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Measurement and CFD prediction of
a two-phase flow in a stirred tank reactor

Boden S., Hristov H.V.



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Objectives

Gas-liquid mixing and the gas-inducing impeller

Experimental equipment

X-Ray cone beam tomography (Stephan Boden)

Setting up the problem into CFX

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Objectives

Measurement and CFD prediction of a two-phase flow in a stirred tank reactor

Why doing it?

Detailed picture of the flow and phase distribution

Design, optimization, scale-up and hazard analyses

Objectives

Implement the X-Ray con beam tomography

3D phase distribution assessment

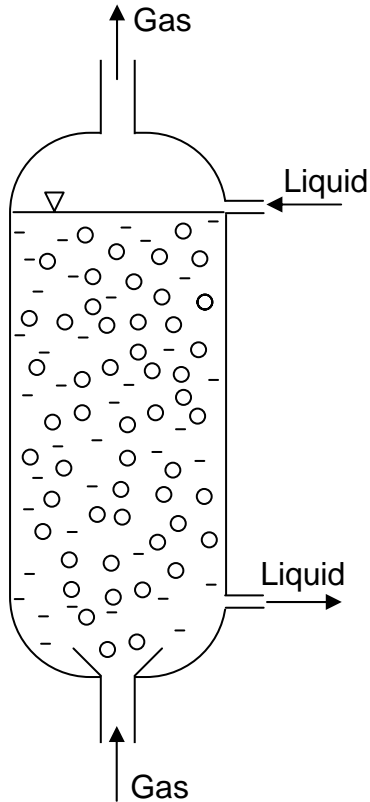
Theoretically asses the gas-liquid mixing process in stirred vessel via CFD

Experimental validation of the numerical predictions

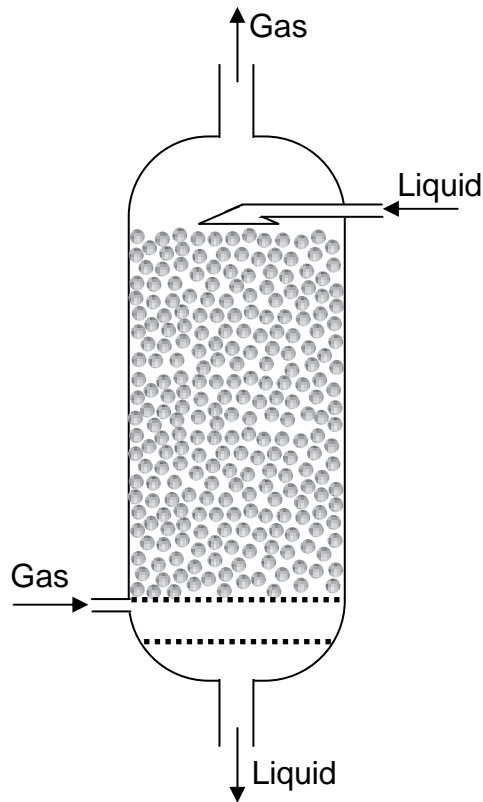


Gas-liquid mixing

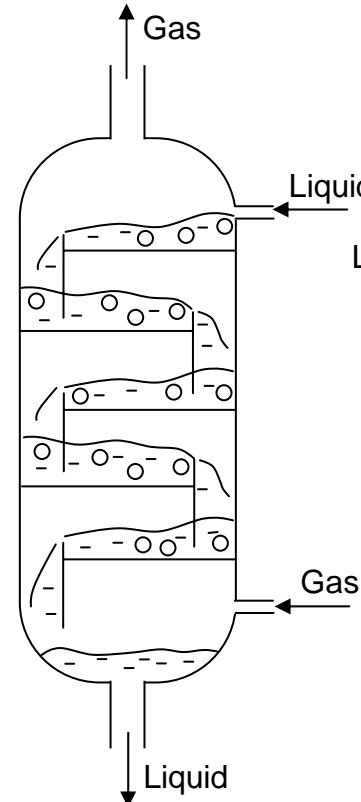
Equipment types for gas-liquid contacting



