Task 2.2: Creation of CFD model for the ettringite process development

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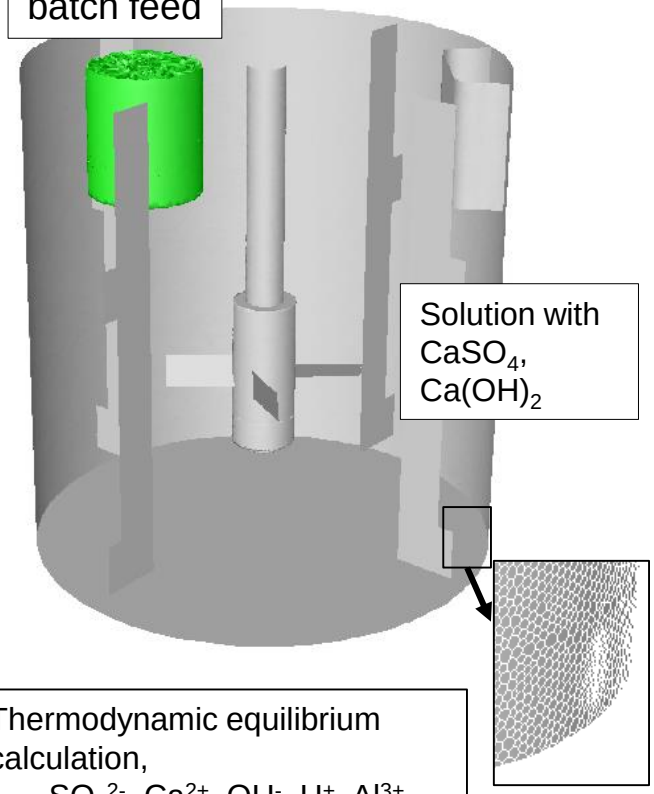
VTT

Task 2.2: Creation of CFD model for the ettringite precipitation process development

- Precipitating solid particles in the process liquid in the reactor
- The modelling of precipitation was based on an assumption of local ion equilibrium in the liquid phase, due to the fast dissociation reactions.
- The mixing process was modelled with multiphase unsteady CFD including species transport and applying MRF (Moving Reference Frame) technique for modelling rotating mesh.
- Solving of thermodynamic equilibrium in system with several chemical components was carried out using HSC software coupled to the precipitation kinetics in CFD (AnsysFluent 18.1)
  - Equilibrium was calculated with HSC 9.1 in every computational cell in every time step during the simulation (EQAqua)
  - Interface for coupling CFD and HSC (HSC 9.1) developed in project was applied
- Batch process modelled
  - Due to the delay in the experiments with continuous process (Task 2.1), the previous results with batch process were applied.

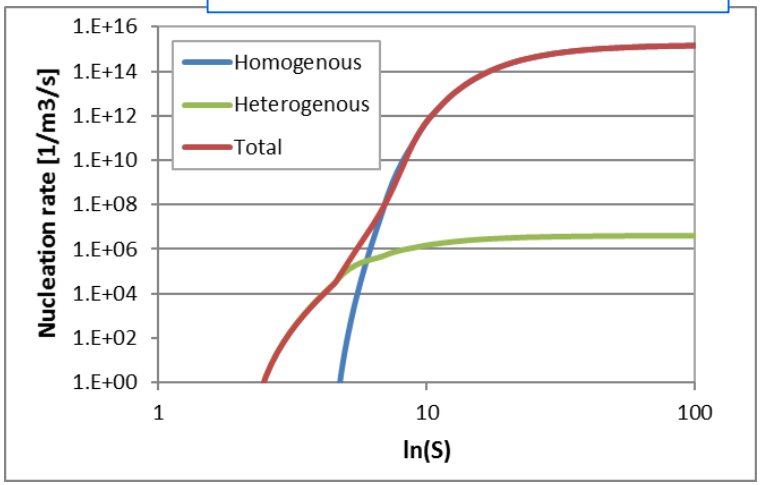
Total volume 5.25 L
Patch region 55.9 mL
150/650 rpm
Grid size: 259 000 cells



Thermodynamic equilibrium calculation,
- SO_4^{2-}, Ca^{2+}, OH^-, H^+, Al^{3+}, Cl^-, $Al(OH)_4^-$
- $Ca(OH)_2$ (portlandite), gibbsite, ettringite

