COMSOL CONFERENCE 2015 GRENOBLE

A numerical Euler-Lagrange method for bubble tower CO_2 dissolution modeling

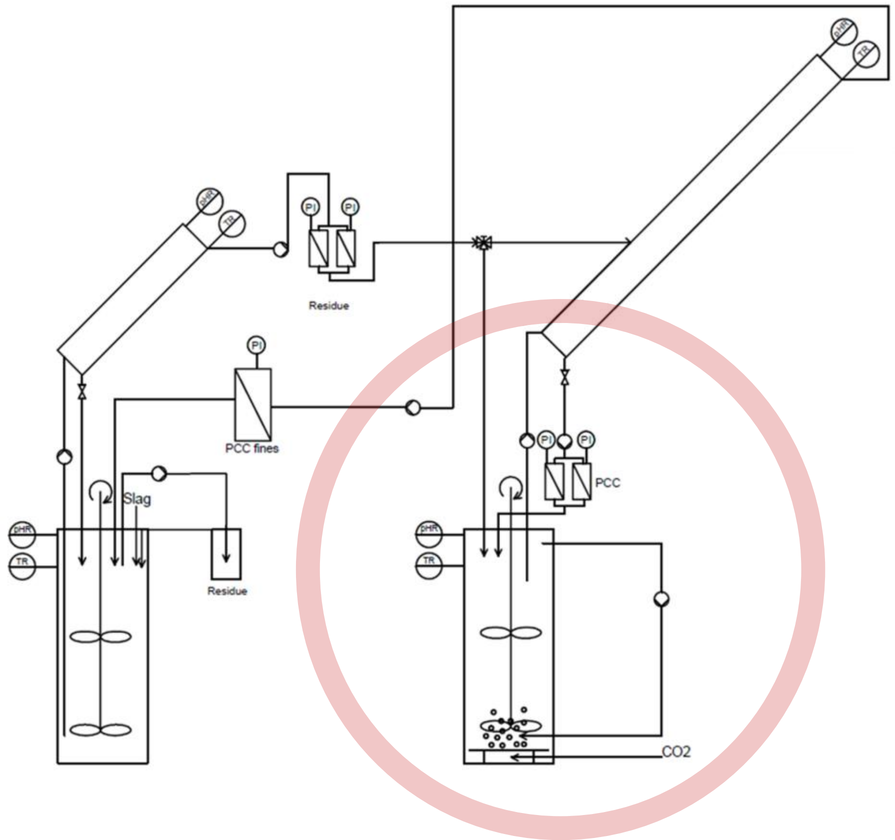
Author: Daniel Legendre
& Prof. Ron Zevenhoven

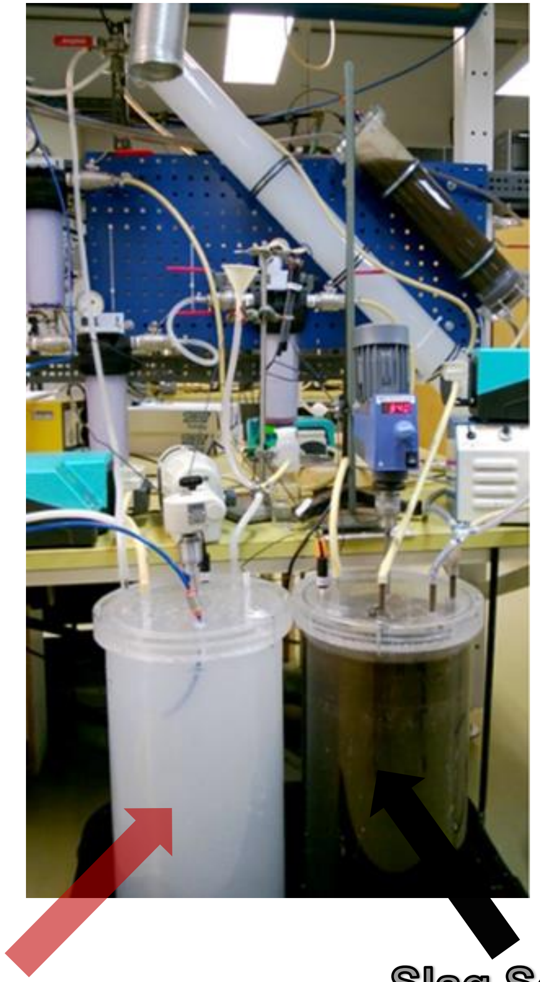
Presentation guidelines

1. Introduction: Slag2PCC process
    1. Project features
2. Eulerian fluid environment
    1. Frozen rotor simulation
    2. Time dependent solution
3. Mass transfer for a single bubble
4. Bubble swarm Lagrangian tracking
    1. Bubble tracking
    2. Bubble dissolution
5. Stacked tower of fluid
6. Bubble dissolution in tower of fluid (water)
7. Conclusions

Introduction : Slag2PCC Process

CO_2 is dispersed in an aqueous solution that contains dissolved calcium (Ca^{2+} ions), that produce PCC (precipitate calcium carbonate $CaCO_3$) [Mattila and Zevenhoven, 2014]