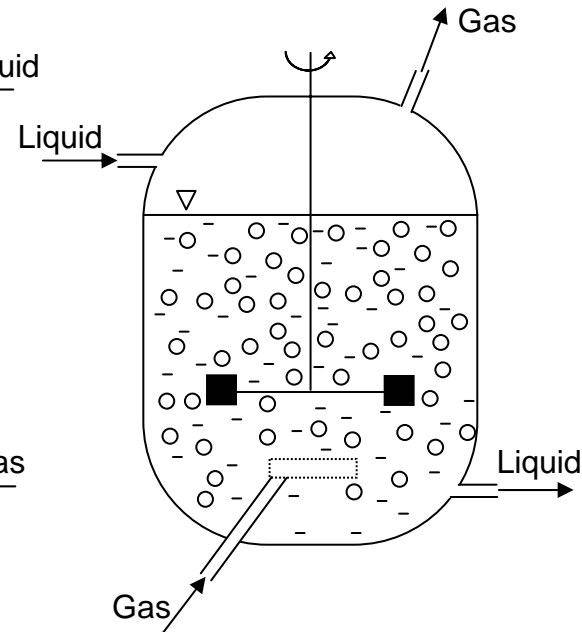
Bubble column



Packed column



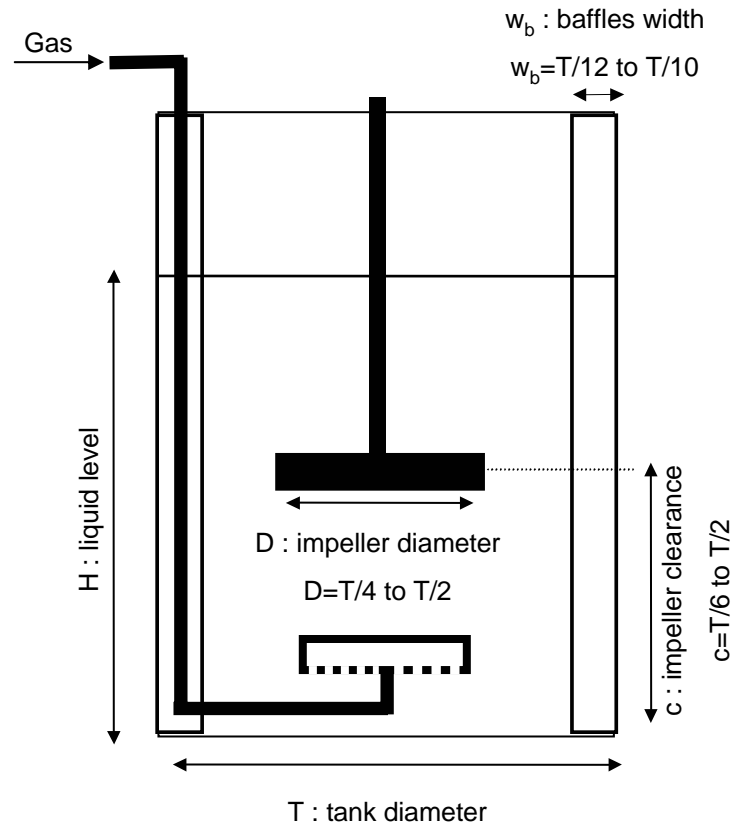
Tray column



Stirred tank

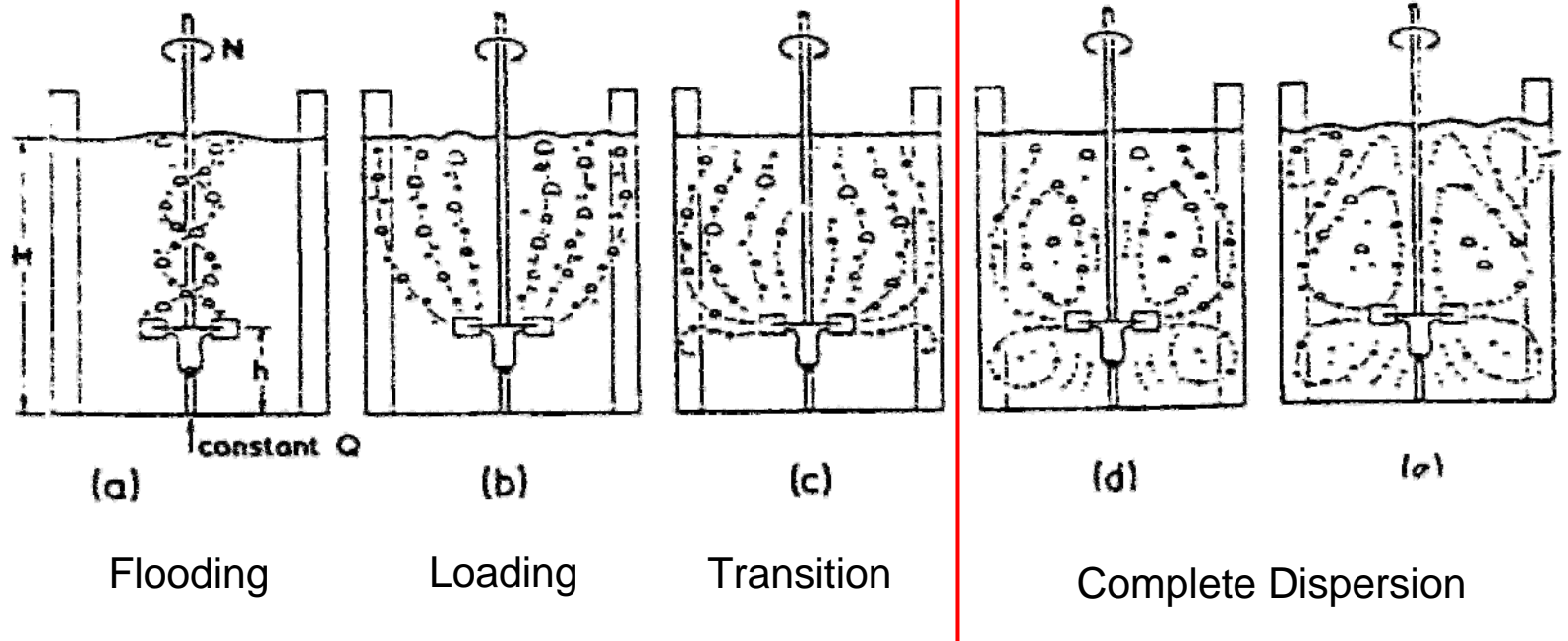
Gas-liquid mixing

Gas-liquid mixing in stirred tank reactors



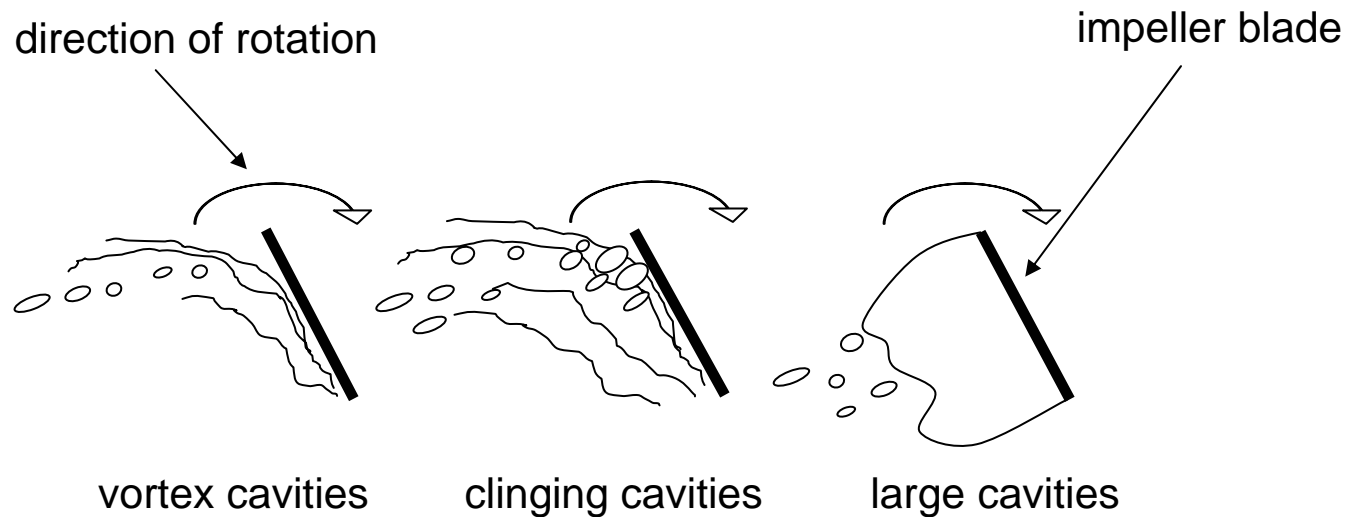
Gas-liquid mixing

Gas-liquid regimes in stirred tank reactors (Nienow et al, 1977)



Gas-liquid mixing

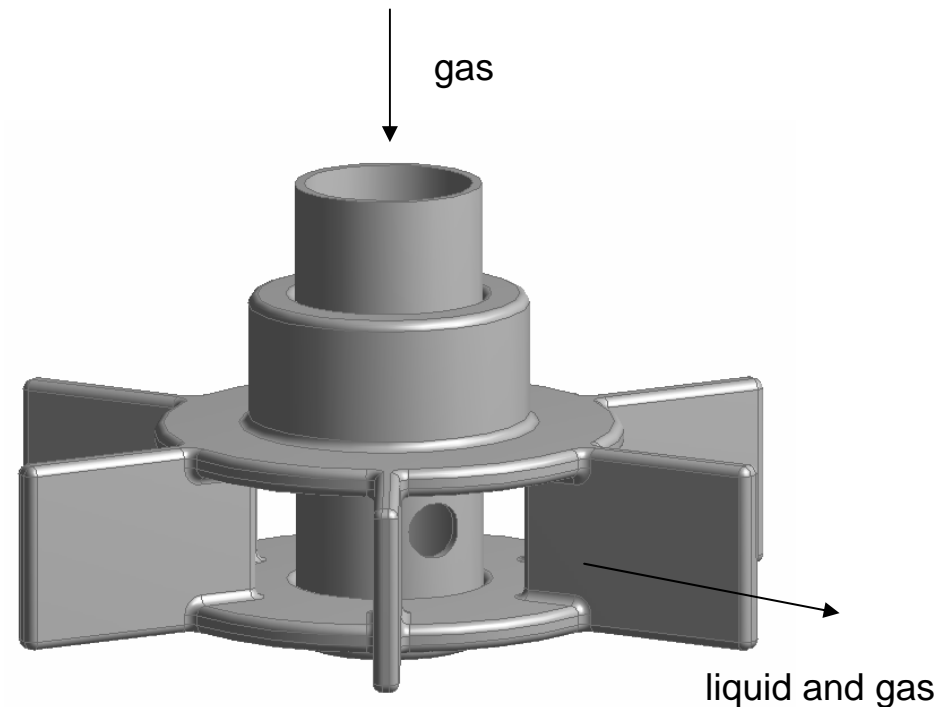
Gas cavity formation behind the impeller blade



