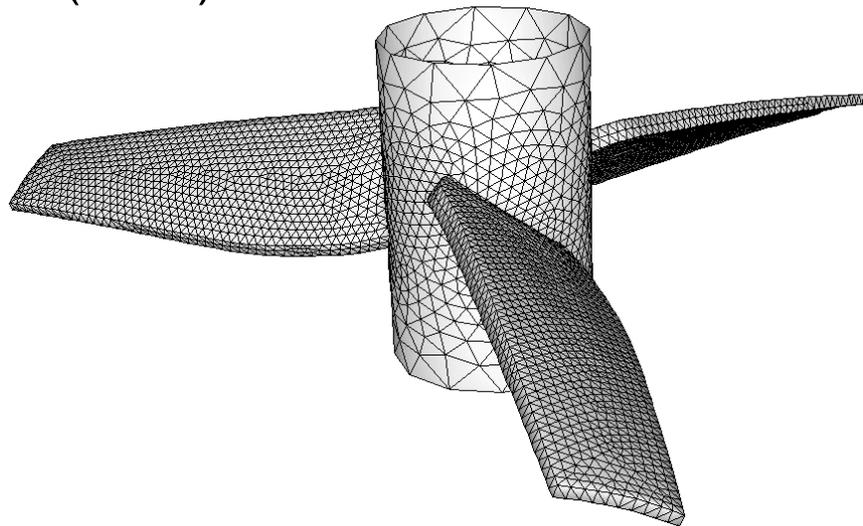
$$r_G = \frac{-r_X}{Y_{X/G}}$$

- Implemented in FLUENT with UDFs.
- SCHEME functions for GUI inputs of model constants.

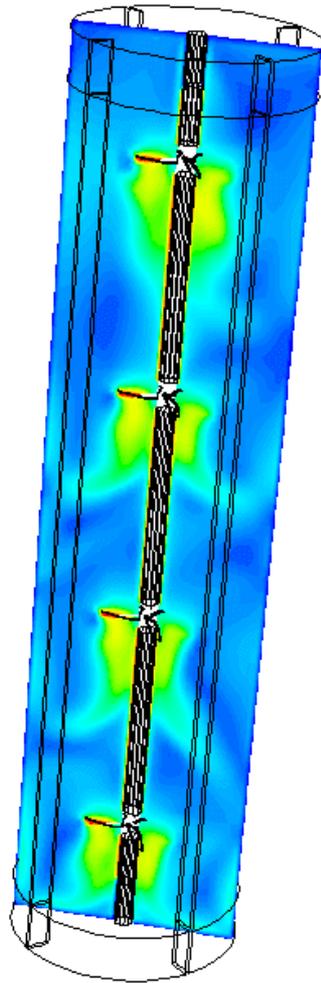
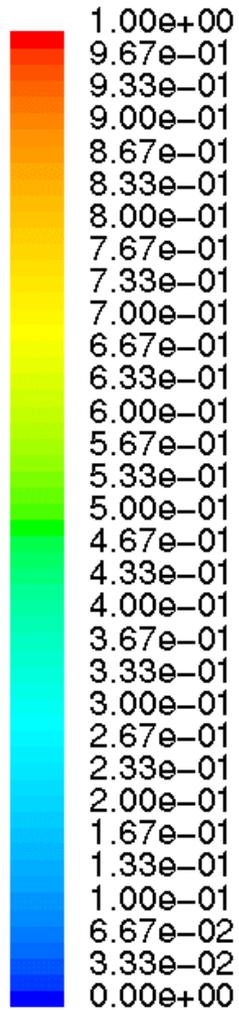


# Full scale batch test case

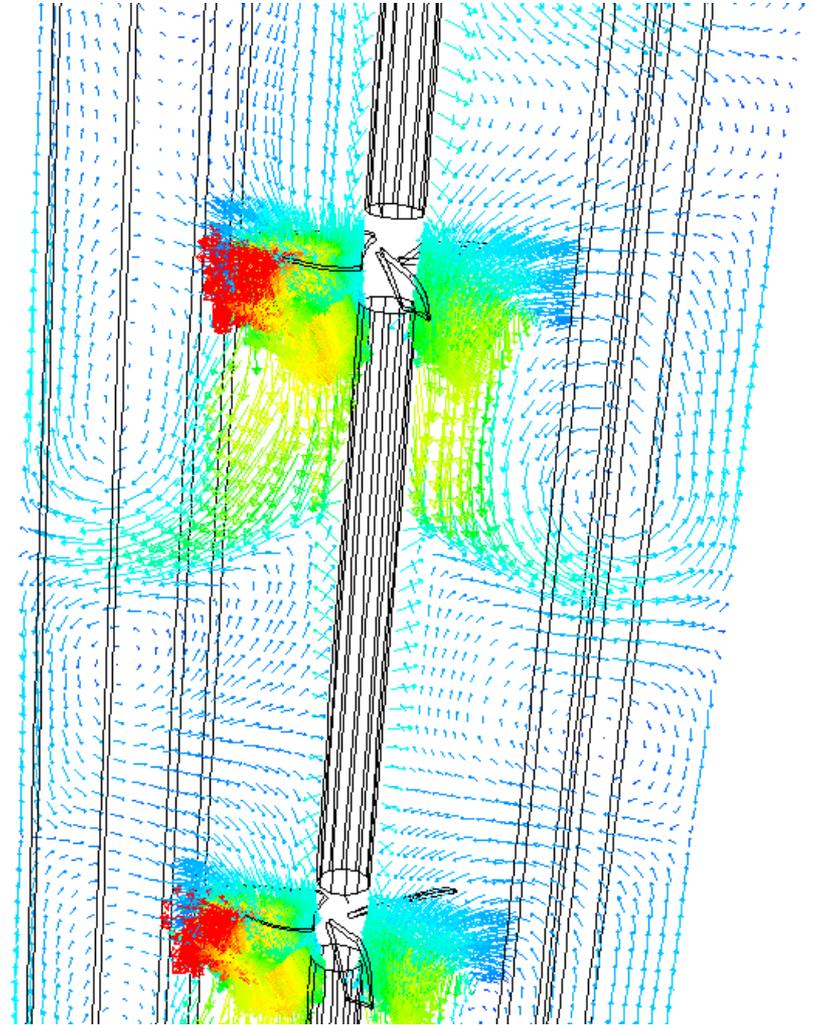
- This example shows high aspect ratio 10 m<sup>3</sup> fermenter equipped with four axial flow impellers (Lightnin A310).
- The system is modeled using a mesh with 433,000 computational cells.
- The flow induced by the impellers is modeled using the multiple-reference frame (MRF) model.



# Flow field



Velocity Magnitude (m/s)