Bubble reactor

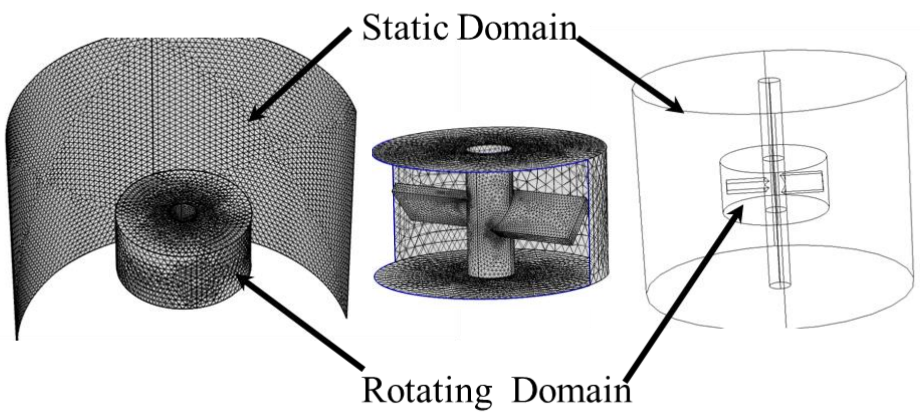
Slag Solution

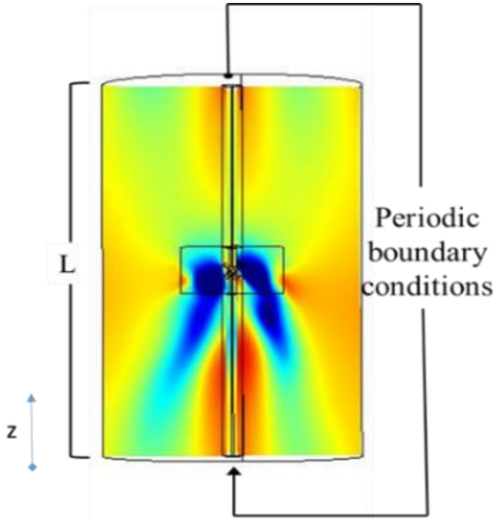
Project features

- Modelling efforts focus on the bubble reactor
- Improvement of PCC particle quality and efficiency of CO_2 use after dissolution
- Goal: CO_2 gas outlet minimization
- Improvement and limit testing of CFD commercial codes:
  - Eulerian stacked tower of fluid
  - One way coupling
  - Lagrangian bubble tracking
  - Variable bubble size and mass
  - Bubble swarm dissolution

Eulerian fluid environment

- Fluid dynamics ruled by impeller motion
  - Eulerian flow lines depend on geometry constraints and impeller characteristics (Turbulence modelling)
  - Bubble disturbance effect on fluid dynamics negligible
  - Periodic Boundary conditions
  - Impeller shaft velocity outside the rotating domain is modelled as a moving wall with velocity Ω x R, with "Ω" the rotational speed and "R" the radial coordinates of the shaft

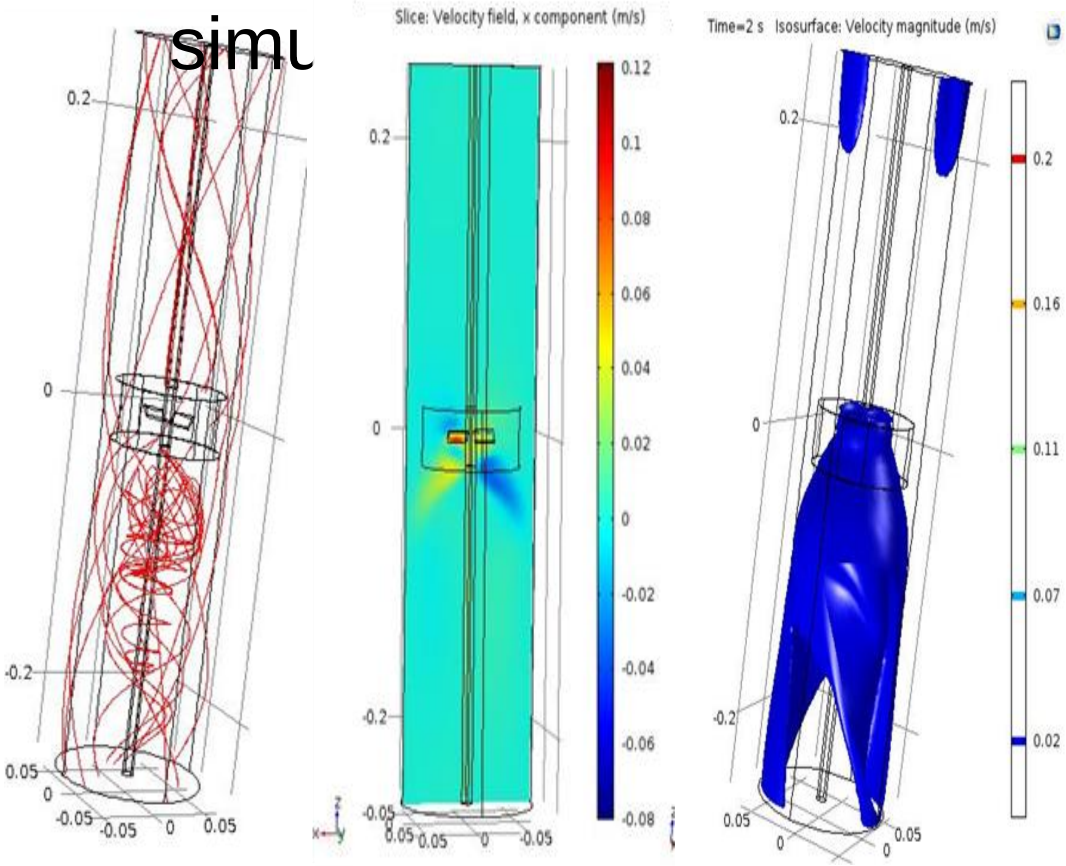




The system consist of a section of a vertical pipe of diameter [D1= 127 mm] with an internal cylindrical rotating domain that contains the impeller geometry with varying diameter of 50- 75% of the outer pipe.