Gas inducing impeller

Gas inducing turbine impellers

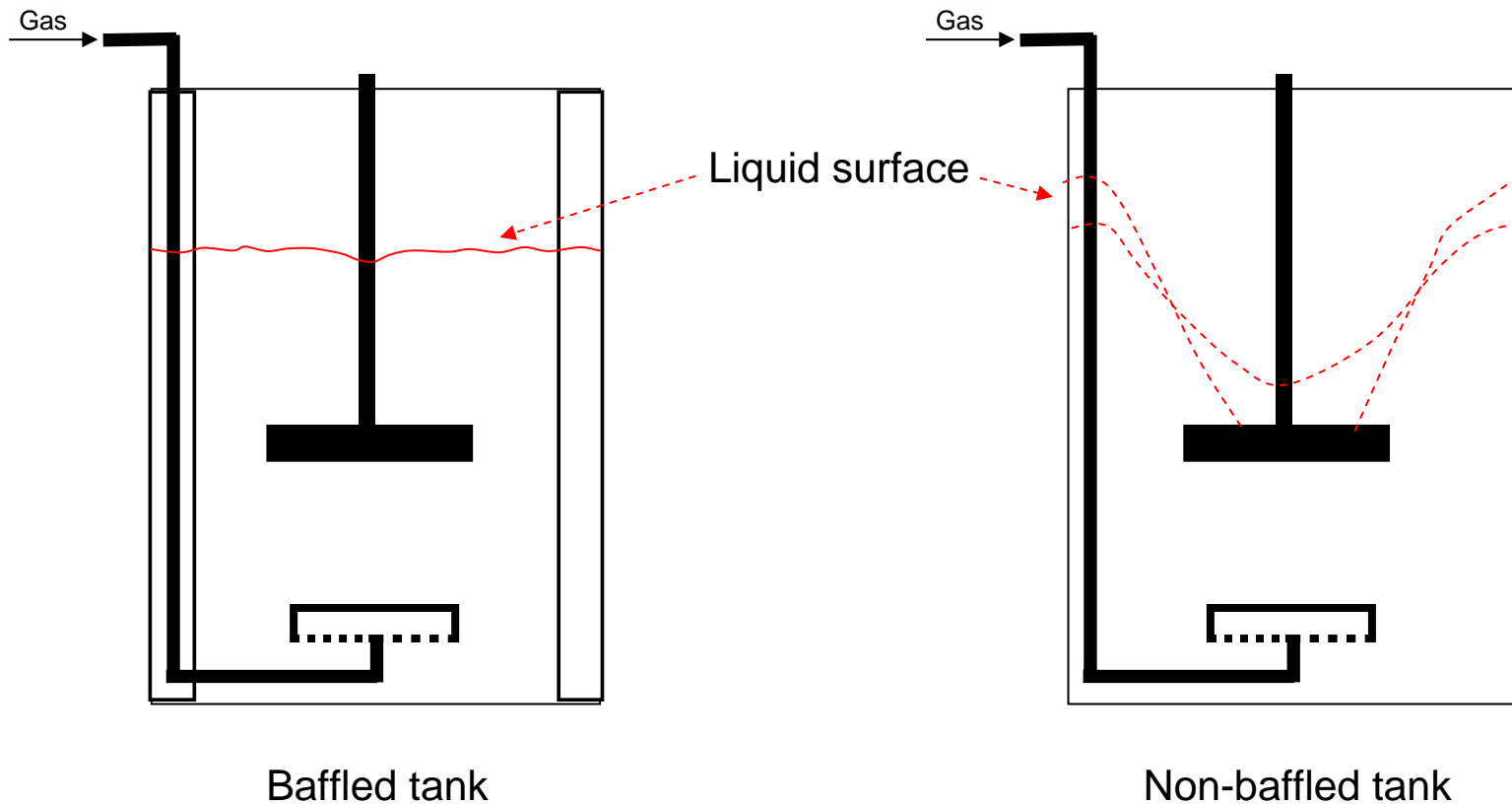
- Ensure gas presence in the tank
- Break-up the gas bubbles
- Disperse the gas
- Operate in the complete dispersion regime



Gas inducing turbine impeller,
Büchi, Laborrührautoklav BEP

Gas-liquid mixing

Gas-liquid mixing in stirred tank reactors



Experimental Equipment

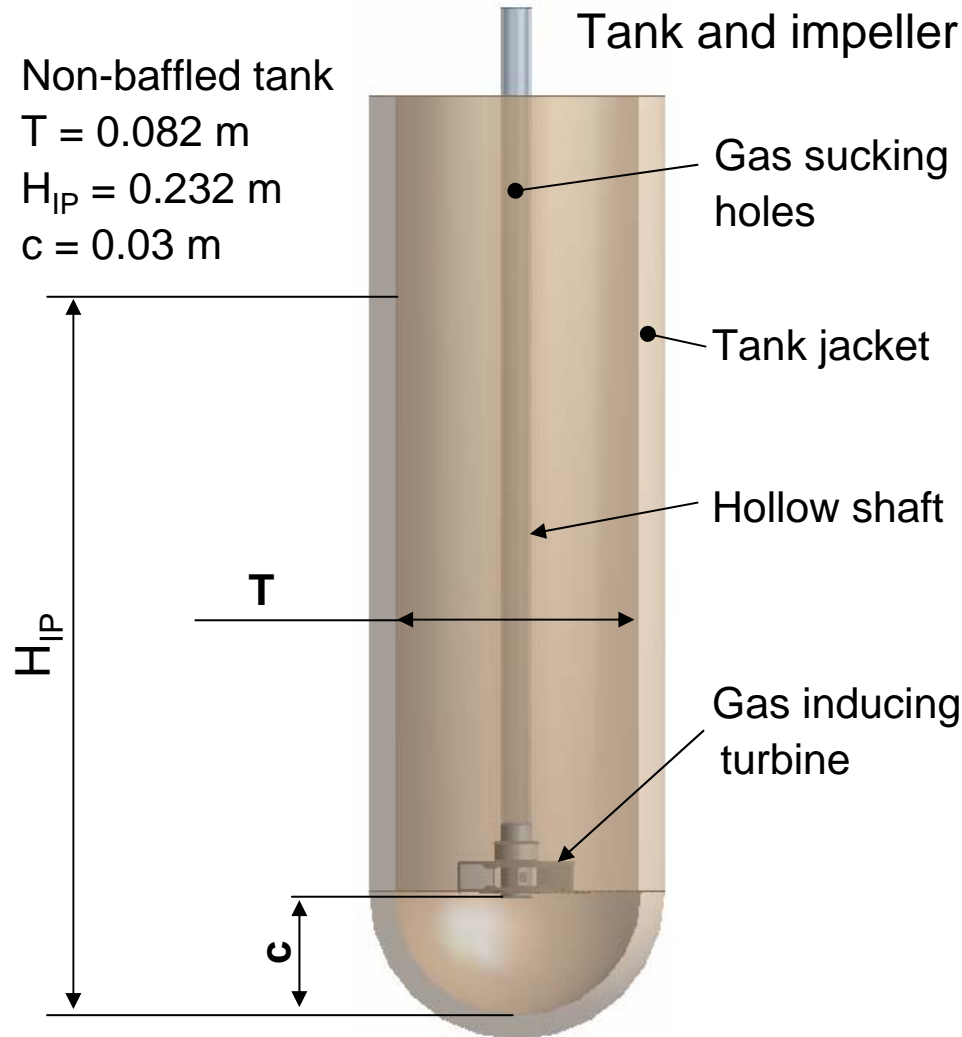
Tank and impeller geometry

Non-baffled tank

$T = 0.082 \text{ m}$

$H_{IP} = 0.232 \text{ m}$

$c = 0.03 \text{ m}$



Two-phase gas-liquid flow:

Gas : Air

Liquid: Isopropanol

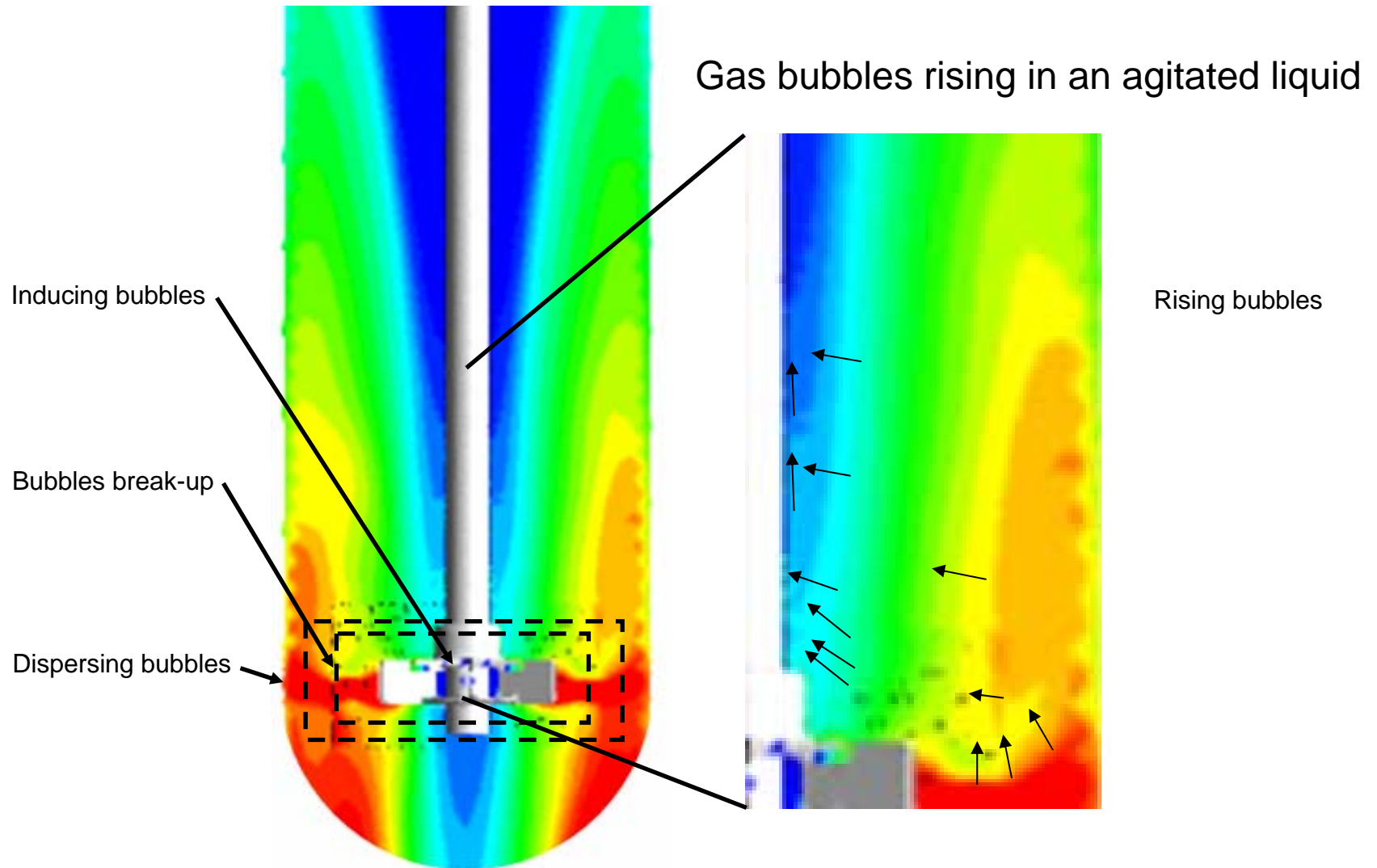
Isopropanol:

Density : $781 \text{ [kg m}^{-3}\text{]}$

Viscosity : $2.06 \cdot 10^{-3} \text{ [Pa s}^{-1}\text{]}$

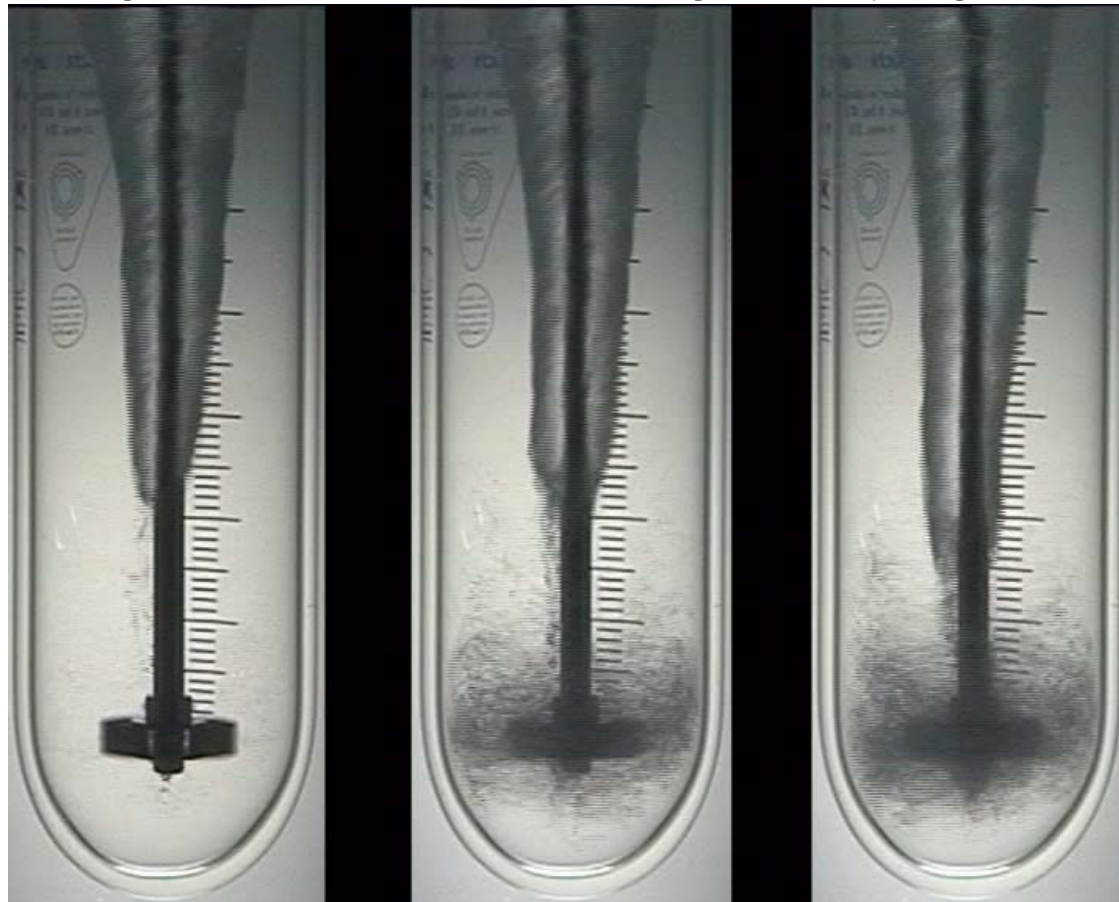
Surface tension coefficient :
 $2.1 \cdot 10^{-2} \text{ [N m}^{-1}\text{]}$

Gas-liquid mixing



Gas-liquid mixing

Gas-liquid mixing in a stirred tank reactor agitated by a gas-inducing turbine



1050

1150

1200

Stirrer speed [rpm]