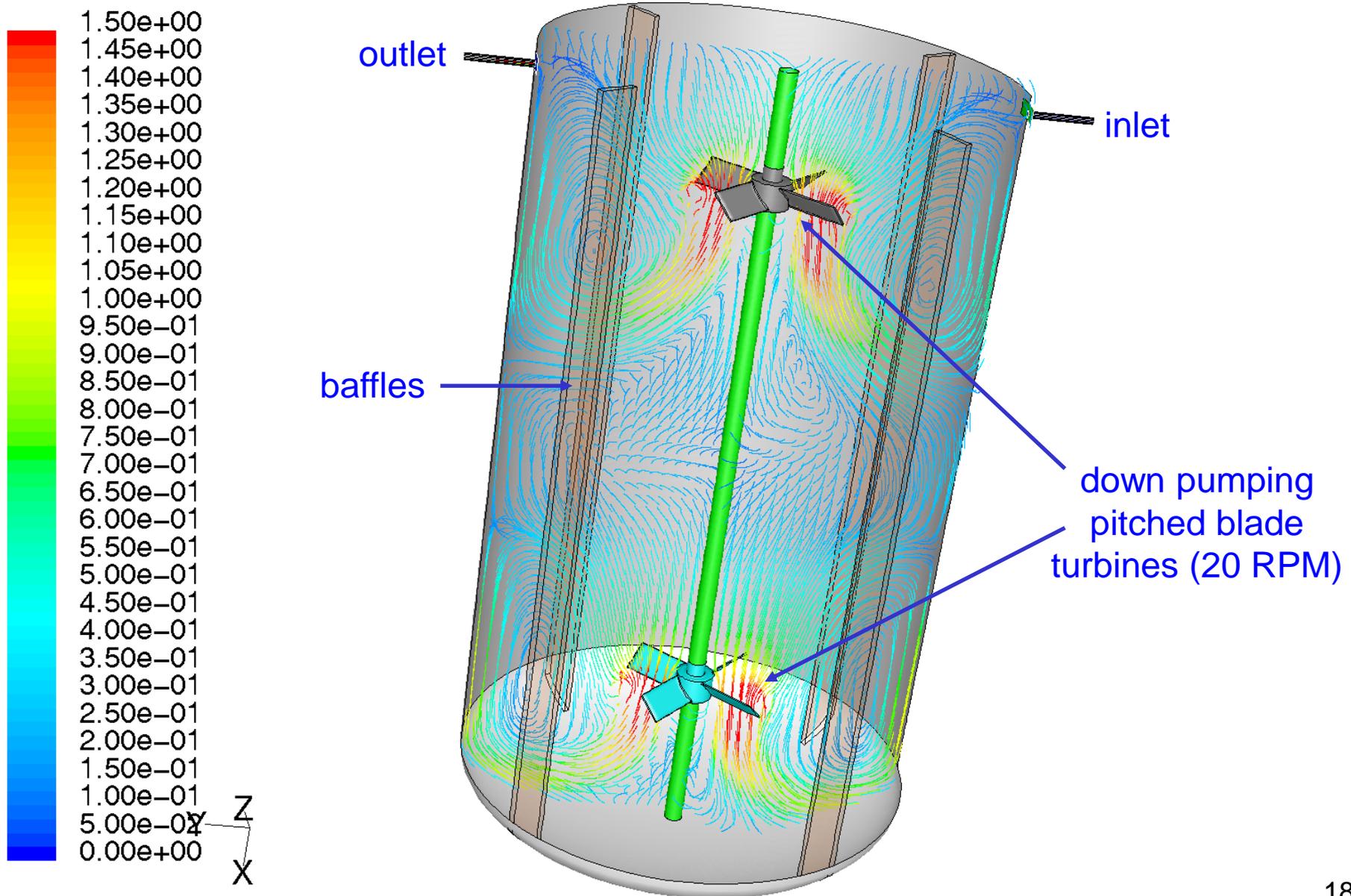


Velocity Vectors

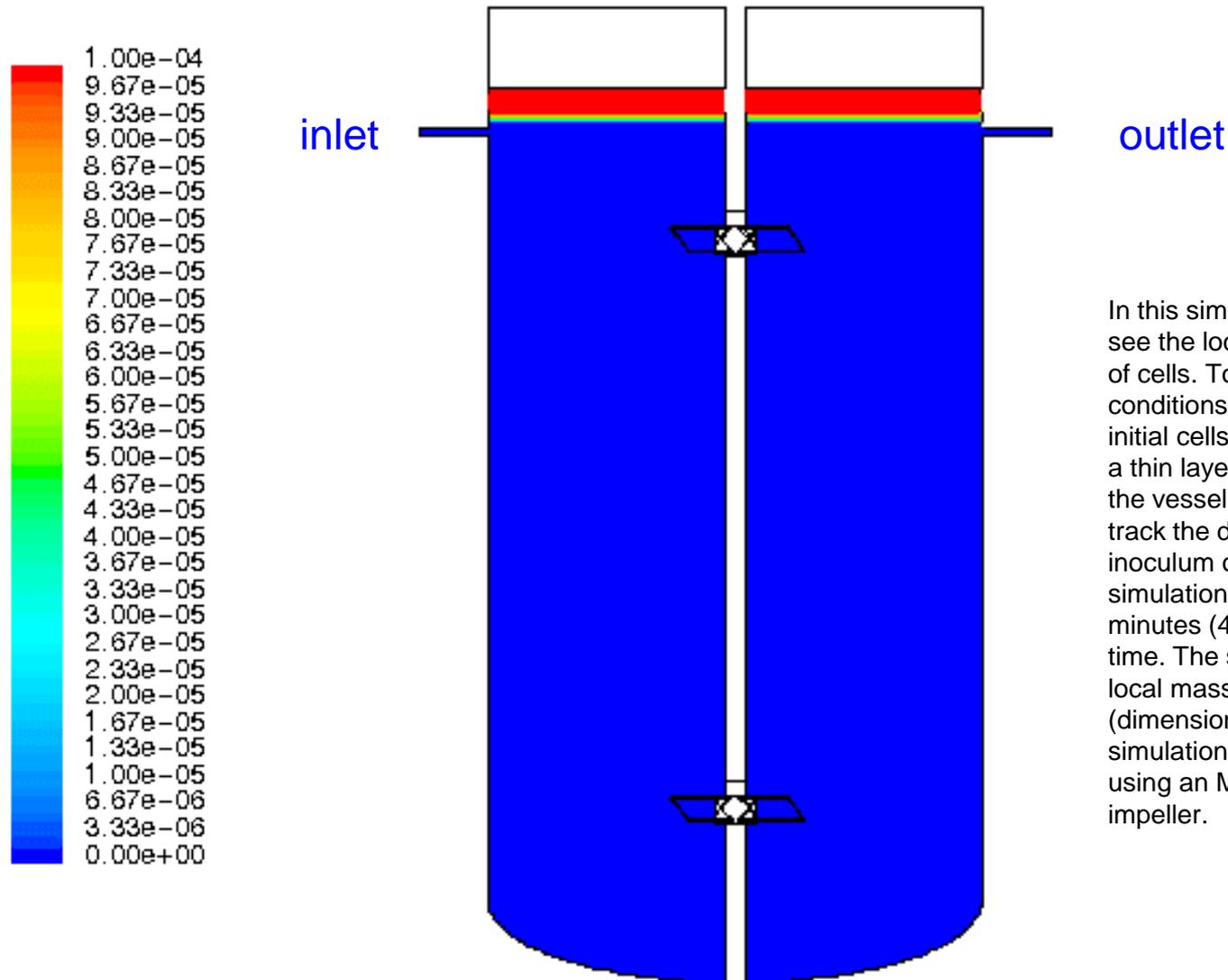
# Large scale fermenter

- 500,000 gallon (1900 m<sup>3</sup>) fermenter.
- Diameter of 36 ft (10.8 m).
- Aspect ratio 1:2.
- Residence time 18 hours.
- Stirred by two pitched blade turbines.
- Impeller diameter 12 ft.
- 20 RPM.
- Impeller power input predicted by CFD model is 54kW. Would require minimum of 100HP motor.

# Large scale fermenter

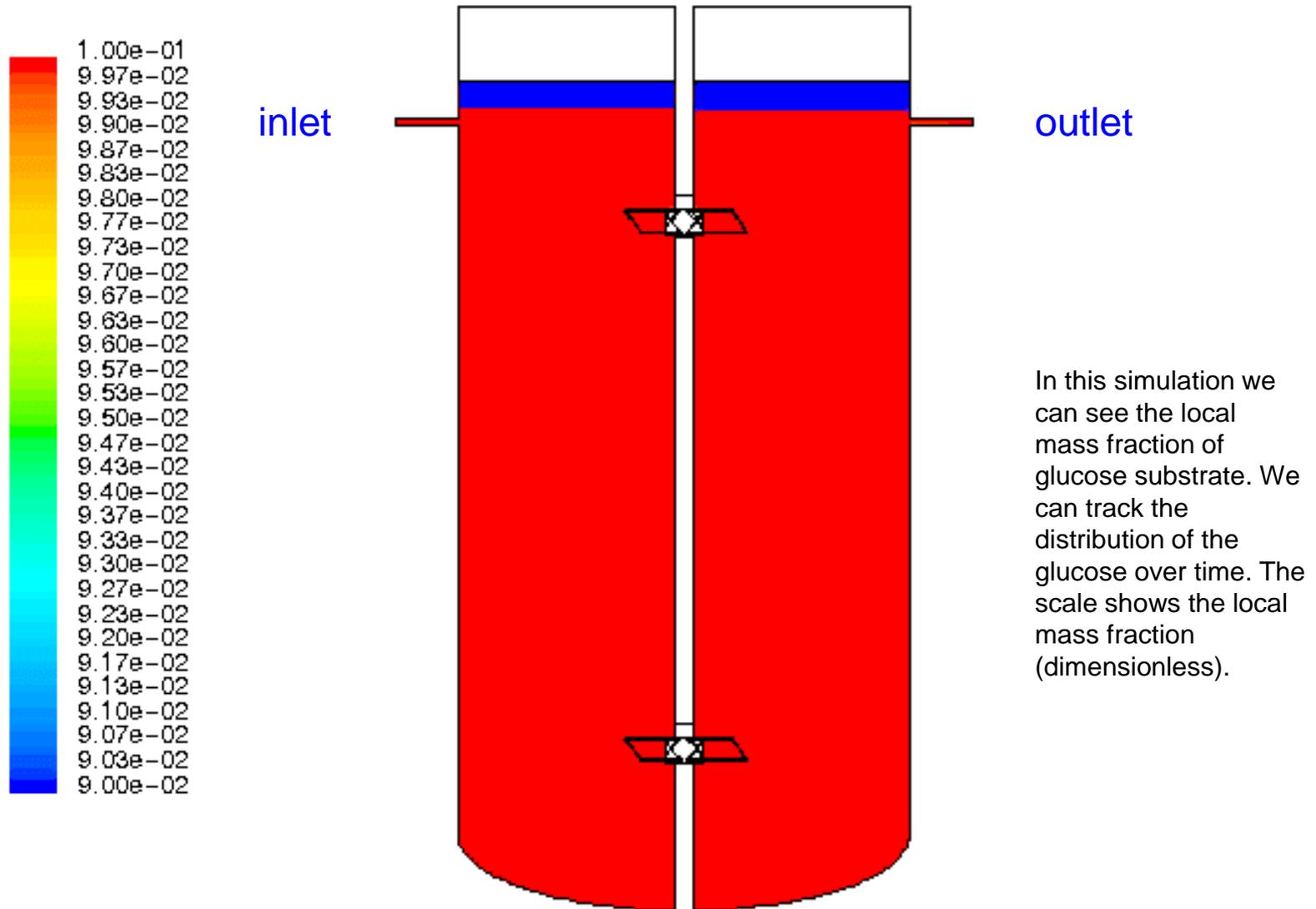


# Mass fraction of cells – initial condition

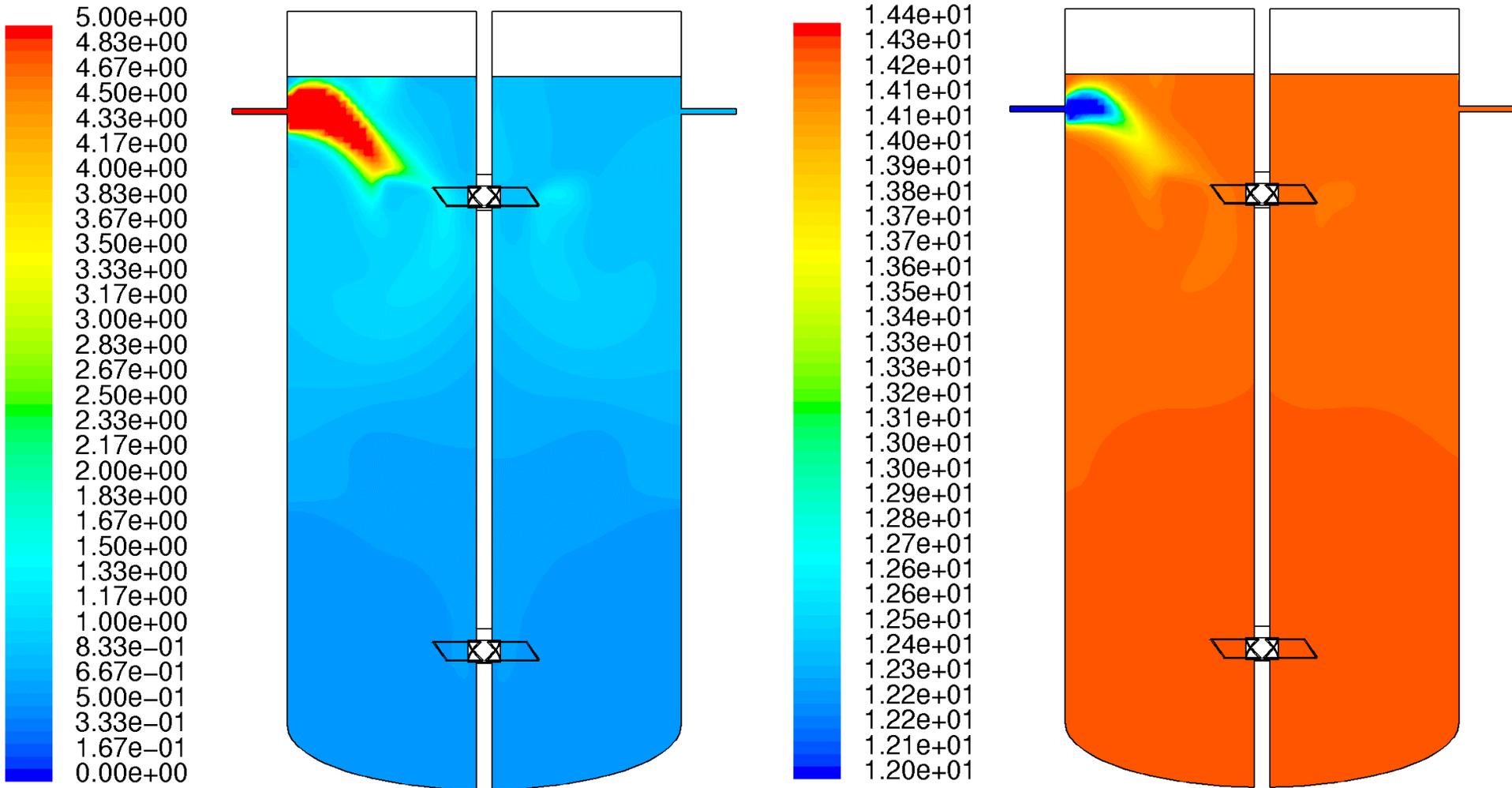


In this simulation we can see the local mass fraction of cells. To model startup conditions, we place the initial cells, the inoculum, in a thin layer on the top of the vessel. We can then track the distribution of the inoculum over time. The simulation covers seven minutes (420 seconds) real time. The scale shows the local mass fraction (dimensionless). The simulation was performed using an MRF model for the impeller.