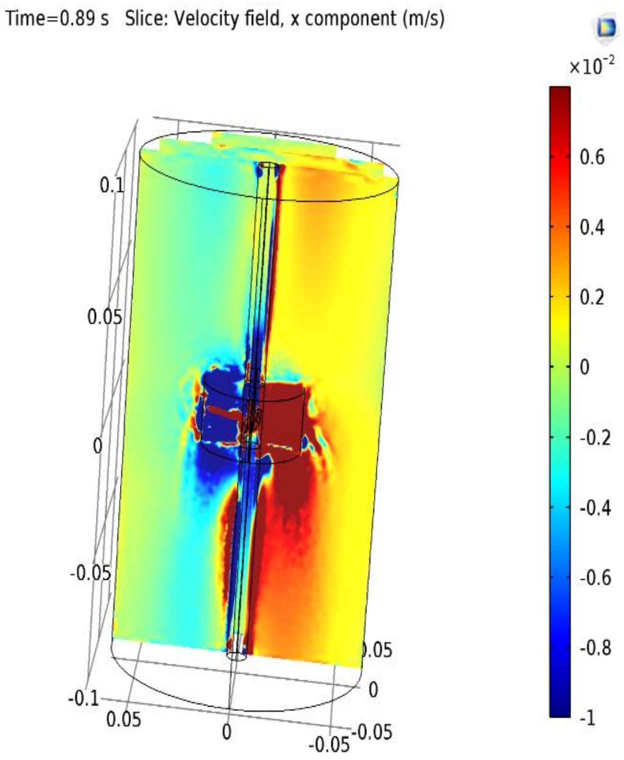
Eulerian fluid environment

- Frozen rotor simu



Velocity field: stream lines (Mixing pattern)
Ω =100 rpm L=50 cm

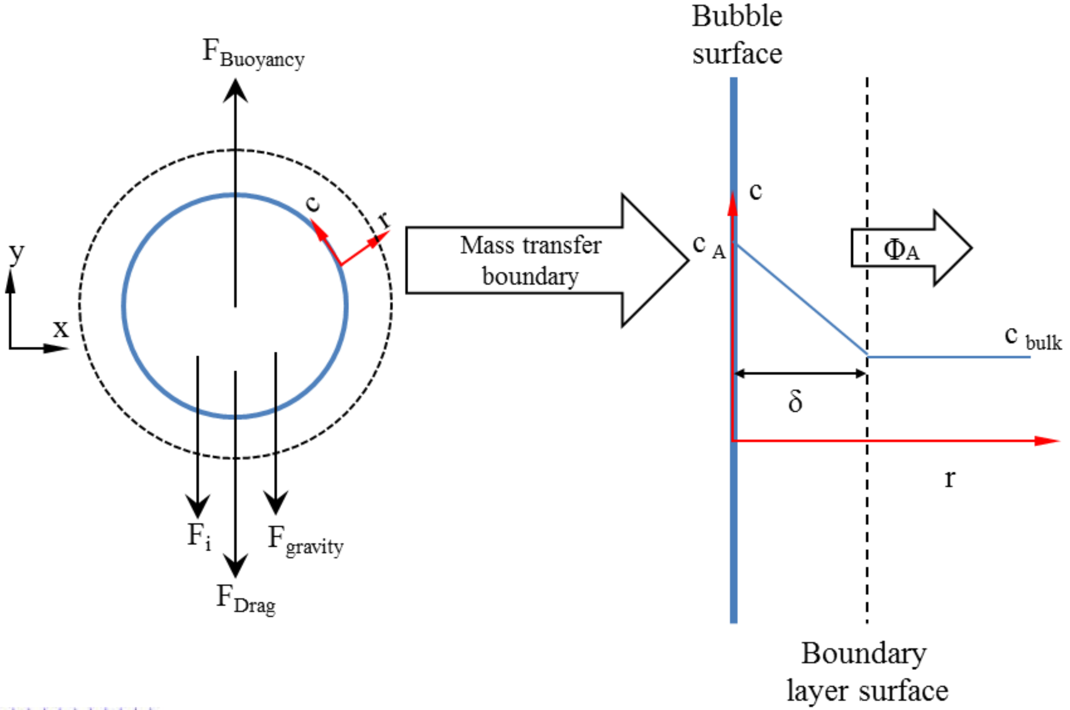
- Time dependent solution



Numerical errors arise causing the results to be unstable

Åbo Akademi

Mass transfer for a single bubble

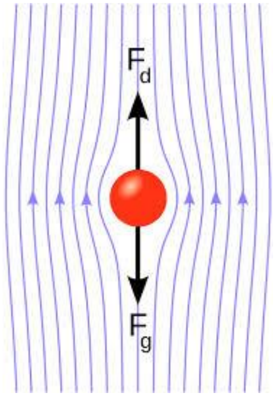


$$Sh = \frac{2\, k_{mass}\, r_{Bubble}}{\mathcal{D}}$$

$$Sh = 2 + 0.6\, Re^{1/2} Sc^{1/3}$$

$$Sc = \frac{\upsilon_{fluid}}{\mathcal{D}}$$

$$Ha = \sqrt{(\mathcal{D}\, k_{reaction})} \;/\; k_{mass}$$



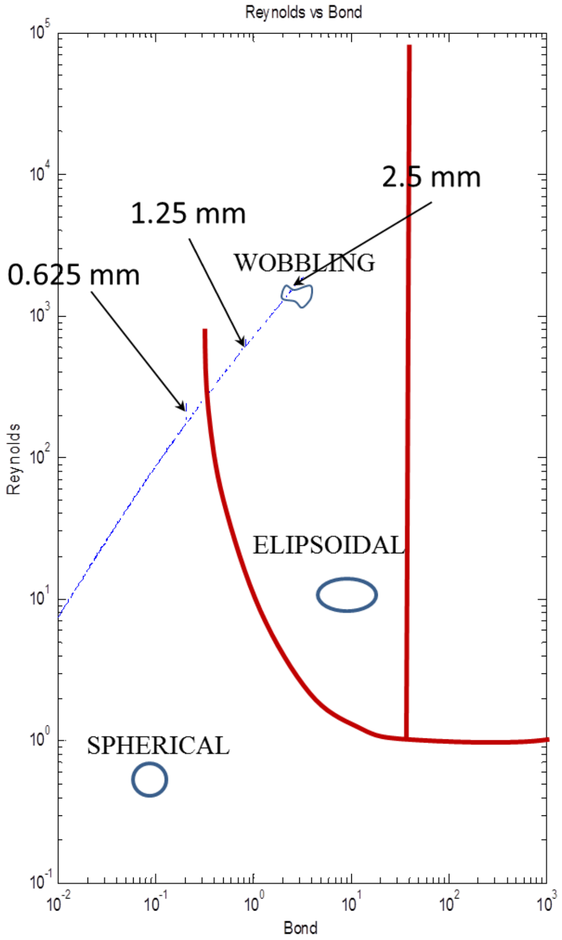
$$m\frac{d\vec{v}}{dt} + \vec{v}\frac{dm}{dt} = \vec{F}_{Bouyancy} + \vec{F}_{gravity} + \vec{F}_{Drag}$$