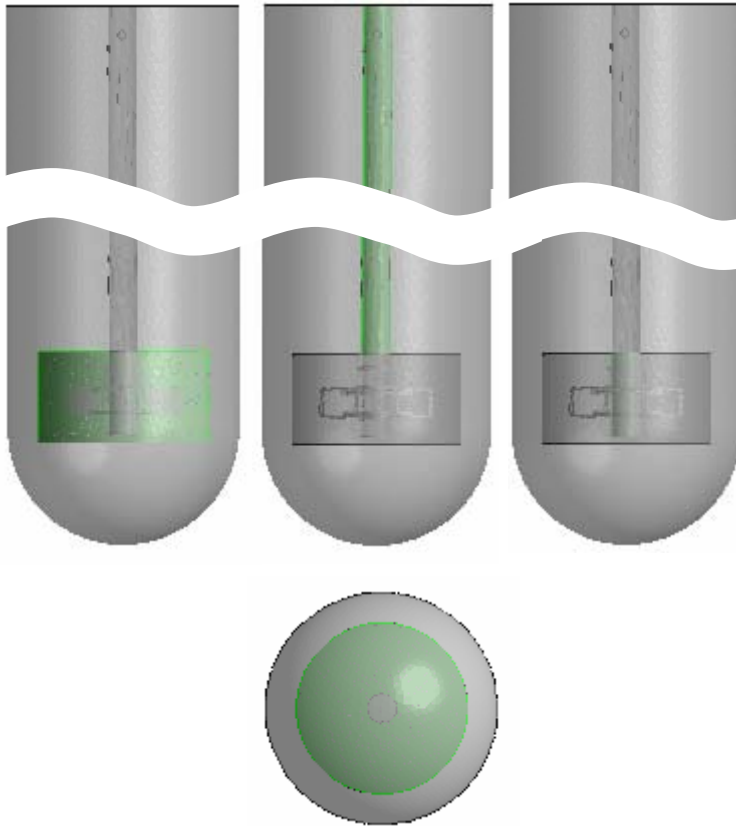
**Forschungszentrum
Rossendorf**

Member Institution of the Scientific Association Gottfried Wilhelm Leibniz

Institute of Safety Research

Setting up the problem into CFX

Geometry



Tetrahedral mesh with total of 1 500 000 elements

Three rotating domains

One stationary domain

Multiple frame of references / Frozen Rotor

Domain interphases

Frame change

Frozen Rotor

Transformation type: automatic

Pitch chance automatic

Setting up the problem into CFX

Steady state simulation

Four simulations at : 200 – 800 rpm
threshold 200 rpm

Five simulations at : 1000 – 1200 rpm
threshold 50 rpm

Two-phase flow

inhomogeneous model

continuous phase : isopropanol

dispersed phase : air

mean diameter : 1mm

Turbulence

Isopropanol : k- ϵ turbulence model

Air : dispersed phase
zero equation

Buoyant flow

Momentum transfer : Drag Force – Grace

Non-drag forces :

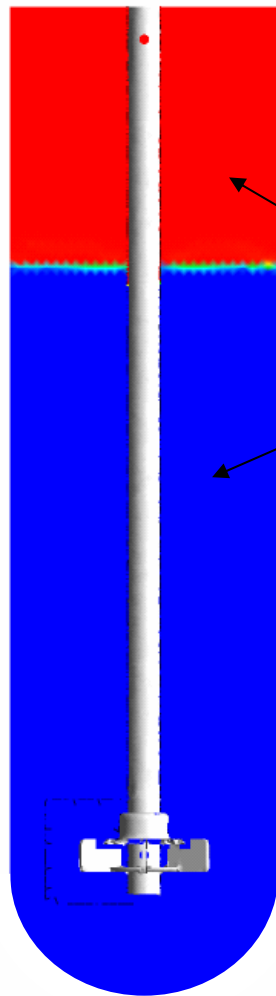
Turbulent dispersion force

Lopez de Bertodano

Turbulence transfer : Sato Enhanced
Eddy Viscosity



Setting up the problem into CFX



Initial conditions

Steady state simulation at stirrer speed of 200 rpm

Air

Isopropanol

Zero initial velocity field for both phases for the steady state simulation at stirrer speed of 200 rpm

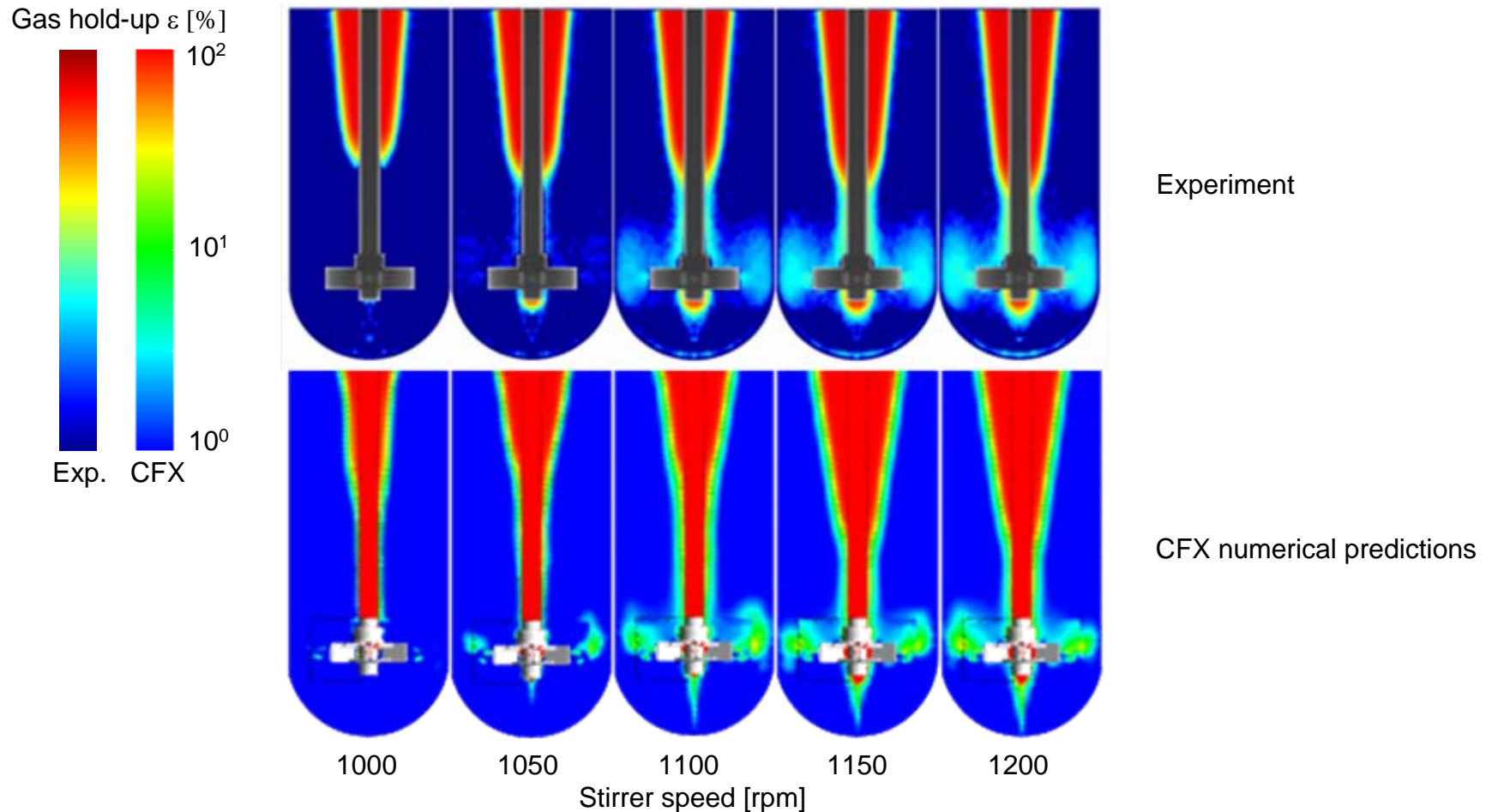
Parallel processing on 2 x Opteron 64 Linux based PC