# Mass fraction of glucose – initial condition

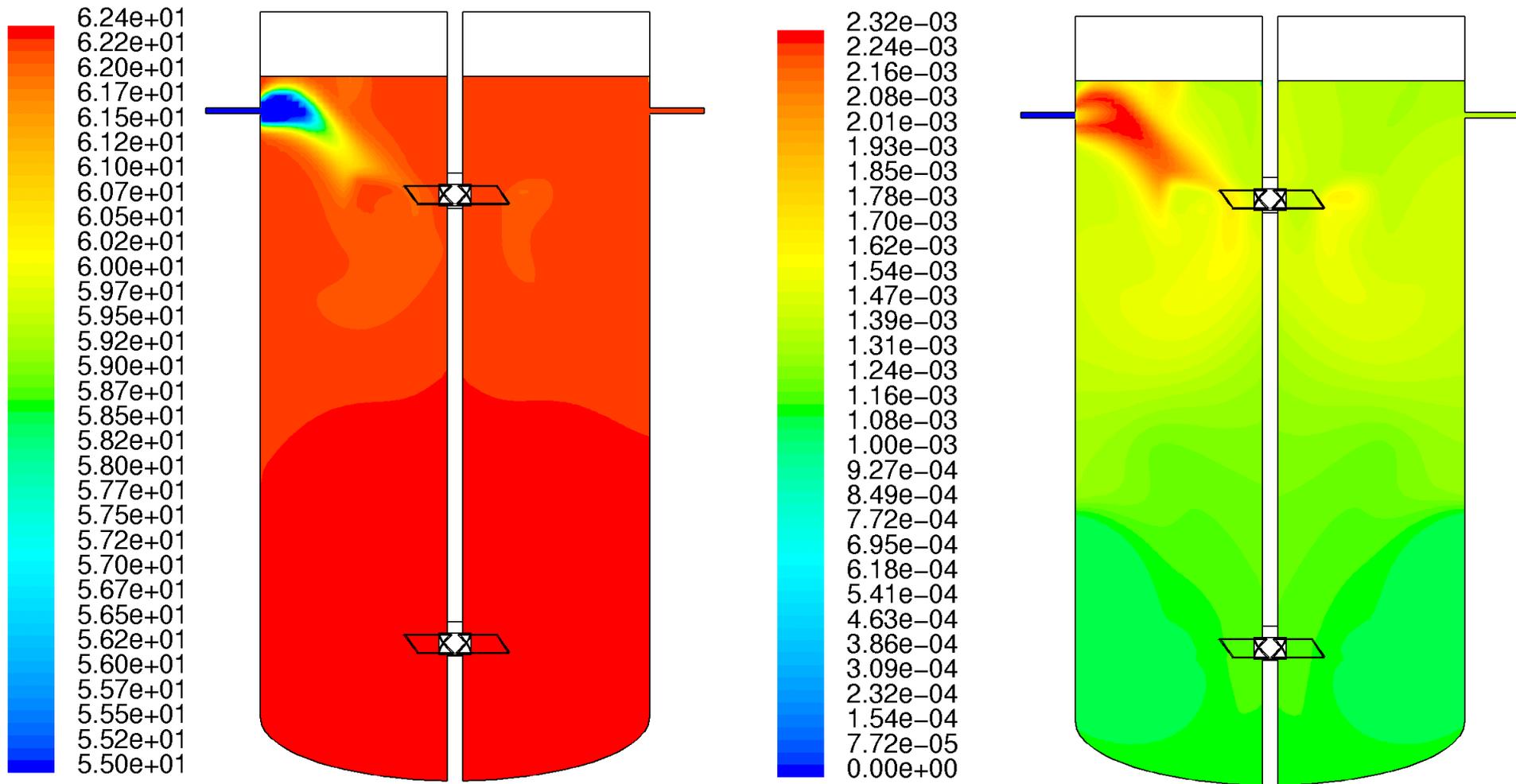


# Final glucose and cell concentration



Here we see the final glucose (left) and cell concentrations (right). The concentrations are in g/L. A plume forms at the inlet, with locally high glucose and low cell concentrations.

# Ethanol concentration and production rate



We see similar plumes form for the ethanol concentration (left) and the ethanol production rate (right). Concentration is in g/L and production rate in g/L/s. You can see that there is at least a factor of two difference in the ethanol production rate in the vessel.

# What about solids?

- Solids can be handled in one of the following ways:
  1. Settling velocity of the solids is negligible: model as a dissolved species. Use an effective viscosity for the slurry, e.g.:

$$\mu_{\text{slurry}} = \mu_{\text{liquid}} \frac{1 + 8.203 x^5}{1 - 2.478 x + 18.456 x^5 - 20.326 x^6}$$

$x = \text{volume fraction solids}$

Kawase and Ulbrecht. Chem.Eng.Comm. Vol. 20, pp. 127-136 (1983)

2. Settling velocity of the solids is low: use the Mixture model. This is a multiphase flow model with one set of shared momentum equations for all phases.
3. Fast settling solids with significant segregation: Eulerian granular model with separate momentum equations for each phase.

# Effective diameter of solid particles

- Solid particles do not usually all have the same size.
- The mass weighted average diameter  $d_{43}$  is best used as the effective diameter of the solids:

$$d_{43} = \frac{\sum_i d_i^4}{\sum_i d_i^3}$$

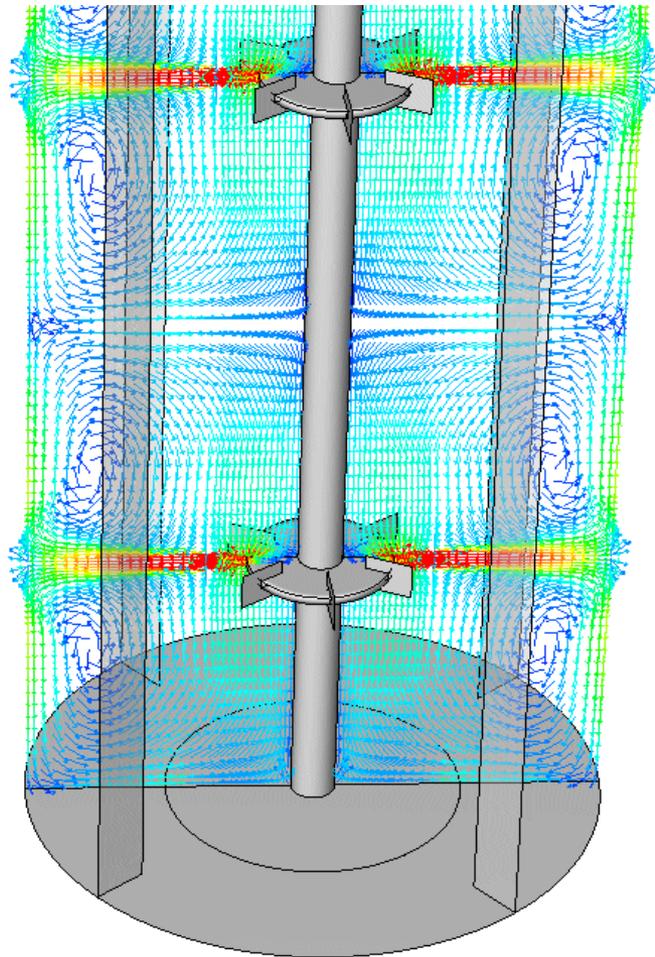
Here  $d_i$  denotes the diameter of particle  $i$ . The sums are over all particles  $i$ .

- If a particle weight distribution is known, the same can be approximated as:

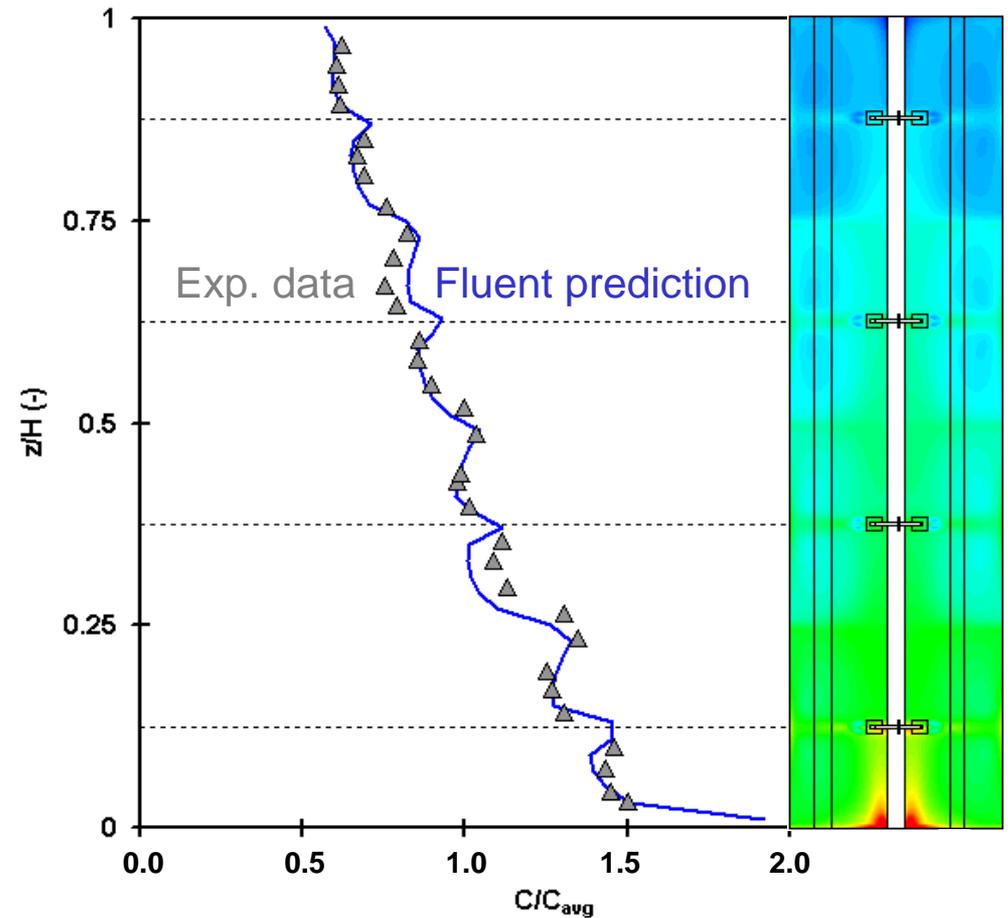
$$d_{43} = \frac{\sum_j M_j d_j^4}{\sum_j M_j d_j^3}$$

With  $M_j$  being the mass of particles in size group  $d_j$ .

# Solids suspension - validation



Color indicates velocity magnitude



Color indicates solids volume fraction

Experimental data for multiple Rushton turbine system are courtesy of University of Bologna: D. Pinelli, M. Nocentini and F. Magelli. *Solids Distribution In Stirred Slurry Reactors: Influence Of Some Mixer Configurations And Limits To The Applicability Of A Simple Model For Predictions*. Chem. Eng. Comm., 2001, Vol. 00, Pp. 1-18.

