Virtual Upscaling:
Modelling Ettringite precipitation process

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CFD model: Ettringite precipitation process

Computational Fluid Dynamics

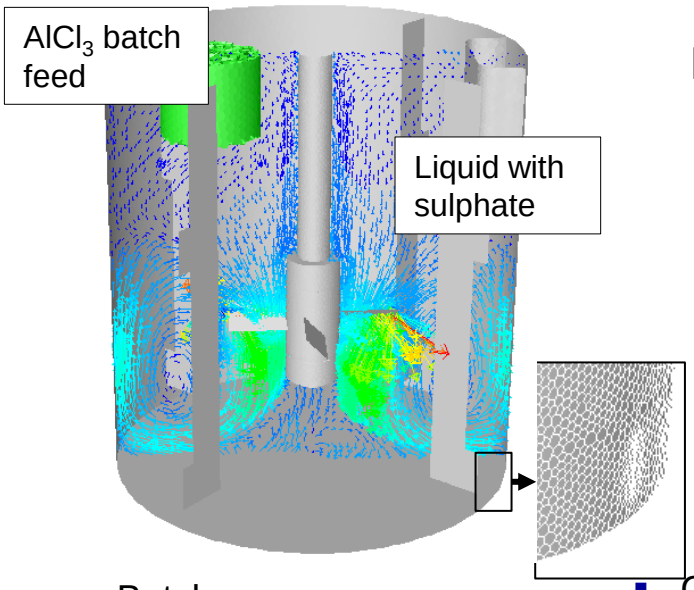
Thermochemical equilibrium

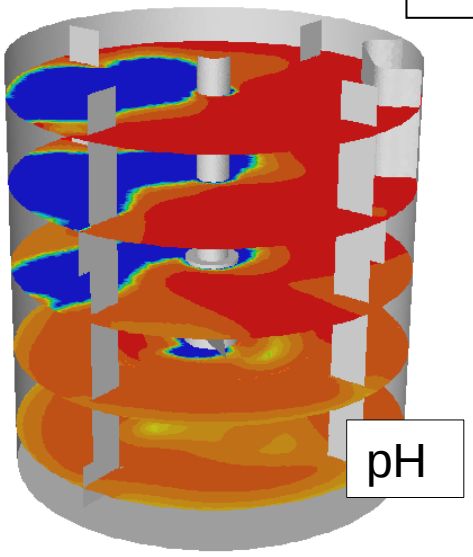
supersaturation is driving force for precipitation

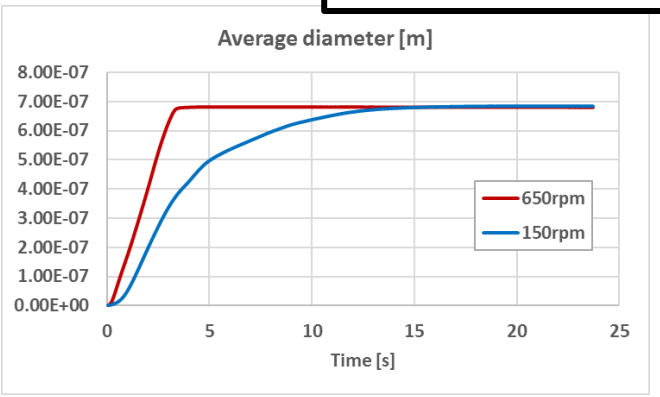
Precipitation kinetics

Nucleation rate

Crystal growth rate







- Batch process
- The mixing process is modelled with multiphase unsteady CFD including species transport

- Calculation of thermodynamic equilibrium in the liquid phase
  - Thermodynamic equilibrium is solved in every computational cell at the end of every time step (at the present: ChemApp)

- Monitoring as a function of time: average over the total reactor, or point monitors, e.g.
  - precipitated mass
  - particle size distribution
  - species concentration
  - pH