Simulation time: approximately 17 hours per simulation

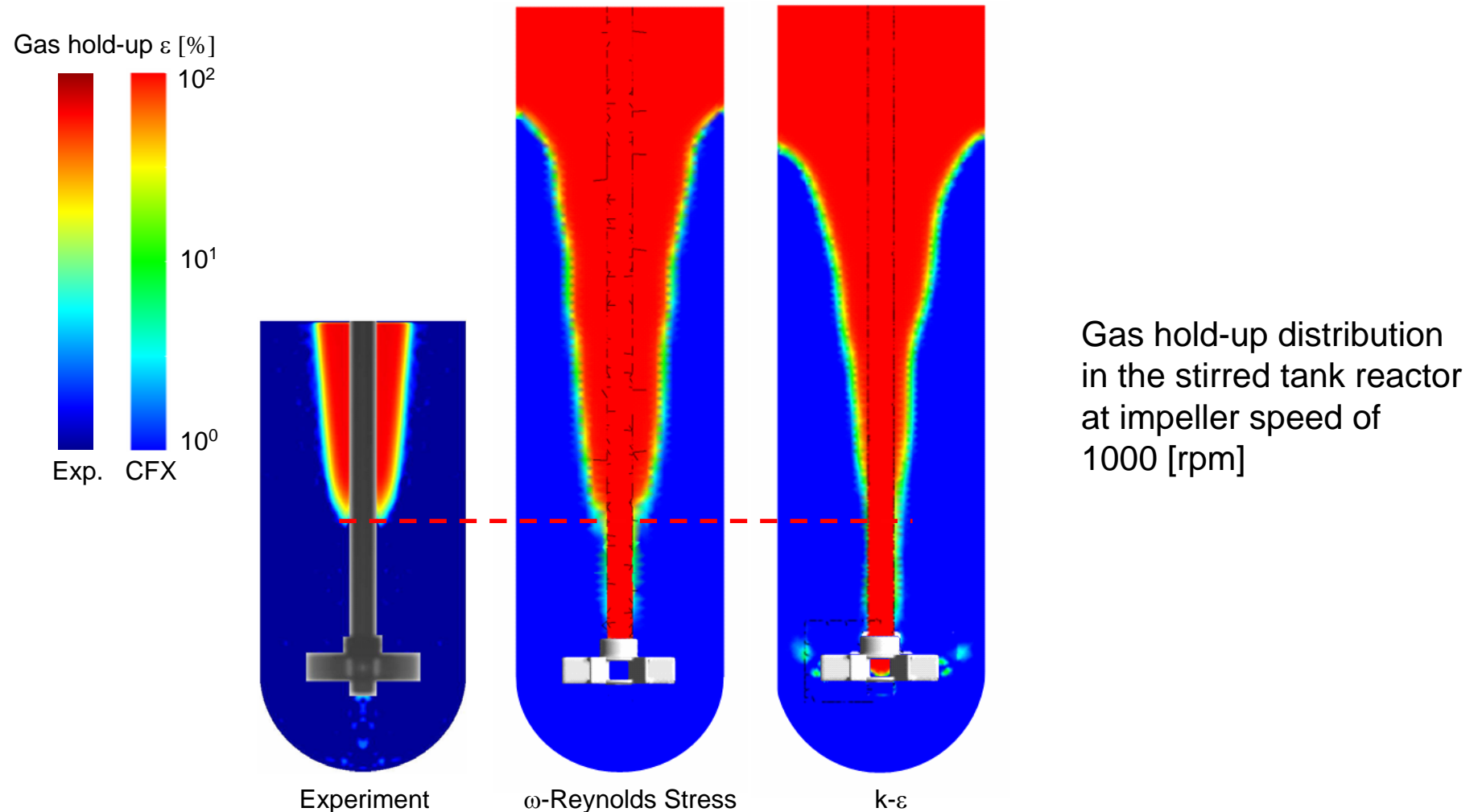
2 nodes on hades app. 60 hours

Results

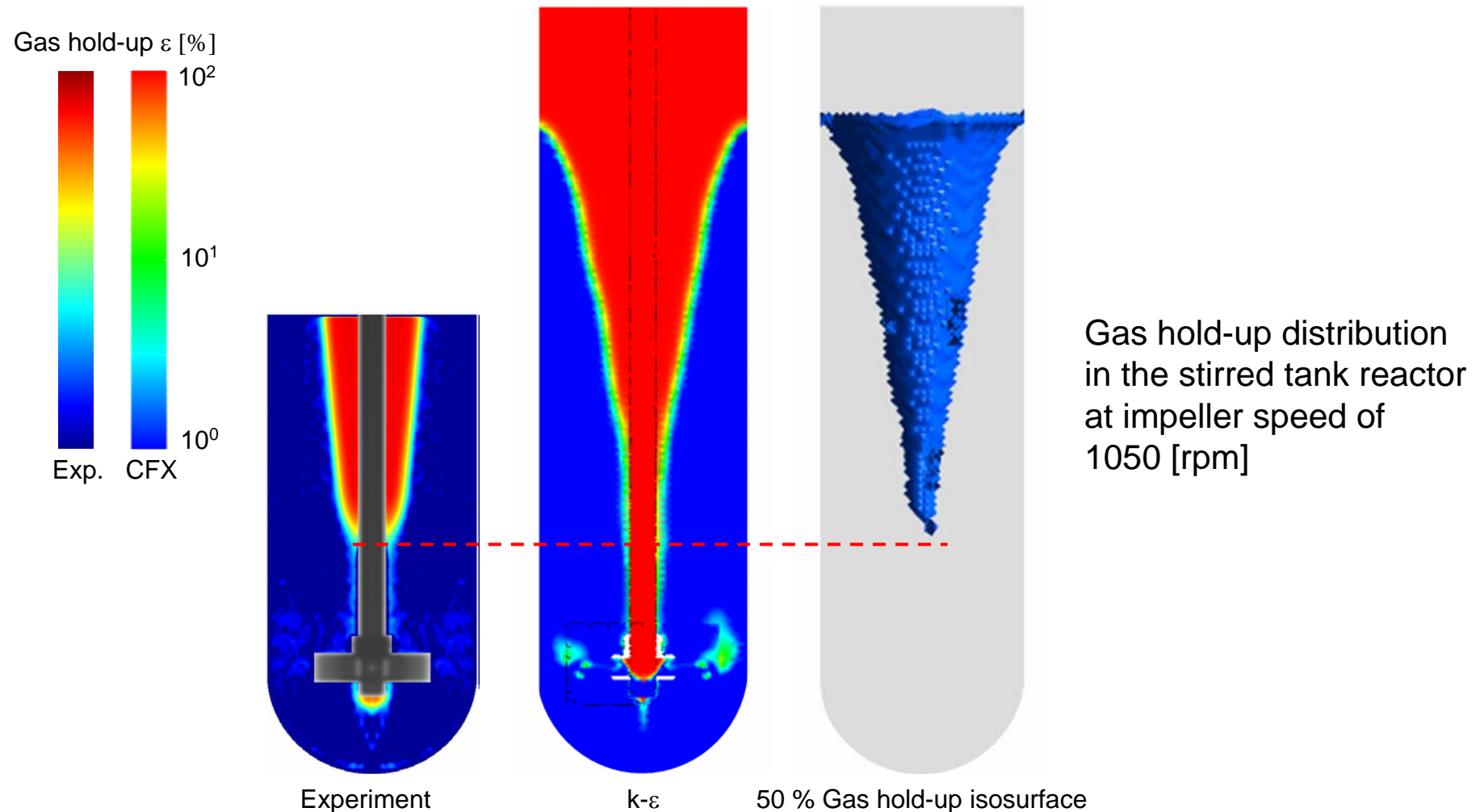
Gas hold-up in stirred tank reactor at different impeller speeds