# Aerobic fermenters

- The sparged gas requires multiphase flow modeling.
  - Usually done with either an Eulerian multiphase flow model or the Mixture model.
  - CPU time intensive transient models required.
  - Degassing requires inclusion of the headspace above the liquid.
  - Mass transfer between phases usually requires UDFs.
- Bubble size can be treated as follows:
  - Calculate using scalar equations using method of moments.
  - Calculate a size distribution.
  - Use a single effective diameter.

# Estimating local $k_l a$

- Both  $k_l$  and  $a$  can be calculated from the local flow conditions.
- Local  $k_l$  is calculated from the turbulence intensity, e.g.:

$$k_l = 0.301 (\varepsilon \nu)^{1/4} \text{Sc}^{-1/2}$$

Kawase and Moo-Young (1990) Chem.Eng.J. **43**, B19-B41.

- Here  $\varepsilon$  is the turbulent dissipation rate,  $\nu$  is the liquid kinematic viscosity, and Sc is the Schmidt number ( $\nu$  over the diffusion coefficient).
- Presence of chemicals, such as oils, will affect  $k_l$ . Verify that your system matches the system described in the literature source.
- The interfacial area  $a$  is calculated from the volume fraction of gas and the bubble size:

$$a = \frac{6\phi}{d_b}$$

- The local volume fraction of gas  $\phi$  is calculated by the multiphase flow model.

# Estimating the average bubble diameter

- One method to estimate the average bubble diameter is from literature correlations for the bubble diameter.
- A commonly cited correlation is:

$$d_b = 4.15 \left[ \frac{\sigma^{0.6}}{(P/V)^{0.4} \rho^{0.2}} \right] \phi^{0.5} \left( \frac{\mu_{gas}}{\mu_{liquid}} \right)^{0.25} + 0.0009$$

Calderbank (1958) *TransIChemE*, **36**, 443.

- Later work (e.g., Sridhar and Potter, *Chem.Eng.Sci.* 35, 683, 1980) resulted in enhanced versions of this correlation taking into account gas-liquid density ratio and sparged gas power input.
- As always review source to make sure that your system falls within the range studied for which the correlation was developed.

# Estimating the effective bubble diameter

- Another method is to estimate bubble diameter from the volume fraction of gas  $\phi$  and the mass transfer coefficient  $k_l a$ .
- These can also be estimated from correlations, e.g.:

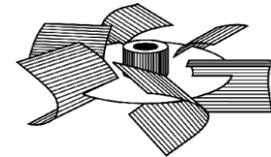
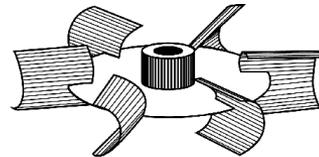
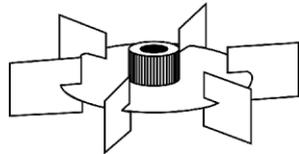
$$\phi \propto v_{sg}^{\alpha} (P/V)^{\beta}$$

$$k_l a \propto v_{sg}^{\gamma} (P/V)^{\kappa}$$

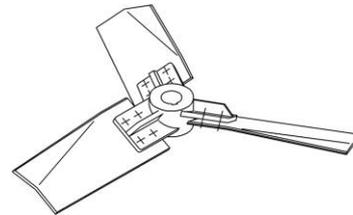
- The superficial gas velocity is defined as  $v_{sg} = 4Q_g(\text{m}^3/\text{s})/(\pi T(\text{m})^2)$ .
- With previous relationship for  $k_l$  and  $d_b = 6\phi/a$  this gives sufficient information to estimate  $d_b$ .
- See literature, e.g., the mixing handbook or Tatterson (*Fluid Mixing and Gas Dispersion in Agitated Tanks*, McGraw-Hill, 1991) for model constants or more references.
  - Note that many correlations are for air-water!
  - Presence of chemicals, e.g., salts or anti-foam will affect gas holdup and mass transfer coefficient. Use correct model constants!

# Impellers used in gas-liquid mixing

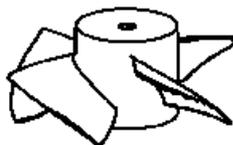
- Radial pumping gas dispersion impellers:  
D-6 (Rushton), CD-6 (Concave blade), BT-6.



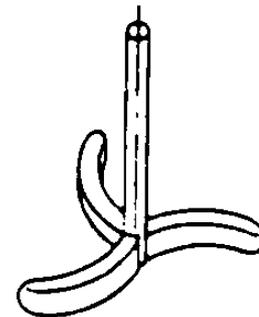
- Axial pumping impellers (lower shear, high flow):  
– HE-3 (narrow blade hydrofoil).



- Maxflo-T (wide blade hydrofoil).

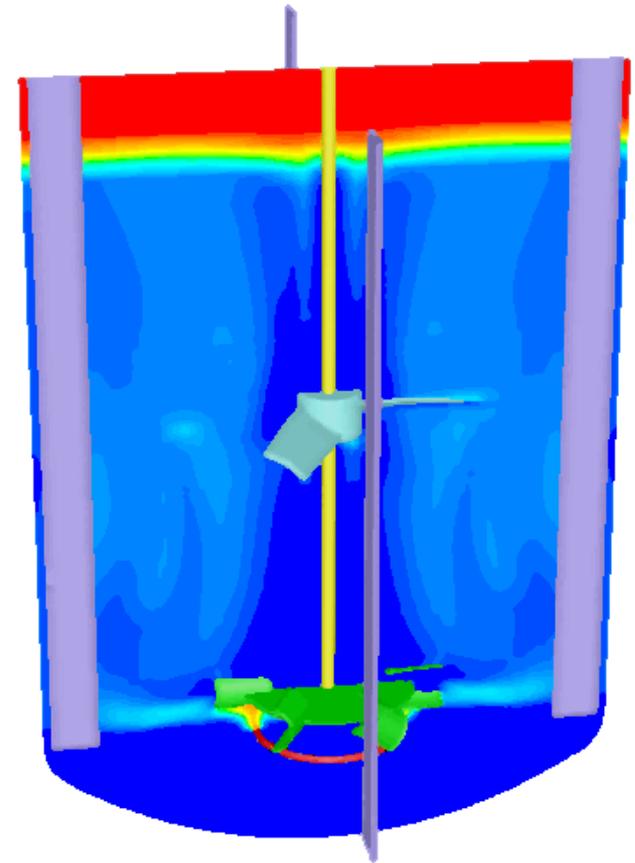
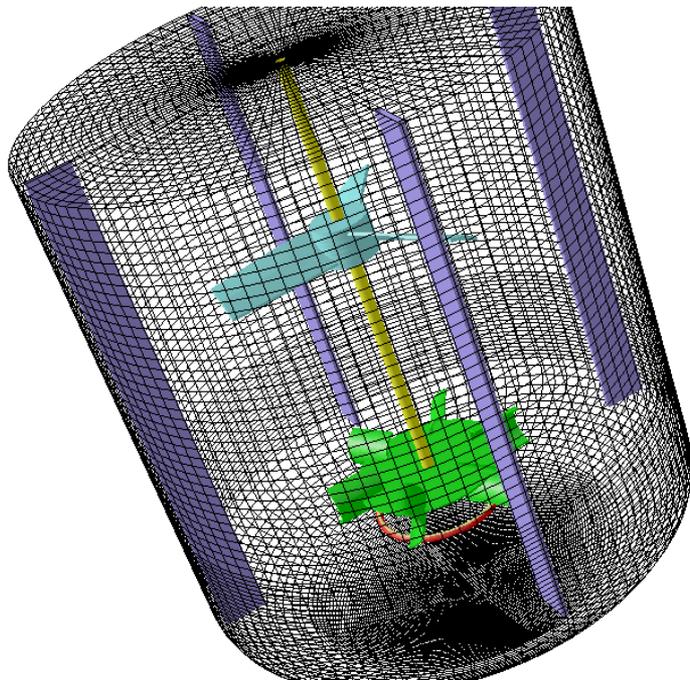


- Pfaudler Retreat Blade: glass lined < 40 m



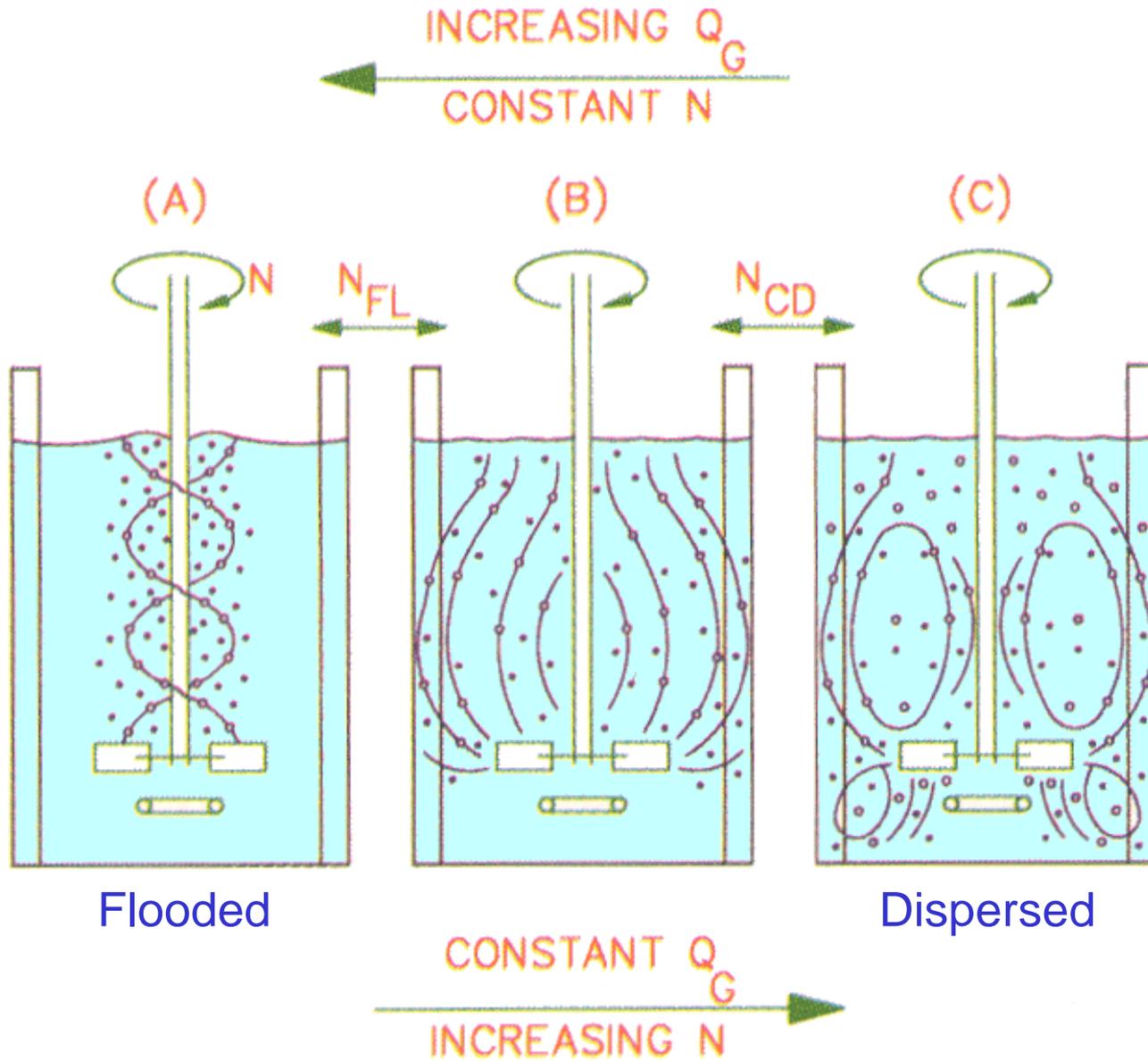
# Example - gas-liquid mixing vessel

- Combinations of multiple impeller types used.
- Bottom radial flow turbine disperses the gas.
- Top hydrofoil impeller provides good blending performance in tall vessels.