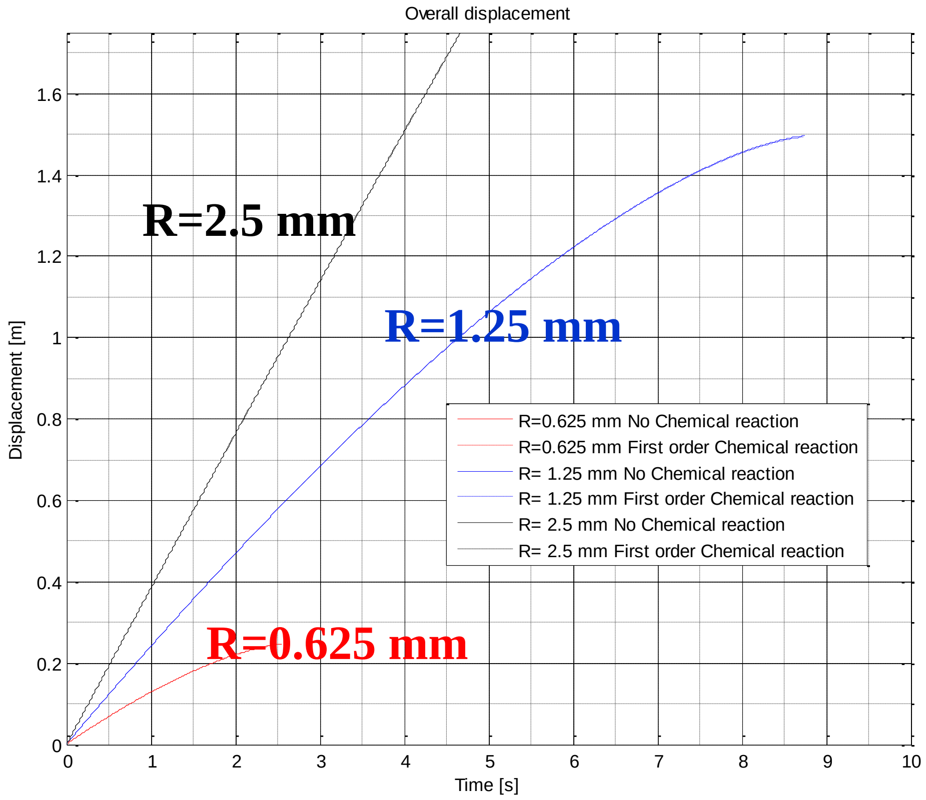
$$\frac{dm}{dt} = \Phi_A = -k_{mass} A_{sup} (C_A - C_{Bulk})$$

$$\frac{dm}{dt} = \Phi_A = -k_{mass} A_{sup} \sqrt{(1 + Ha^2)}\, (C_A - C_{Bulk})$$

A link between mass transfer boundary layer and bubble force is established through the mass time derivative of the dissolving bubble