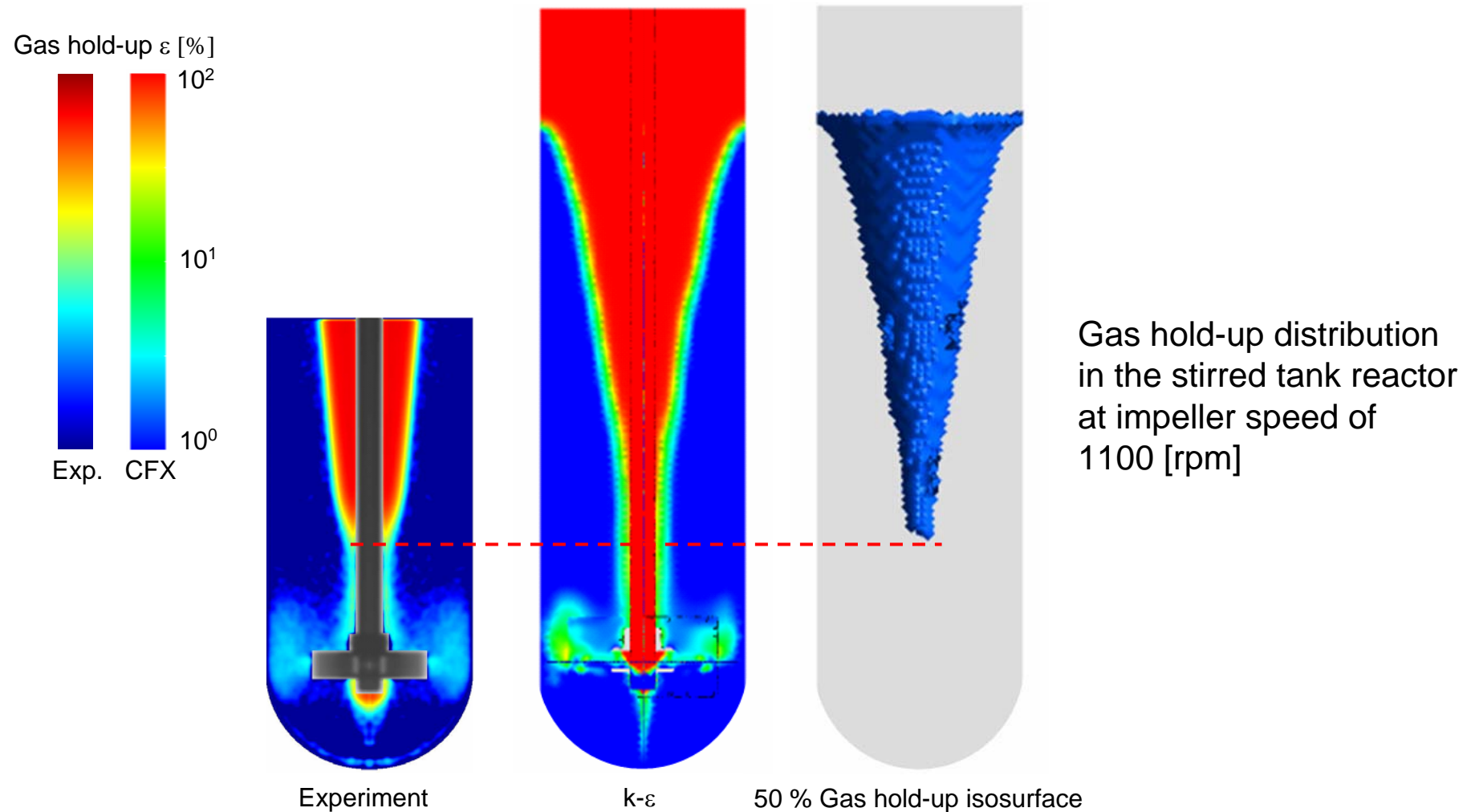
Results : Stirrer speed 1000 [rpm]



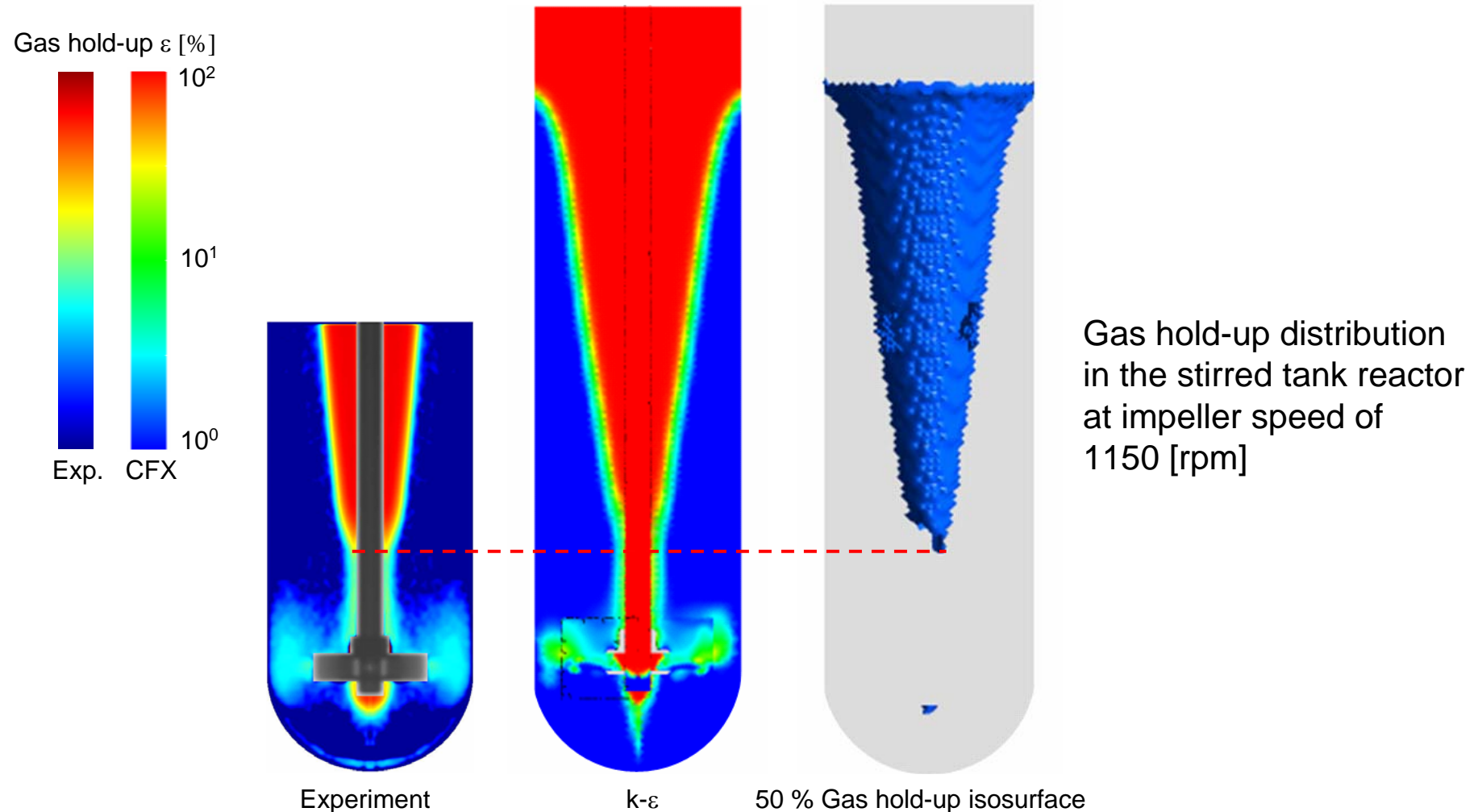
Results : Stirrer speed 1050 [rpm]