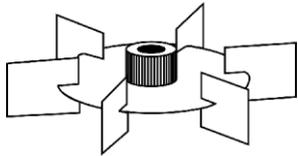
Eulerian gas-liquid simulation  
Color indicates gas fraction

# Gas-liquid flow regimes

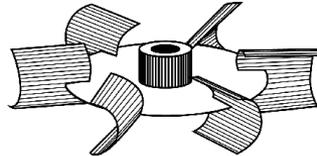


# Impeller performance

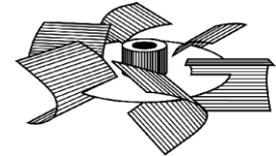
- Example: gas dispersion retrofit comparison.
- Gas flow rate 13 vvm ( $v_{sg}=0.1\text{m/s}$ ).



Rushton

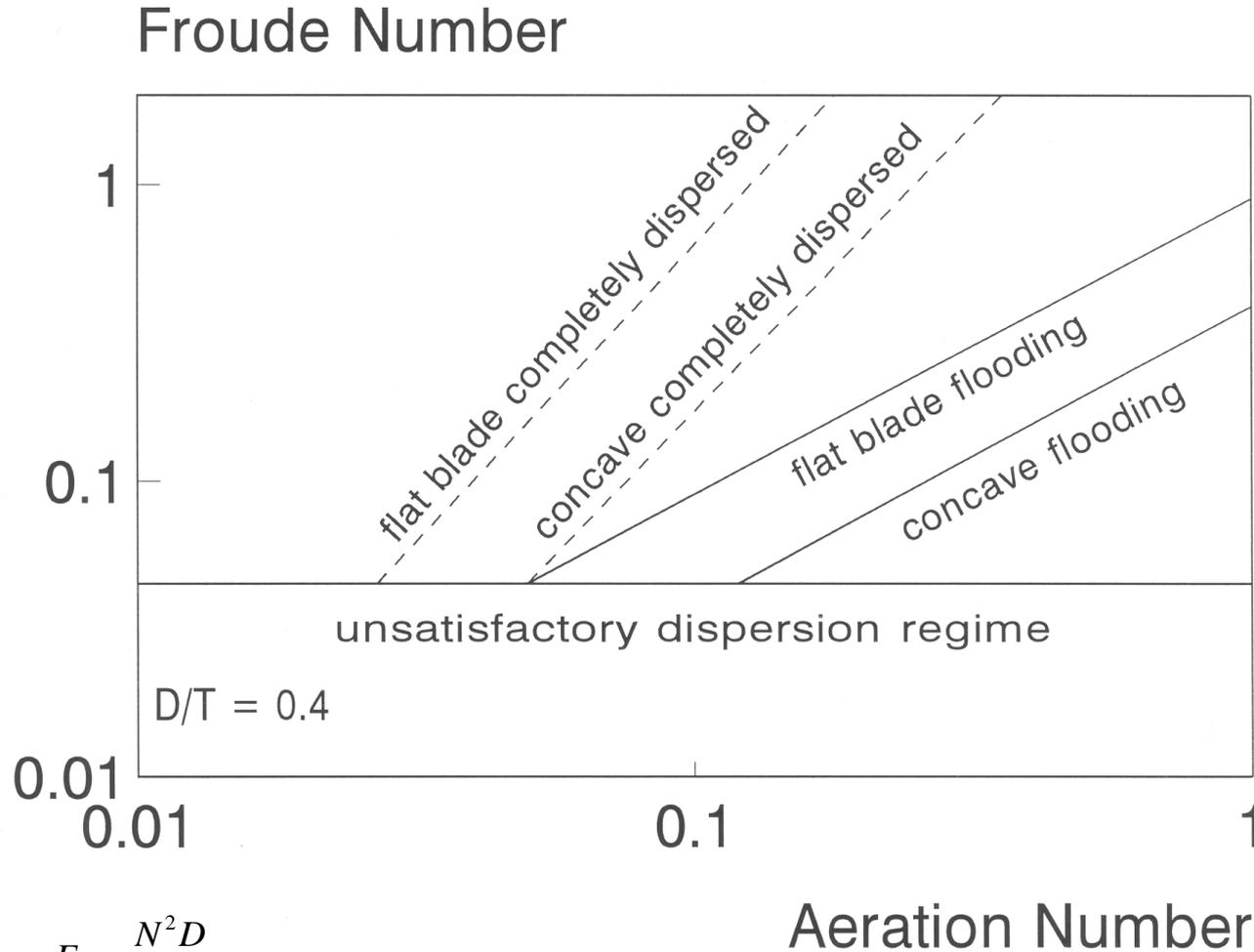


CD-6



BT-6

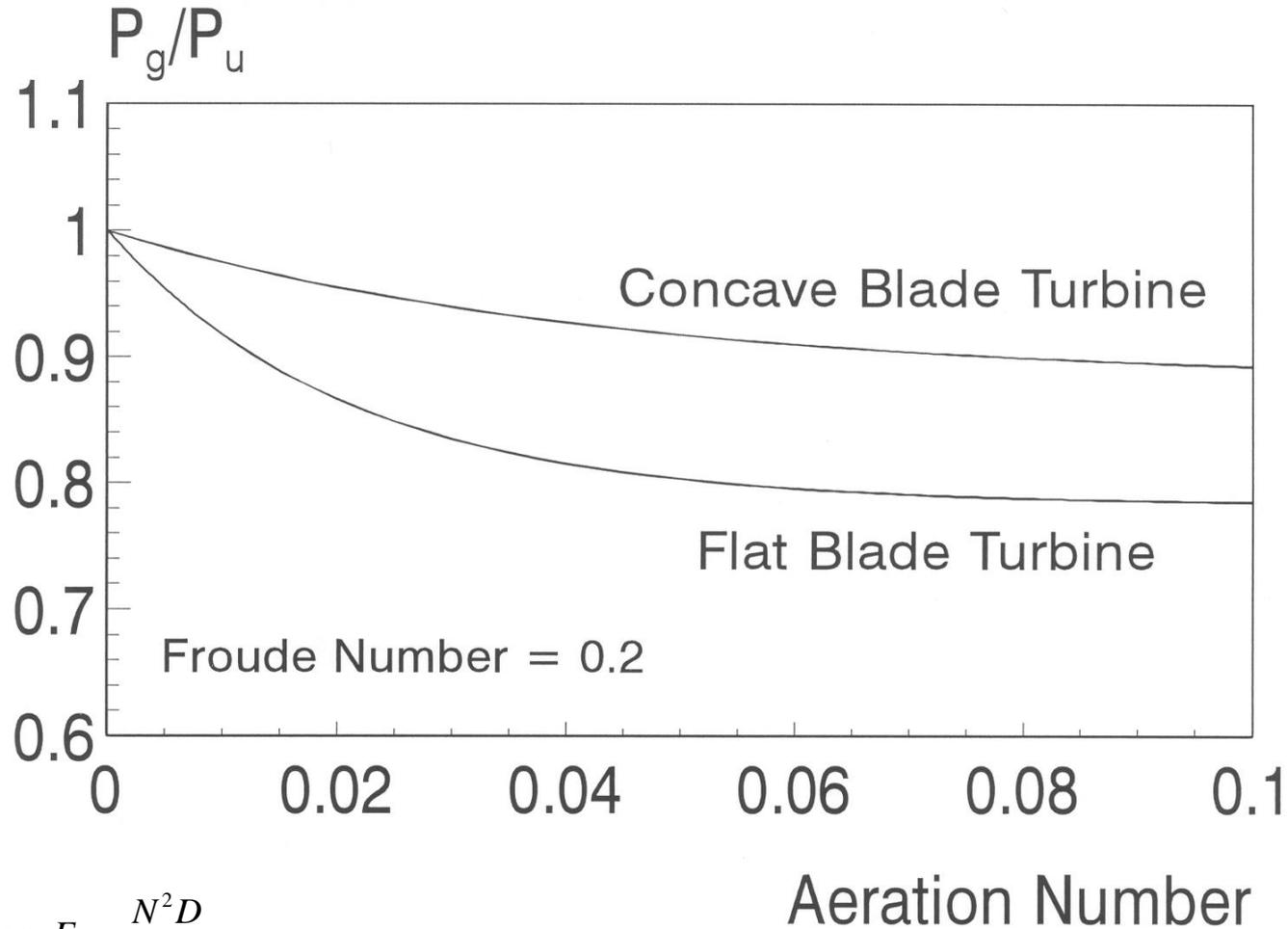
# Flow regime comparison D-6 and CD-6



Froude number:  $Fr = \frac{N^2 D}{g}$

Aeration number:  $Fl_g = N_A = \frac{Q_g}{N D^3}$

# Ratio gassed to ungassed power draw



Froude number:  $Fr = \frac{N^2 D}{g}$

Aeration number:  $Fl_g = N_A = \frac{Q_g}{N D^3}$

# Aerobic fermenter modeling

- Gas-liquid multiphase flow.
- Full Eulerian multiphase flow modeling:
  - Used to model droplets or bubbles of secondary phase(s) dispersed in continuous fluid phase (primary phase).
  - Allows for mixing and separation of phases.
  - Solves momentum, enthalpy, and continuity equations for each phase and tracks volume fractions.
- Impellers can be modeled transient using the sliding mesh method.
- Key design parameters are gas holdup and mass transfer coefficient  $k_L a$ .