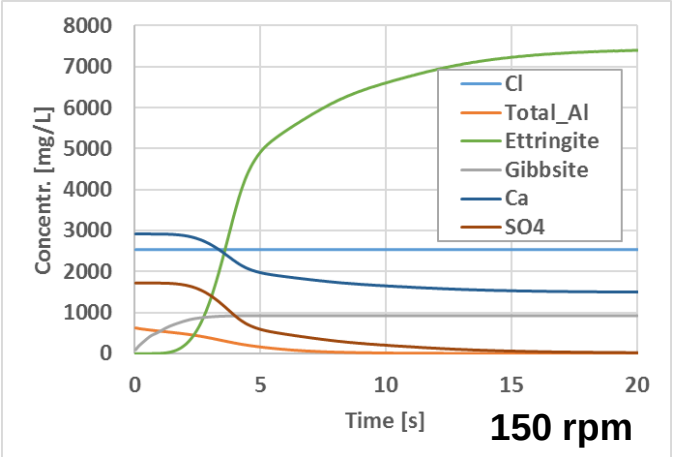
CFD model: Ettringite precipitation process

Benefits of CFD:

- Region for precipitation inside the reactor visible
- Effect of rotor type or mixing speed on precipitation realized
- Effect of feeding location of reactive agents can be studied

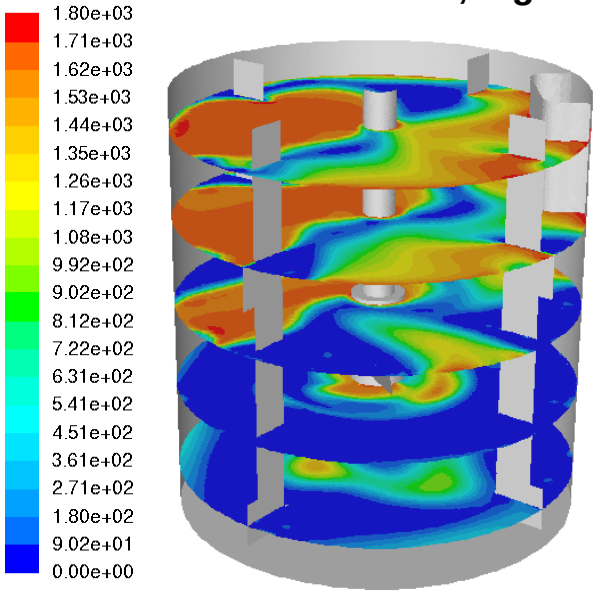
Needs for development:

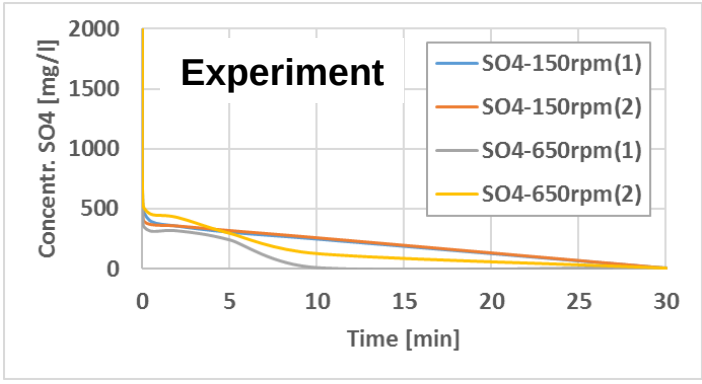
- Validation with experiments showed the need of redefine the set of species included
- Parameters for the kinetic models of precipitation need to be determined



150 rpm

SO_4^{2-} concentration at time instant 5 s, mg/l





Virtual Upscaling: Ettringite precipitation process

- Batch ettringite precipitation studies using Reaction Calorimetry (RC) (Tommi Kaartinen, VTT)
  - Thermodynamics and kinetics involved in the reactions related to the sulphate removal are determined
  - Temperature, type of stirrer (anchor, propeller), stirrer speed, dosing rate and seeds are to be focused in the experiments.
- Piloting ettringite precipitation with FLEXMET bench pilot equipment (Tommi Kaartinen, VTT)
  - Continuous pilot runs for SO_4-removal are executed.
- CFD model development for the ettringite precipitation process
  - Application of HSC for calculation of thermodynamic equilibrium
  - Determination of model parameters based on experiments
  - Is the amount of considered species sufficient?
- System level studies using process simulation
  - Interface between CFD and process simulation tool HSC Sim process is developed