Precipitation kinetic models:
Nucleation and growth rate

$$J_{Total} = J_{\text{het}} + J_{\text{hom}}$$



- Precipitation from a solution includes several sub-processes
  - In here, nucleation and crystal growth are considered
  - Solubility of Ettringite is very small

$$c^*(Ettrinigite) = 1.26\text{e-}45 \text{ mol/L}$$

  - Saturation ratio is modelled as

$$S_\beta = \frac{c(Ettringite_{(aq)})}{c^*(Ettringite)}$$

$$J_{het} = 4.0 \cdot 10^6 \exp\left(\frac{-100.0}{\ln^2 S_a}\right) \qquad J_{\text{hom}} = 1.5 \cdot 10^{15} \exp\left(\frac{-800.0}{\ln^2 S_a}\right)$$

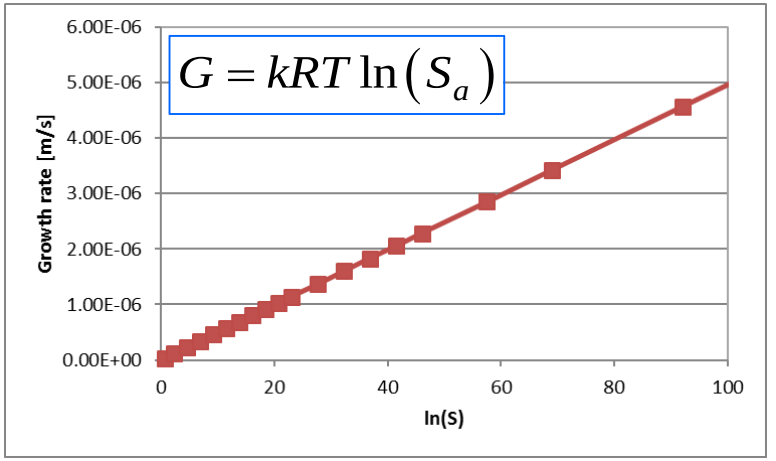
Thermochemical equilibrium

supersaturation is driving force for precipitation

Precipitation kinetics

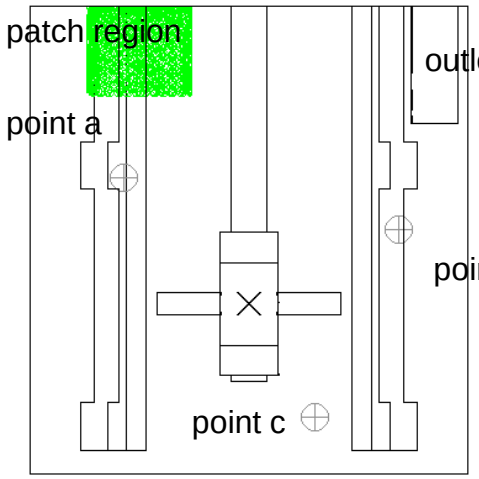
Nucleation rate

Crystal growth rate

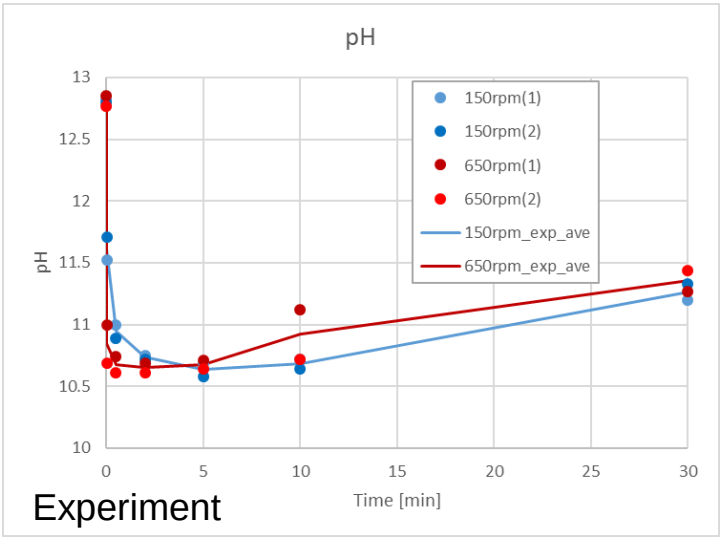


k=2.0e-11

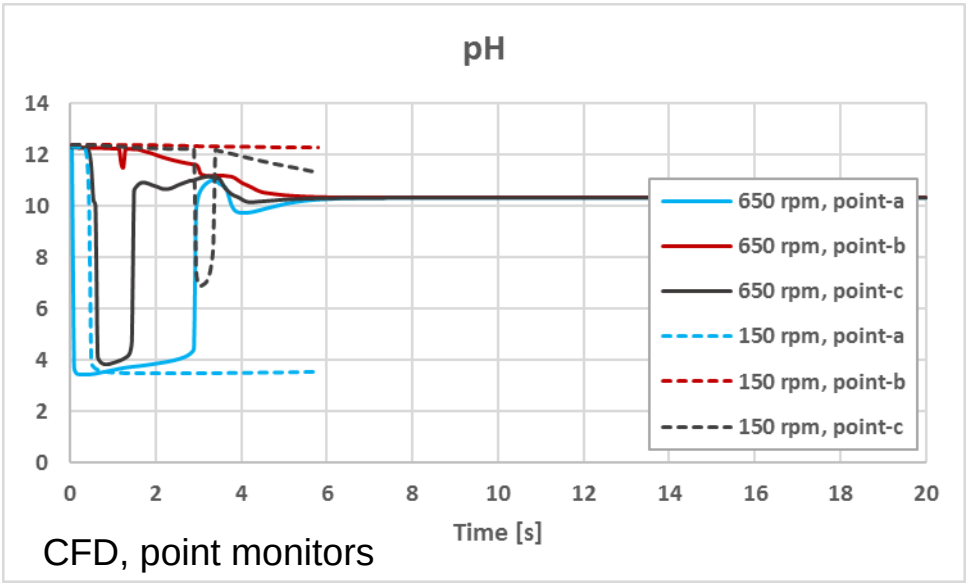
CFD results for pH



Point monitors are placed at the vertical plane through outlet, patch region and axis