# Volume fraction

- Eulerian multiphase model.
- Volume fraction:

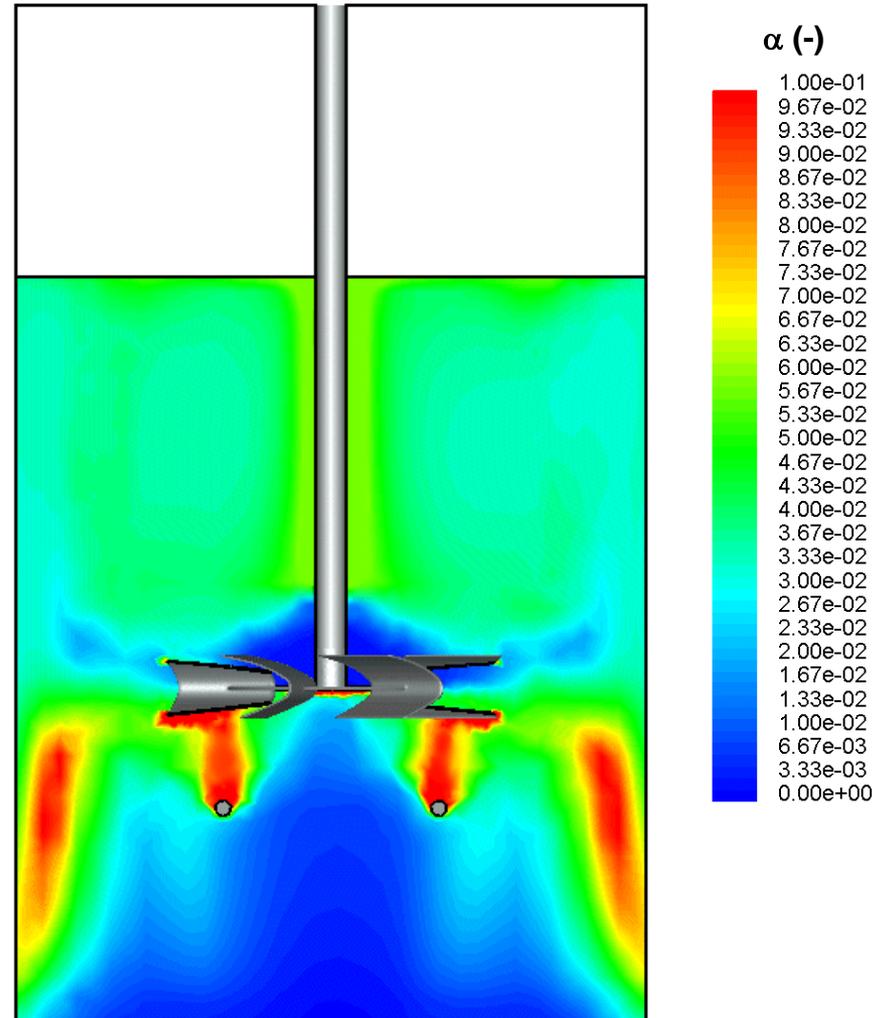
$$\frac{\partial}{\partial t} (\bar{\alpha}_c \rho_c) + \nabla \cdot (\bar{\alpha}_c \rho_c \tilde{U}_c) = S_{\alpha c}$$

- Momentum balance:

$$\frac{\partial}{\partial t} (\bar{\alpha}_c \rho_c \tilde{U}_c) + \nabla \cdot (\bar{\alpha}_c \rho_c \tilde{U}_c \otimes \tilde{U}_c) = -\bar{\alpha}_c \nabla \tilde{p} + \nabla \cdot \tilde{\tau}_c^t + F_{Dc}$$

- Drag forces:

$$F_{Dc} = K_{dc} \left[ (\tilde{U}_d - \tilde{U}_c) - \left( \frac{\overline{\alpha_d u'_d}}{\bar{\alpha}_d} - \frac{\overline{\alpha_c u'_c}}{\bar{\alpha}_c} \right) \right]$$



# Volume fraction

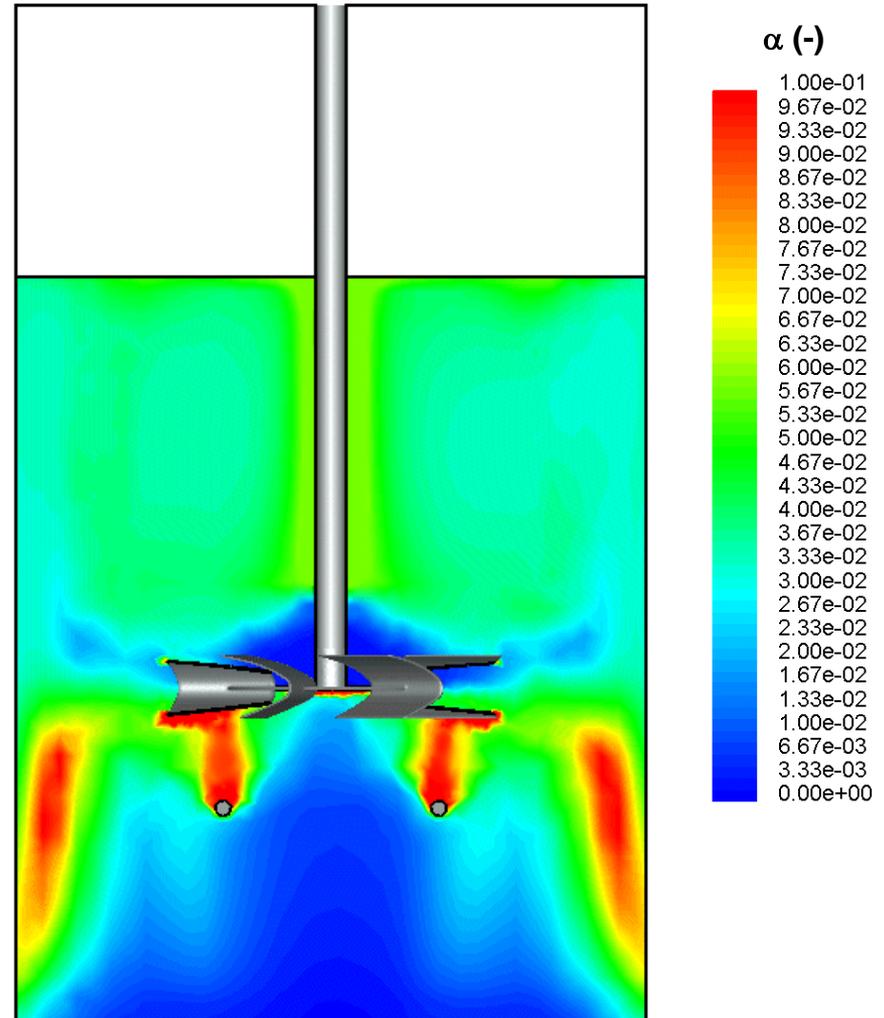
- Using an Eulerian multiphase flow model, we solve a transport equation for the gas fraction. From left to right, the rate of change term plus the convective transport of the phase, equals the phase source term. The tilde over the velocity symbol  $U$  indicates a phase-averaged velocity approach.

$$\frac{\partial}{\partial t} (\bar{\alpha}_c \rho_c) + \nabla \cdot (\bar{\alpha}_c \rho_c \tilde{U}_c) = S_{\alpha c}$$

- In the momentum equation, we have from left to right the rate of change plus the convective momentum transport equaling momentum transport due to the pressure forces, shear forces, and momentum exchange terms including the drag force.

$$\frac{\partial}{\partial t} (\bar{\alpha}_c \rho_c \tilde{U}_c) + \nabla \cdot (\bar{\alpha}_c \rho_c \tilde{U}_c \otimes \tilde{U}_c) = -\bar{\alpha}_c \nabla \tilde{p} + \nabla \cdot \tilde{\tau}_c^t + F_{Dc}$$

- The figure shows the local gas-holdup in a 3-D vessel equipped with a radial pumping BT-6 impeller. The two grey circles below the impeller show the cross section of the ring-sparger. This is where the gas enters the vessel. The gas escapes into the open headspace above the liquid surface. The gas holdup in a cross section in between the baffles is shown. The highest gas volume fractions (denoted by the symbol  $\alpha$ ) are found in the sparger outflow and also near the vessel wall, in the lower circulation loop. In that region the gas and liquid are in counterflow, resulting in higher gas volume fractions.

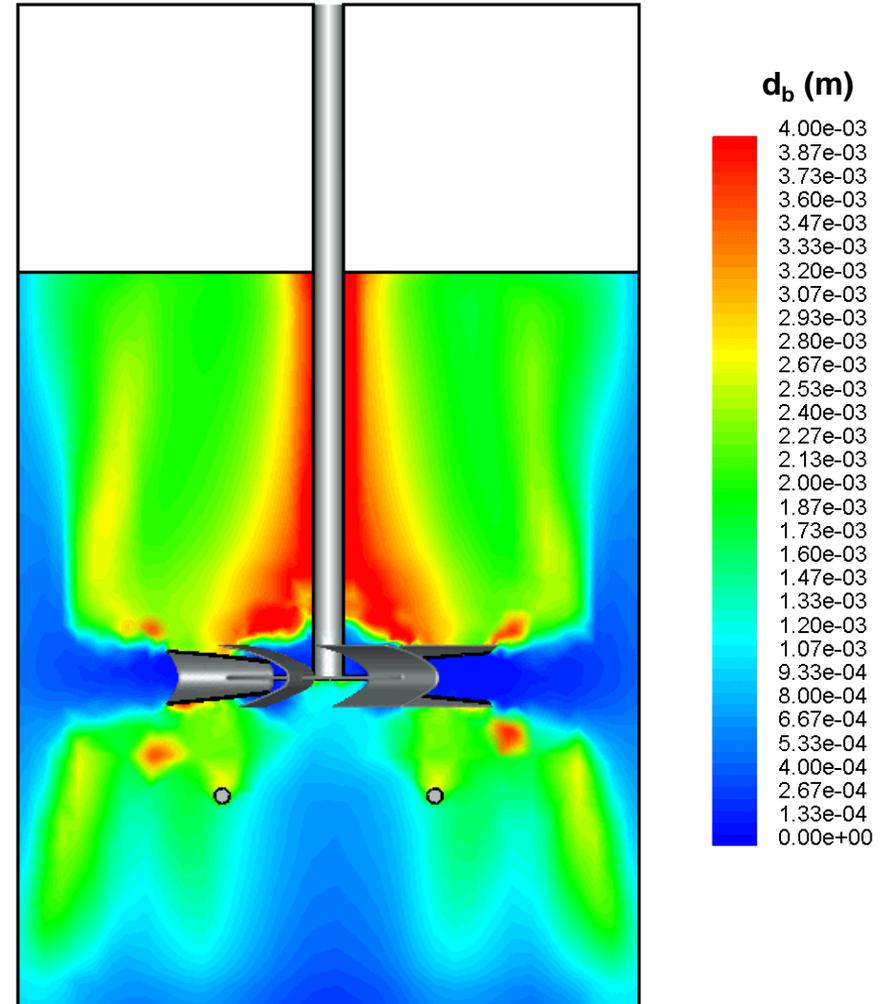


# Bubble size

- A single scalar equation is solved for the local bubble number density:

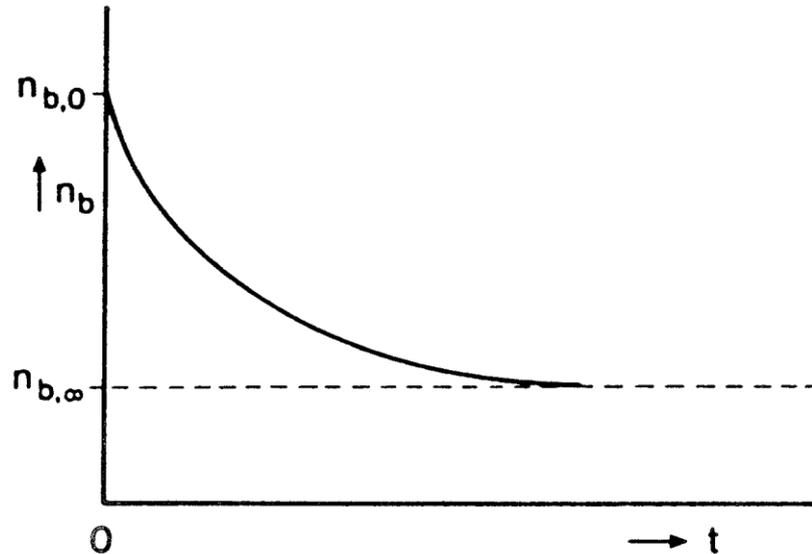
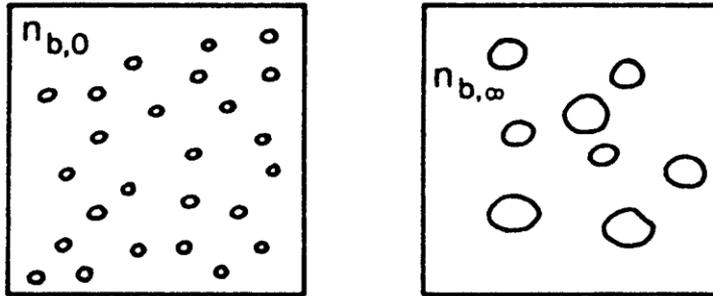
$$\frac{\partial n_b}{\partial t} + \vec{\nabla} \cdot (n_b \vec{u}_g) = S_{bc} + S_{\alpha} / V_{b,in}$$

- This includes coalescence and breakup source terms  $S_{bc}$ .
- These include effects of turbulence on the bubble breakup and coalescence behavior.
- Local average bubble size can be calculated from the bubble number density and the volume fraction:  $n_b = \alpha / V_b$



The figure shows the local bubble size in a cross section of the vessel. Bubbles enter the vessel from the sparger at a given size (here ~3mm). They are broken up by the impeller into smaller bubbles (<1mm). These then coalesce into larger bubbles, and the bubble size increases away from the outflow of the impeller. There are red spots near the tips of the impeller blades where bubble size is larger due to the high gas holdup in the vortices shed by the impeller blades.

# Bubble size modeling



$$\frac{\partial n_b}{\partial t} + \vec{\nabla} \cdot (n_b \vec{u}_g) = \omega (n_{b\infty} - n_b) + \frac{S_g}{V_{b,in}}$$

$$n_b = \frac{\alpha}{V_b}$$

$$\omega = C_\omega \frac{3}{2} \sqrt{2} \frac{\alpha}{d_b} \left| \vec{u}'_g \right|$$

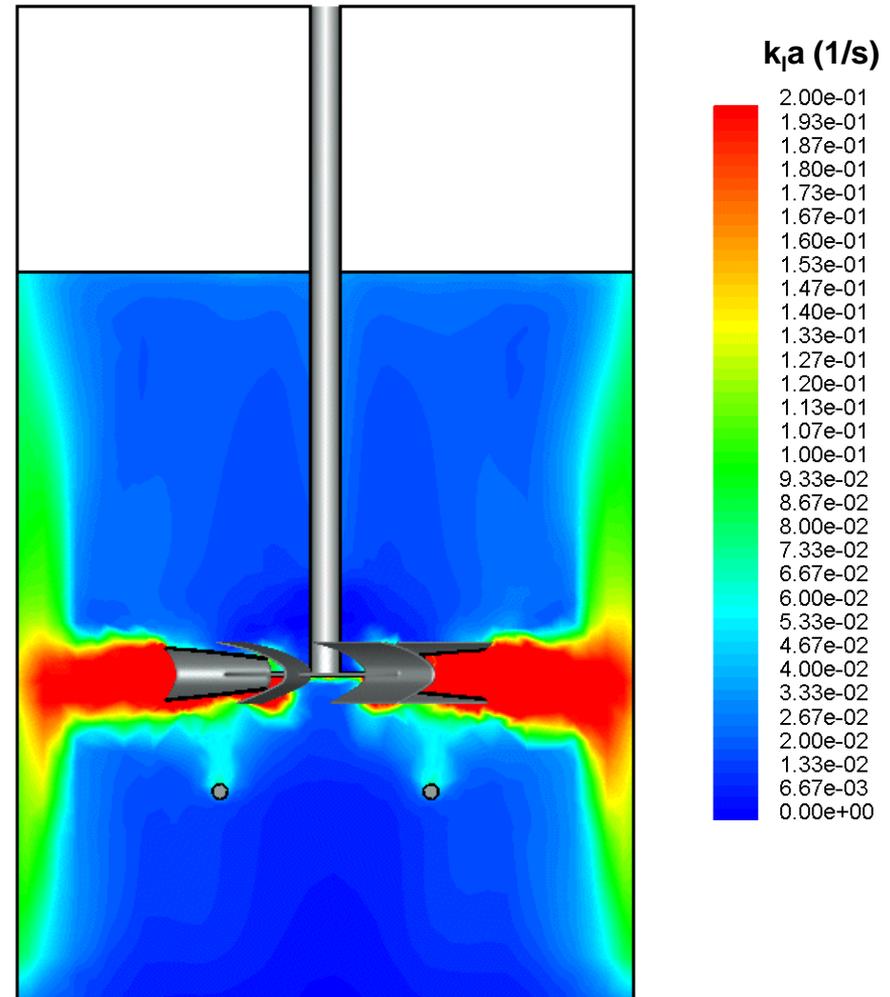
$$d_{b\infty} = C_{b\infty} \left( 12 \frac{\sigma}{\rho_l} \right)^{\frac{3}{5}} \epsilon^{-\frac{2}{5}}$$

# Mass transfer coefficient $k_l a$

- Interfacial area can be calculated from local gas holdup and bubble size.
- The liquid side mass transfer coefficient  $k_l$  is calculated from Kawase and Moo-Young (1990):

$$k_l = 0.301 (\varepsilon \nu)^{1/4} Sc^{-1/2}$$

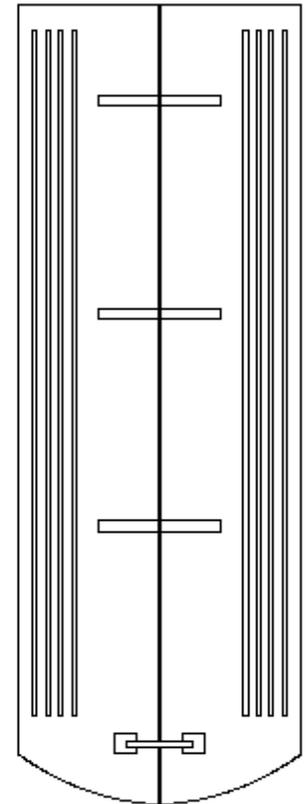
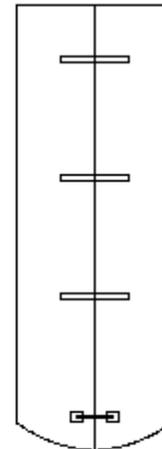
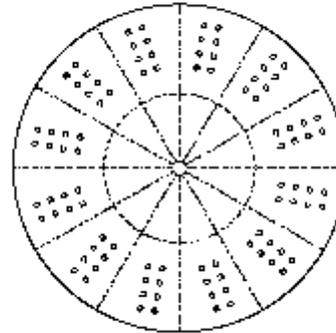
- Most of the mass transfer will occur in the impeller region, where the turbulence intensity is the highest.



The figure shows the local mass transfer coefficient  $k_l a$  in a cross section of the vessel.  $k_l a$  is highest in the impeller region and the impeller outflow, due to the fact that this is where the bubbles are smallest (resulting in a high interfacial area  $a$ ) and also the liquid side mass transfer coefficient  $k_l$  is high due to the high turbulence intensity.

# Fermenters - design example

- Design example:
  - Aerobic fermenter.
  - Vessel diameter 5.8 m.
  - Total height 21 m.
  - Batch volume up to 450 m<sup>3</sup>.
  - Fed batch: batch time 5 days.
  - Viscosity in 50 - 100 mPa·s range.
  - Superficial gas velocity 0.1 m/s or 1 vvm.
- Process requirements:
  - $k_L a$  around 0.1 1/s.
  - O<sub>2</sub> Uniformity: blend time order of  $1/k_L a$  combined with good gas dispersion.
  - No dead zones, rapid mixing of feed.
  - Sufficient flow around cooling coils.

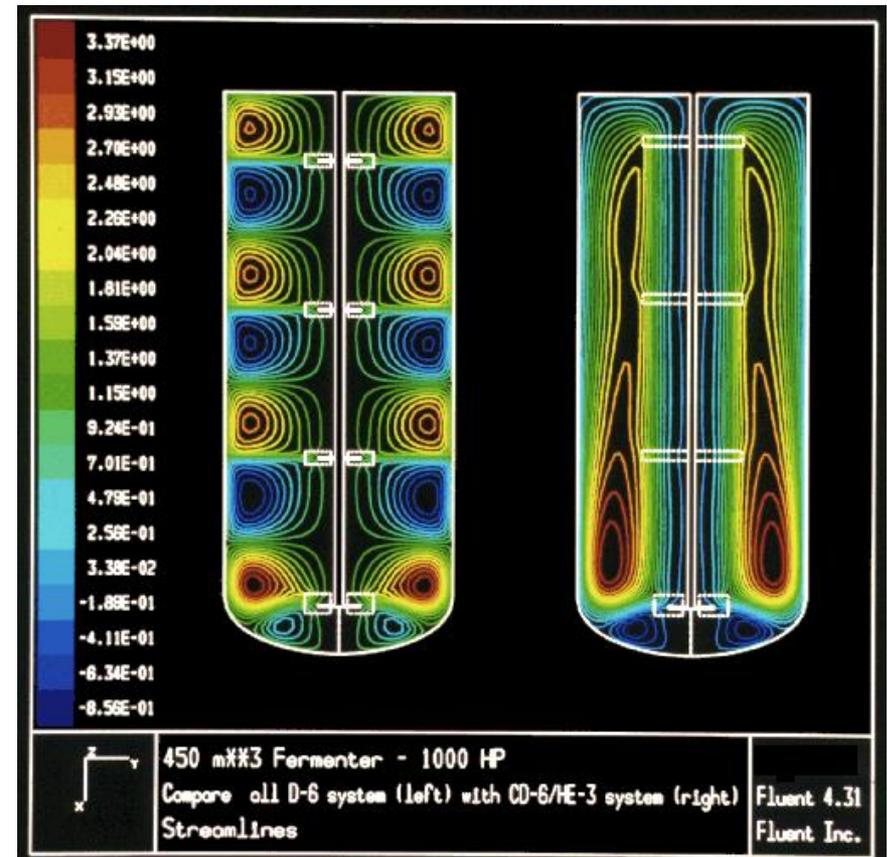
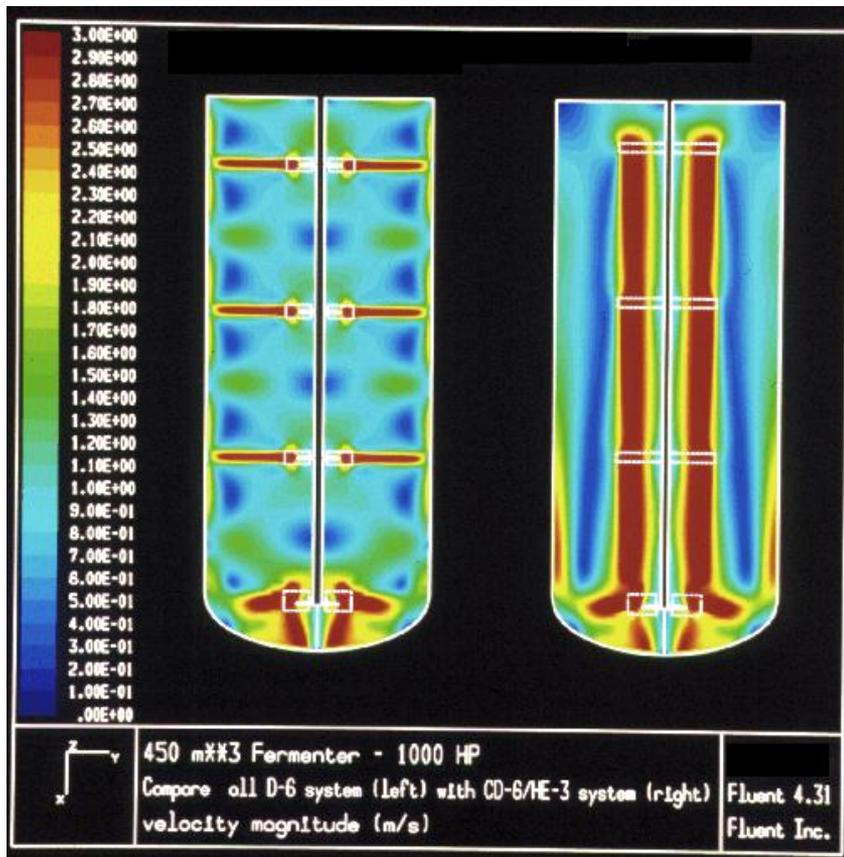