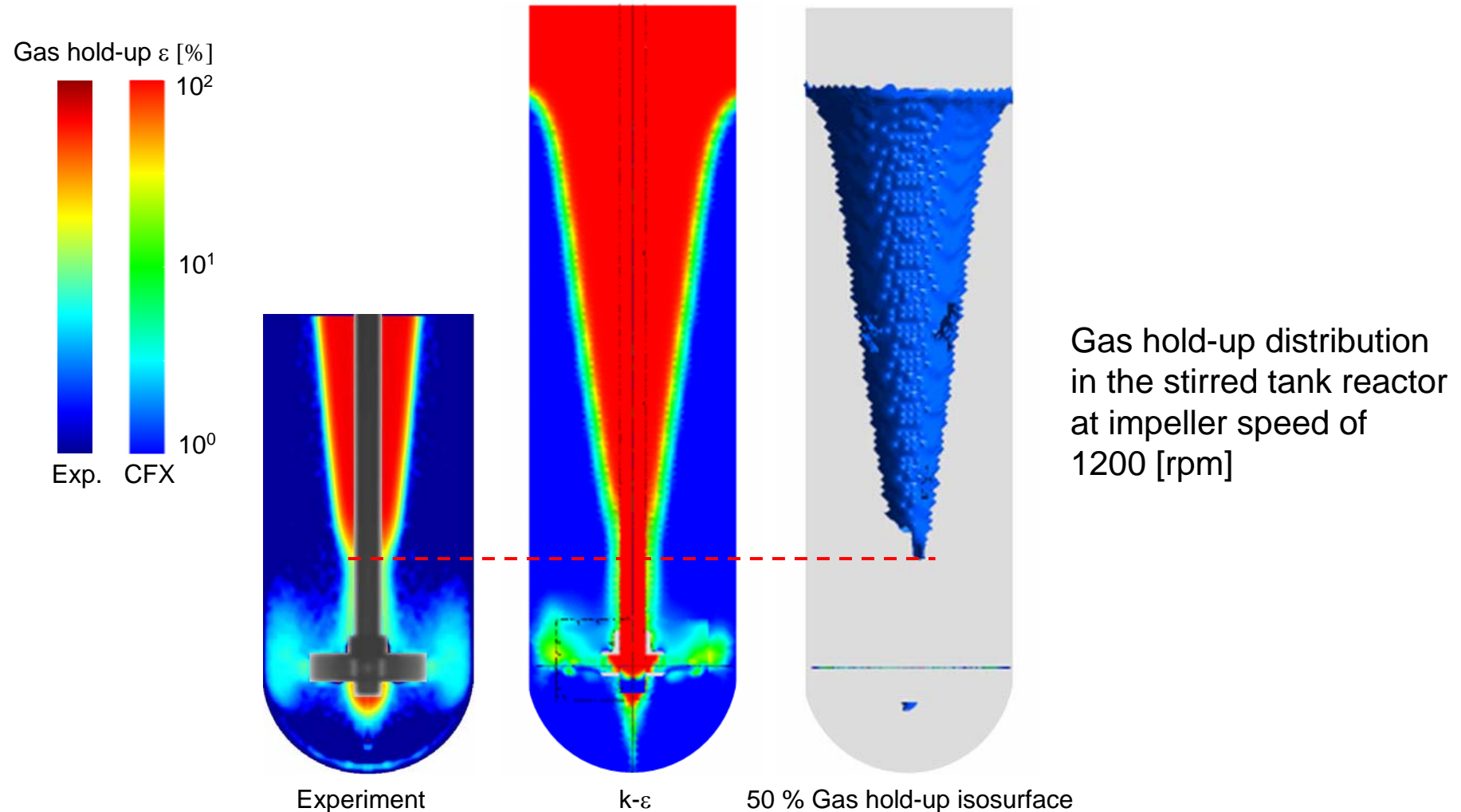
Results : Stirrer speed 1100 [rpm]



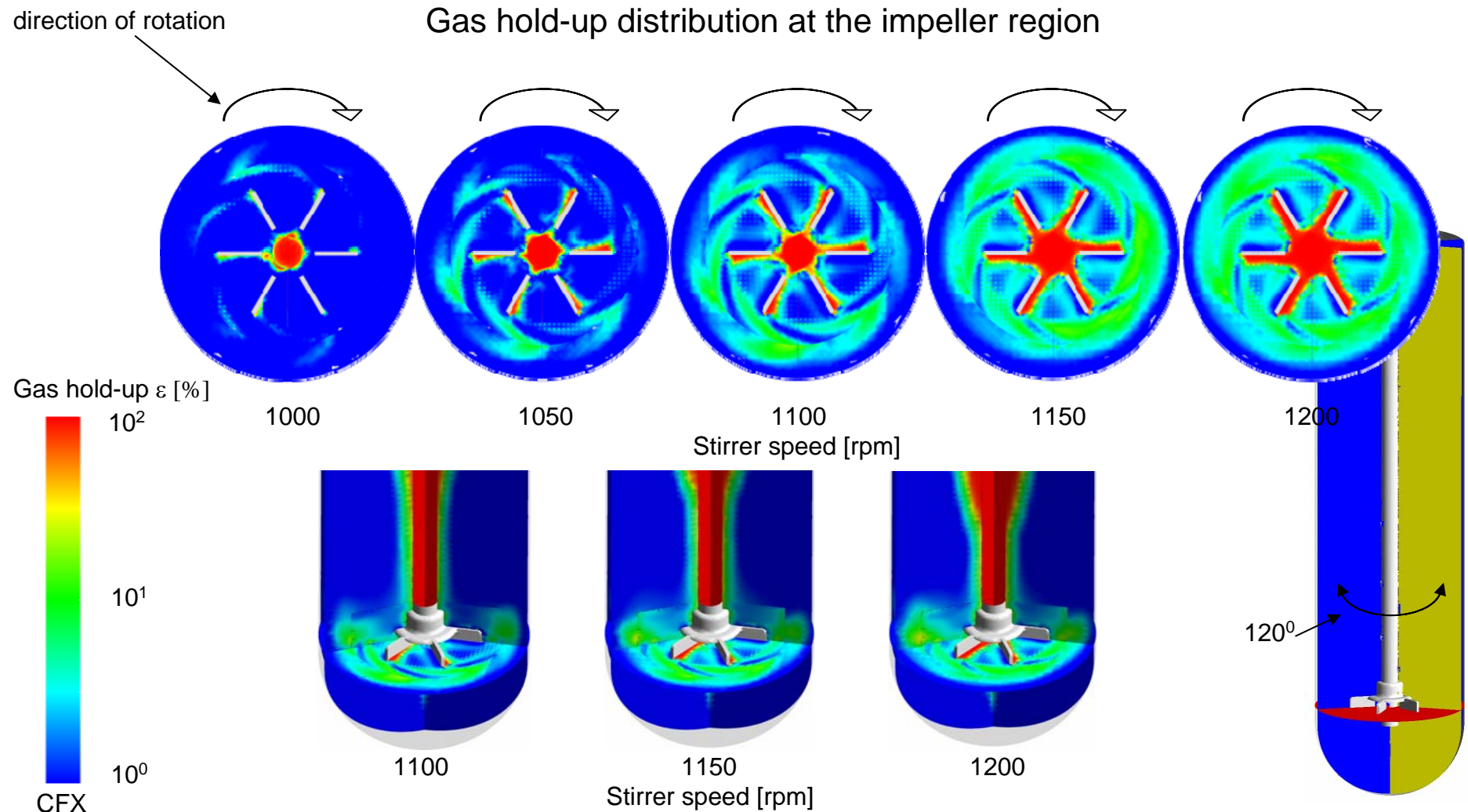
Results : Stirrer speed 1150 [rpm]



Results : Stirrer speed 1200 [rpm]



Results



Conclusions and Further work

Conclusions

- Free surface deformation

 - Slightly under predicted depth of the central vortex by the k- ε turbulence model (lower stirrer speed)

- Local gas-hold-up in the impeller region

- Gas cavities behind the impeller blades

Future work

- Spatial averaging of the gas hold-up

- Dynamic simulations

- Turbulence model

- Bubble mean diameter / multiple diameter gas fractions

- Tank internals

- Scale-up