Mass transfer for a single bubble

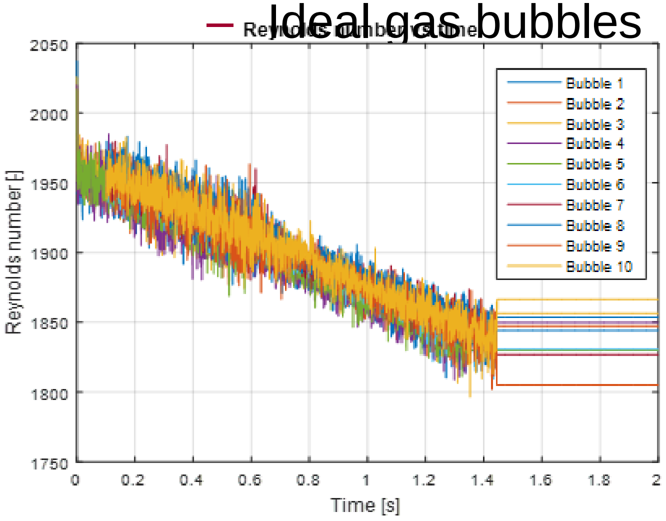


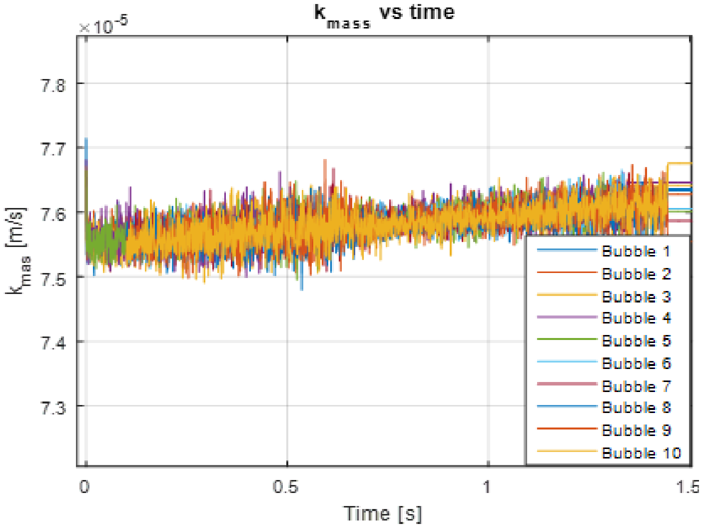


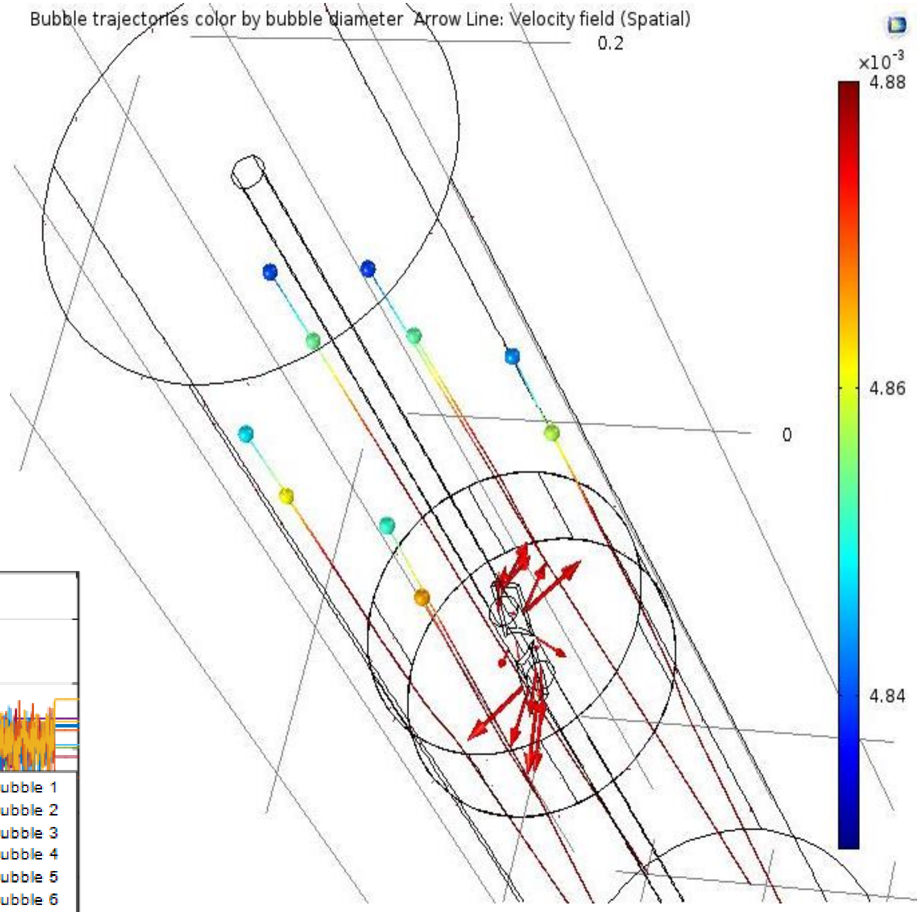
Under ideal conditions a rising CO_2 bubble of initial radius 1.25mm would dissolve after approx. 1,5 m displacement in a bubble tower

Bubble swarm Lagrangian tracking

- Bubble Tracking
  - Single and multiple bubble interaction
  - Mass transfer boundary layer
  - Local internal bubble pressure related to the local fluid pressure drop.
  - Ideal gas bubbles