# Compare flow patterns

- Impeller system options:
  - Multiple impellers required.
  - All radial flow.
  - All axial flow.
  - Bottom up-pumping, top down-pumping.
  - Bottom radial flow, rest axial flow.
- Use computational models to calculate the flow patterns for the various impellers.
- Tank is divided in grid cells (up to 1,000,000 depending on type of model).
- Solve equations of momentum, continuity, etc. for each cell.
- Impellers are modeled using boundary conditions obtained using laser-Doppler velocimetry.

# Flow pattern comparison

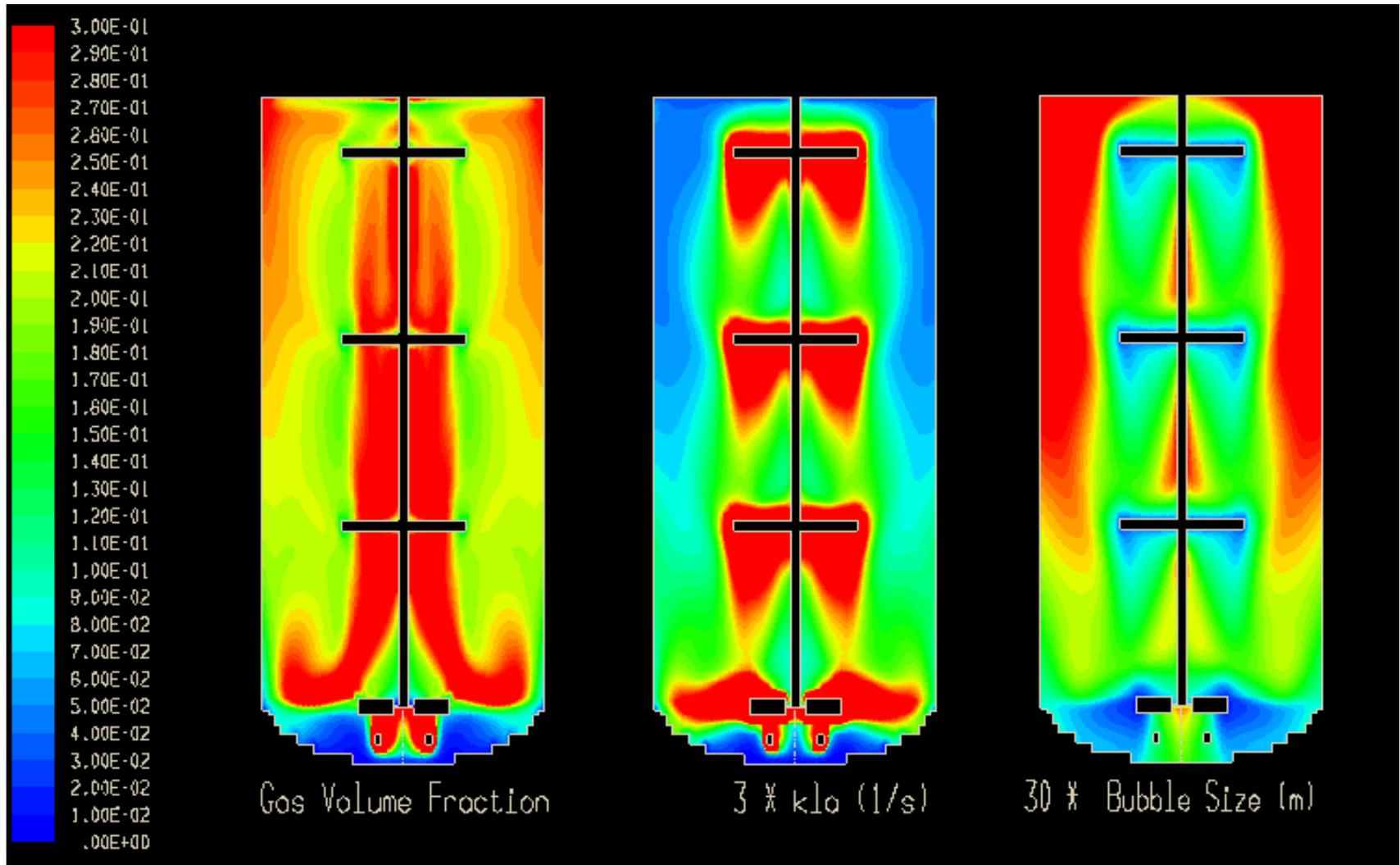
- Blend time of a system with only radial flow impellers is typically about 2.5 times longer than for a system that has upper axial flow impellers.



# Gas dispersion modeling

- Use computational models for full scale predictions.
- Computational model for gas dispersion calculates local gas holdup, local bubble size, and local  $k_L a$ .
- Bubble size model based on population balance and takes effect of break-up and coalescence into account.
- $k_L a$  follows from local holdup, bubble size, and turbulence intensity.

# CFD simulation results



# Heat transfer coils

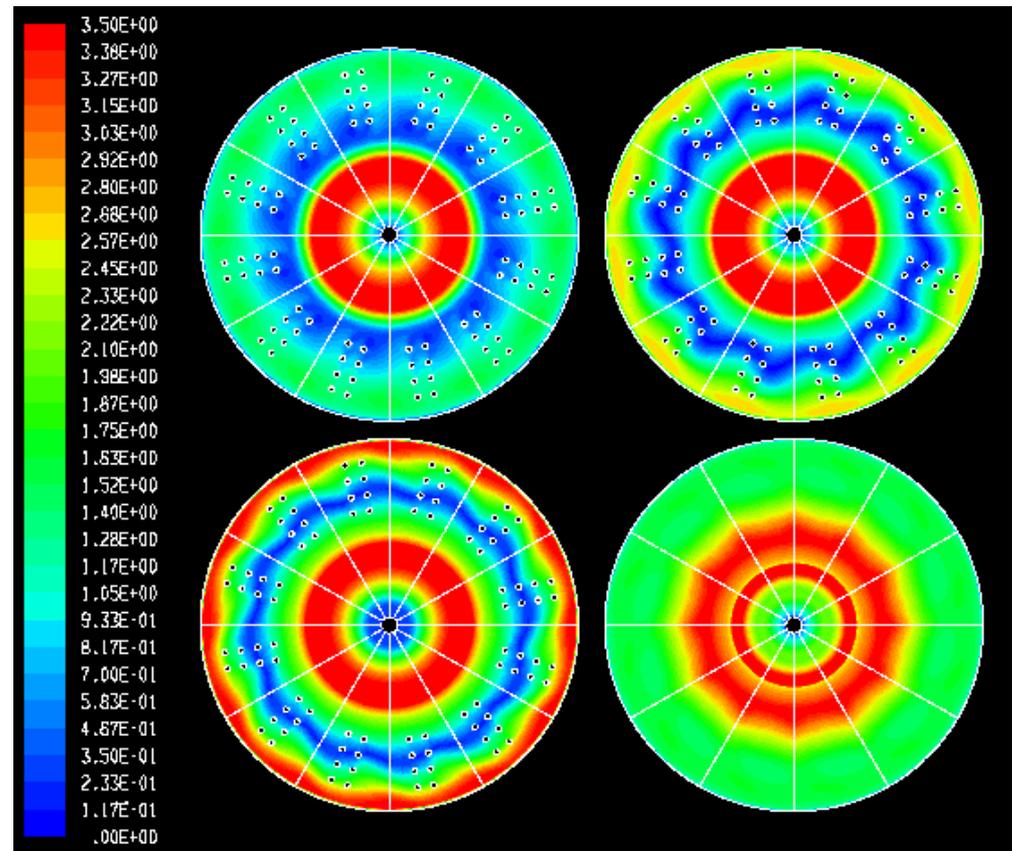
- Twelve sets of eight vertical cooling coils that also act as baffles.
- Water cooled.
- Total heat transfer resistance includes wall resistance, resistance cooling liquid side, fouling, etc.
- Process side heat transfer coefficient:

$$\text{Nu} = k_{imp} f_{geo,visc} \text{Re}^{2/3} \text{Pr}^{1/3}$$

- Process side heat transfer coeff.  $\sim P^{0.29}$ .
- Cooling capacity approx. 8000 kW from correlations.
- Verify there is sufficient liquid movement around the coils.
- Computer model for 30° section of tank; 250,000 nodes.

# Flow field around coils

- This image shows the velocity magnitude in four cross sections. From top left to bottom right, at 0.8, 0.6, 0.4, and 0.2 fraction of the liquid level off the bottom.
- The simulations show that there is sufficient liquid movement around the cooling coils.



# Final design

- 1000 HP motor at 105 RPM loaded 80% under gassed conditions
  - (second speed 52.5 RPM)
  - (hollow shaft 0.42 m diameter)
- One CD-6 and three HE-3 impellers.
- Estimated gas hold-up 23%;  $P_g/P_u = 0.65$ .
- $k_L a = 0.10$  1/s; blend time = 40 s.
- System performed as designed and operates as hoped.
- More than sixty of these 1,000 HP units have been built for various fermentations.
- Total installed CD-6\HE-3 systems approximately 94,000 HP.

# Conclusions

- Full CFD models of fermenters can be developed.
  - Usually, calculations will be CPU time intensive.
- Aerobic fermenters are prone to mixing related performance problems:
  - Gas dispersions can never be homogenous.
  - Most mass transfer will occur in impeller regions.
  - Good top to bottom blending performance is essential.
  - Systems with a lower gas dispersing impeller and upper axial flow impellers are ideally suited for large scale fermentations.

END