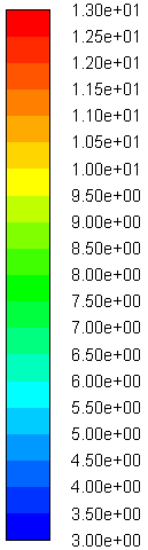


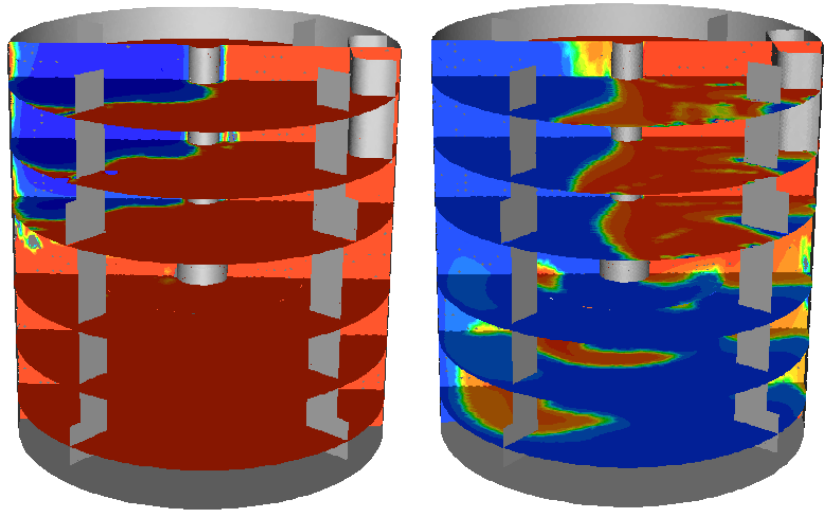
Experiment



CFD, point monitors

Time instant of 1.25 seconds



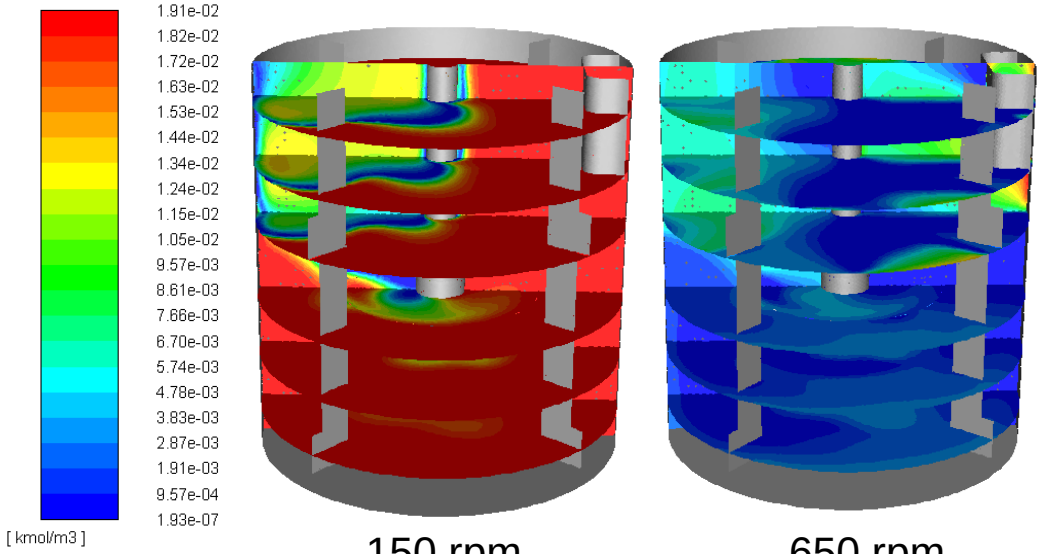


150 rpm

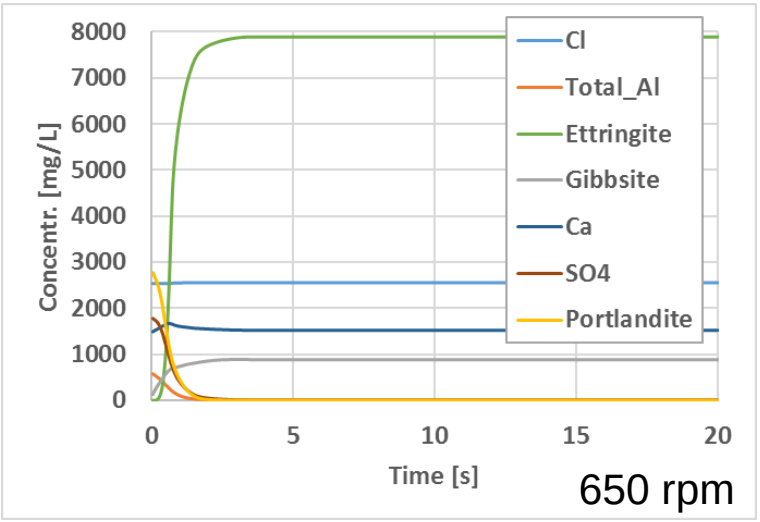
650 rpm

CFD results for species concentrations

Molar concentration of SO_4^{2-}



Average concentrations as a function of time, mg/l



Time instant of 1.25 seconds

Final concentrations:

HSC, Simulation 650rpm :

- Ettringite 7891 mg/L
- Gibbsite 1957 mg/L
- Portlandite 3.51 mg/L
- Calcium 1524 mg/L
- Sulphate 7.48 mg/L
- Aluminium 277 mg/L
- pH 10.32

Experiment (filtering with 0.45µm)

- Average solid concentration
  - 150rpm: 6724 mg/L
  - 650rpm: 6594 mg/L
- Calcium 1100 mg/L
- Sulphate <40 mg/L
- Aluminium ~150mg/L
- pH (30 min) 11.35

Conclusions

- The simulation of ettringite precipitation process was carried out assuming only ettringite in a solid phase. Other constituents were in liquid phase, also gibbsite and portlandite.
- Final pH was lower than with the experiments.
- The simulation result for the solids mass was larger than the final experimental value.
- The time period for the precipitation process in simulated results was much shorter (~ tens of seconds) than in the experiments (~ tens of minutes). This was seen e.g. in the evolution of pH in the solution.
- There was not enough experimental data for determining the kinetic model parameters.
- The simulation is extremely time consuming
  - Attempts were made to apply look-up-tables for the equilibrium values: if the change in the concentrations is inside the predefined limits, the values for concentrations are taken from the table (from previously calculated results)