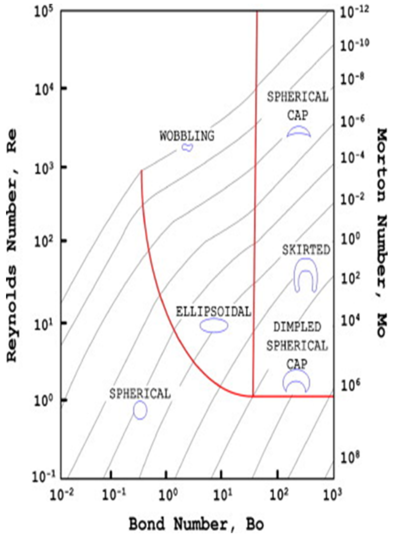


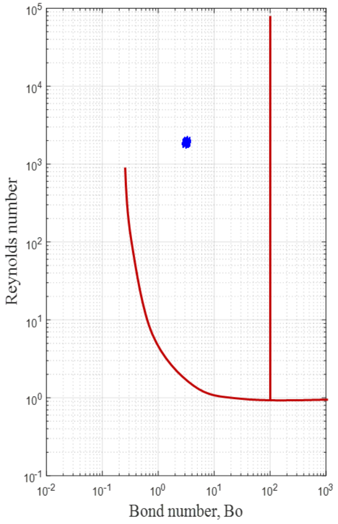


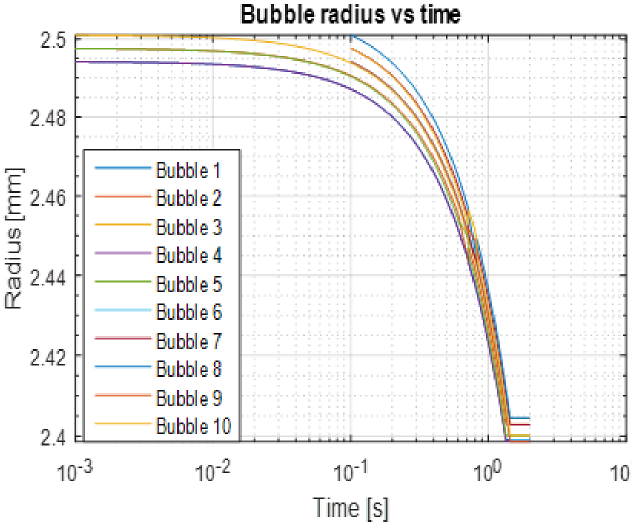


Bubble swarm Lagrangian tracking

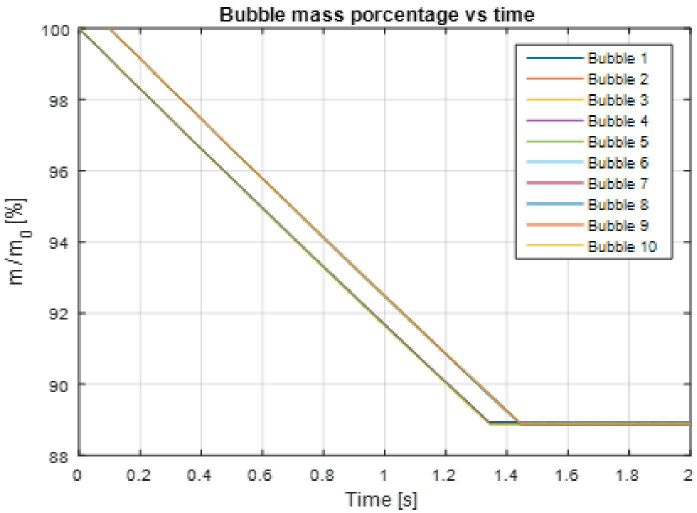
- Bubble Dissolution
  - Bubble shape drag coefficient tracking
  - Chemical reactions effects negligible: maximum values of Hatta number ≤0.0386
  - Mass dissolution







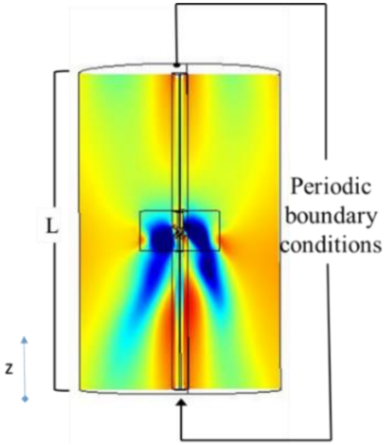
A total mass loss of approx. 11% is found in the first tower section for the bubbles even if the bubbles only experience a 0.2 mm change in diameter.

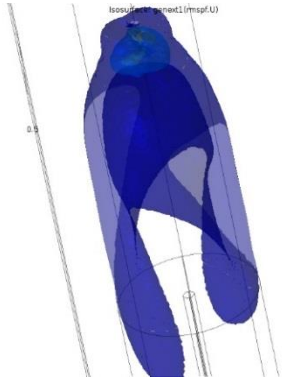


Stacked tower of fluid

- A bubble tower slice of height “L” is modeled

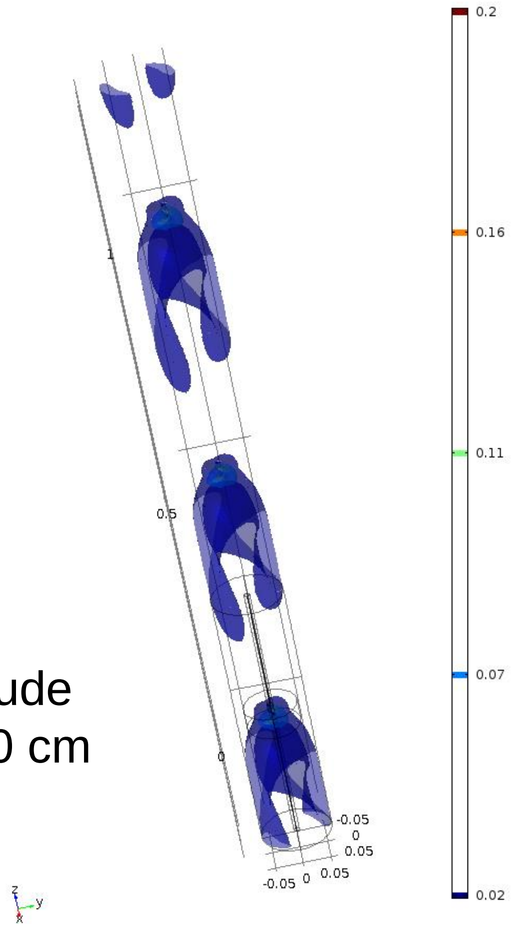
1





- Flow field solution for a slice is copied and stacked to form a

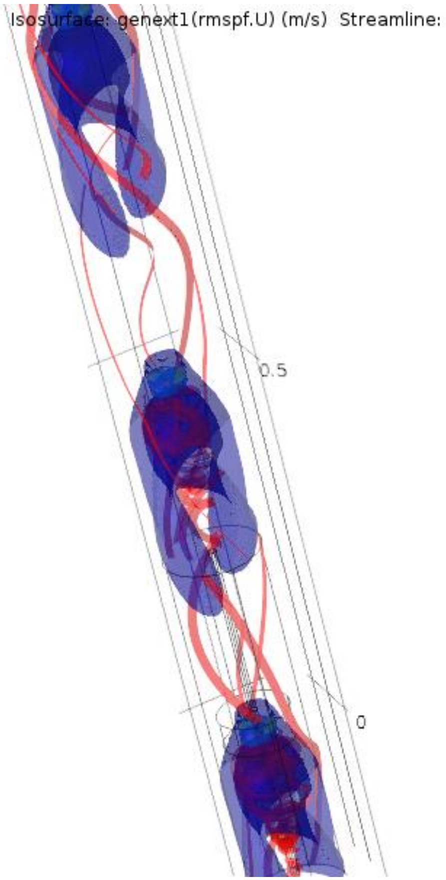
2



Isosurfaces
Velocity magnitude
Ω =100 rpm L=50 cm

- Influence of neighboring impellers is studied

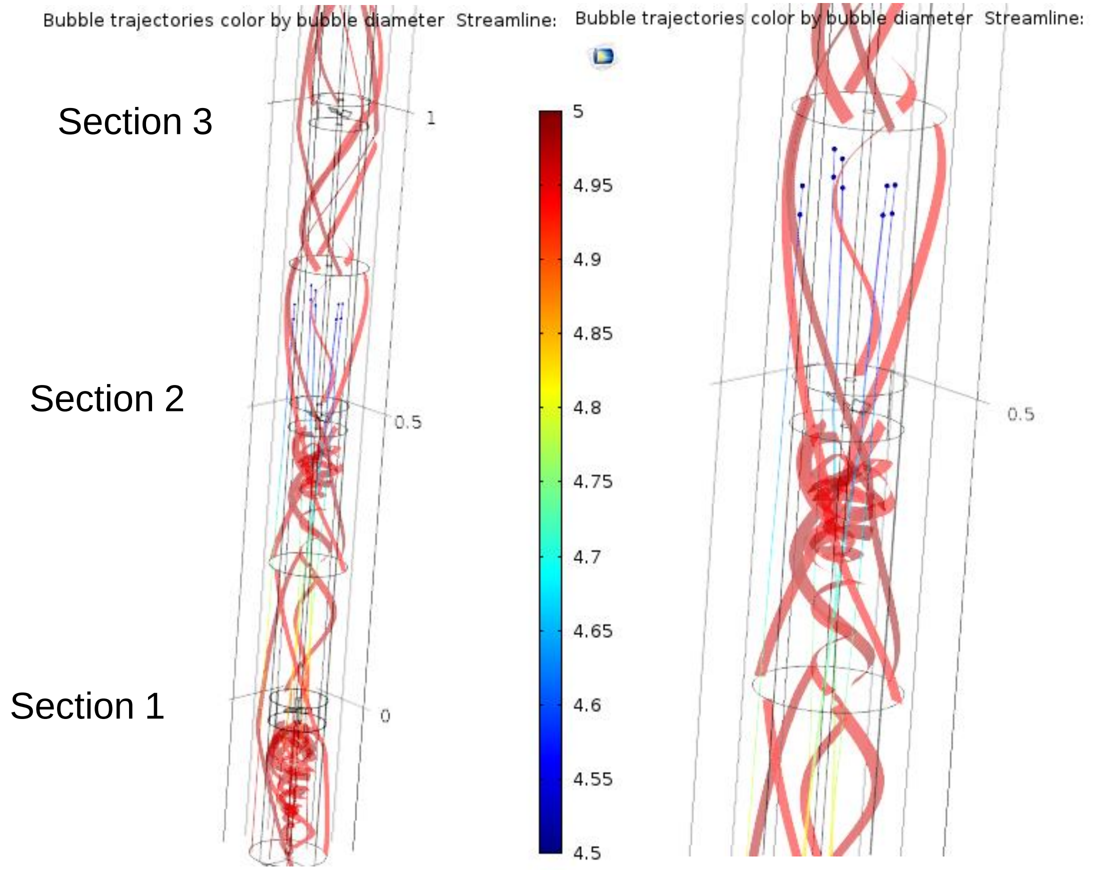
3

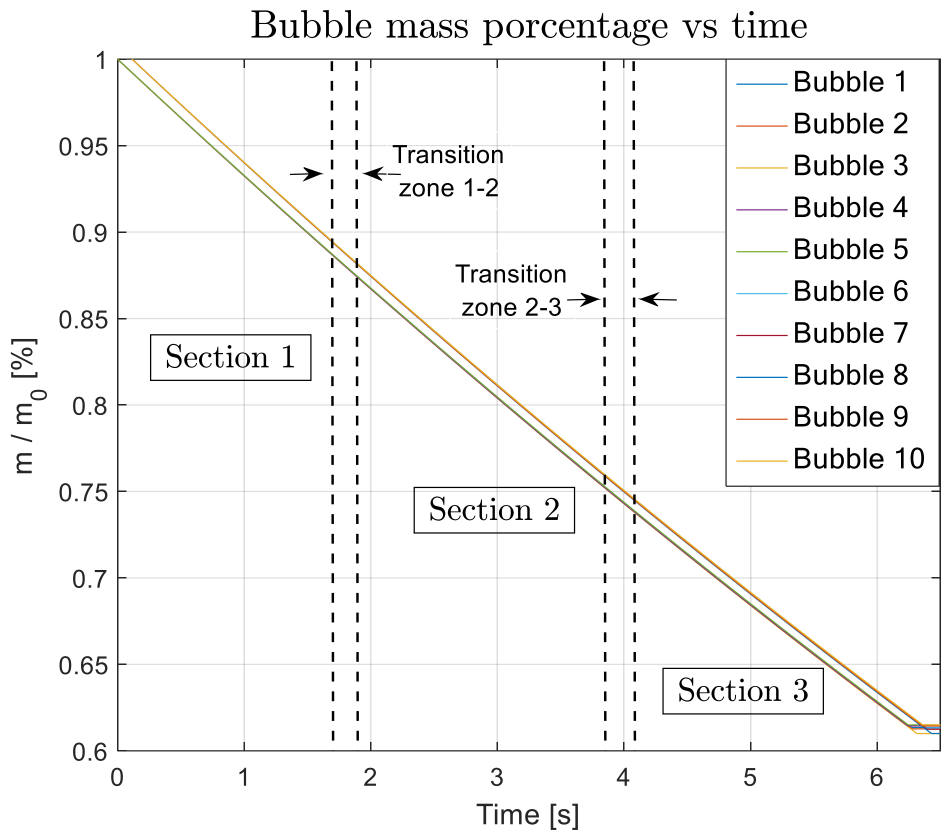


General
Extrusion
Operator

Bubble dissolution in tower of fluid

- Bubble Tracking*

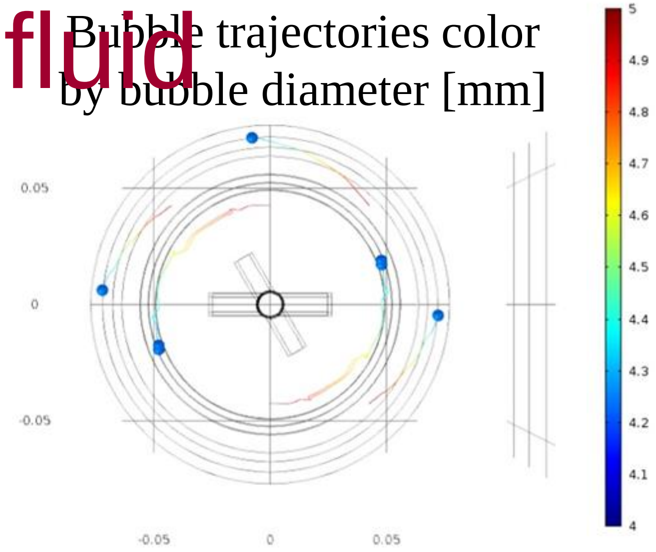


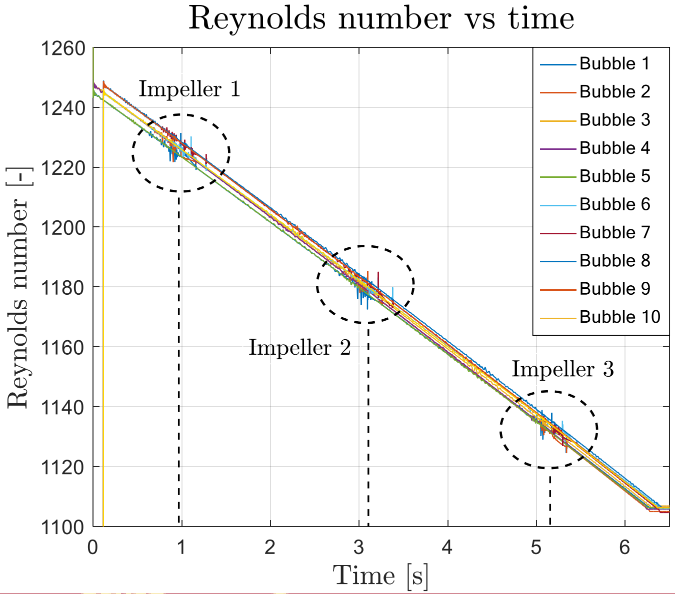


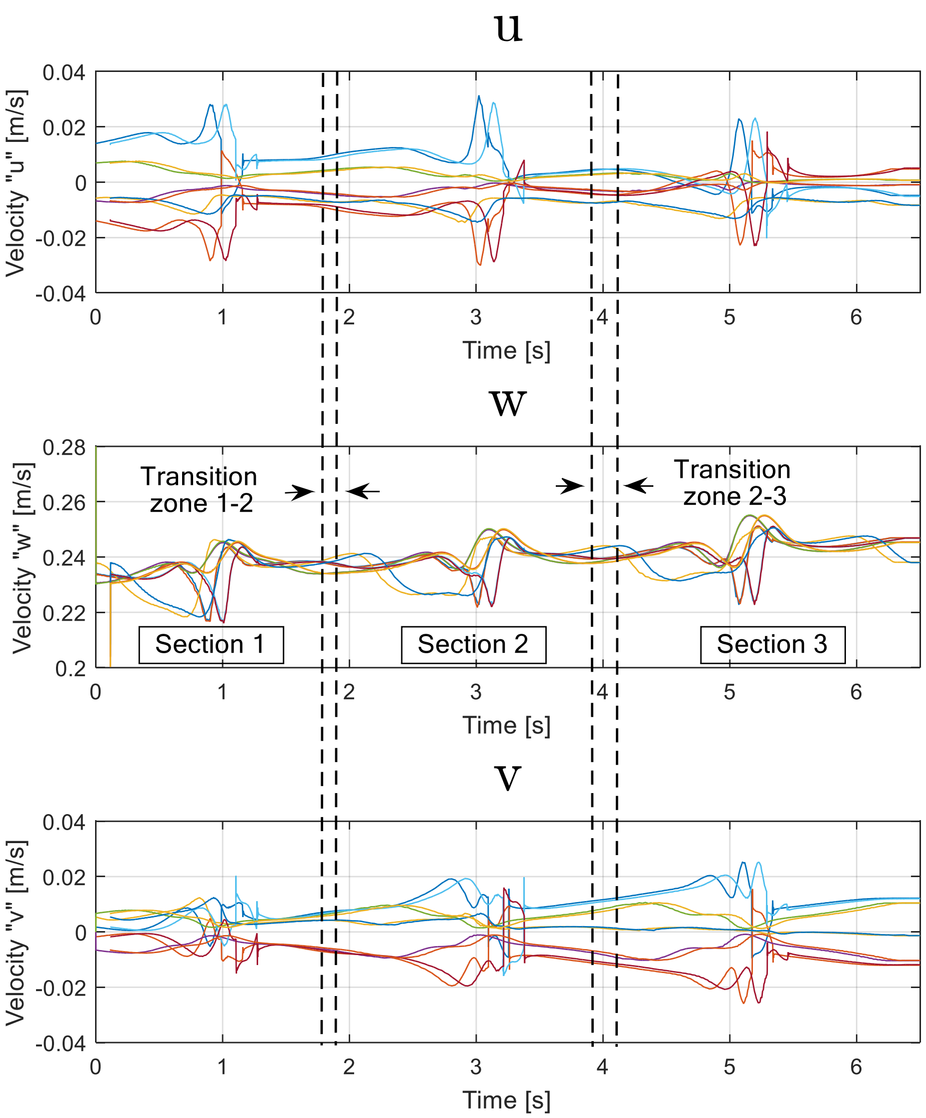
A total bubble mass dissolution of approx. 38% is found in 3 tower sections of 50 cm.

*Spherical shape deviation effects taking into account according to Roghair et al. 2011

Bubble dissolution in tower of fluid







Conclusions

- The mass diffusion profile seems realistic, bubbles become smaller and decrease their Reynolds number
- First order chemical reaction has a minor effect on the total mass transfer
- Deviation from spherical shape tracking is necessary for more complicated trajectories
- The final goal is to fill the gaps between the numerical and experimental approaches, concentration profile modelling with a simple time-dependent exponential profile
- Design a solid hybrid model for bubble reactors

Thank You

Questions
?

Daniel Legendre
PhD candidate, Åbo Akademi University
Daniel.legendre@abo.fi