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Electrochemical water treatment
Process level simulation model

Virtual Upscaling workshop Dec 20 2017

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Outotec Electrochemical Water Treatment

- Modular product to combine water treatment, process design, electrolysis & hydrometallurgy knowhow

- Purification of waste water based on electricity & right combination of electrode materials

- Easy & automated process allowing minimum presence of personnel with high quality & performance

- Modular & containerized plants are ideal for remote locations with minimum transportation and installation needs

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Basic phenomena

- Water flows between electrodes
- Electricity with right electrode materials generates desired oxidative/reductive conditions, dissolves metal from anode to water
- Dissolved metal (for example iron) reacts with impurities & with water itself, forms solid particles
- Electric field affects surfaces of solid particles, enhancing solids separation
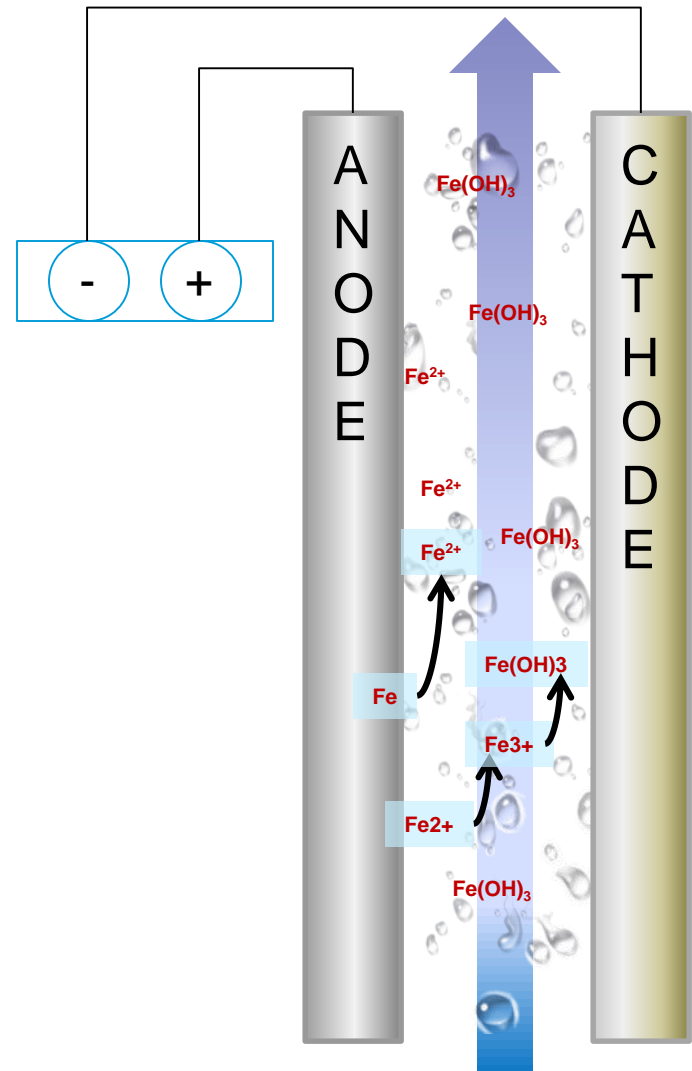
Virtual Upscaling topics

- Upgrade process simulation model, including equipment sizing & design basis
  - →Define relevant chemical equations to simplify complex phenomena
  - →Fine tune control setup
  - →Link downstream logic to upstream setup

- Goals
  - →Better usability for process engineers
  - →Process flowsheet development / mass balance calculations
  - →Opex/Capex calculations
  - →Empirical scale-up factors + other scale-up input
  - →Integrated process design module to a plant configurator
  - →Maintenance frequency (e.g. plate change) estimator
  - →Modelling of dynamic power control

- What can we input from CFD?

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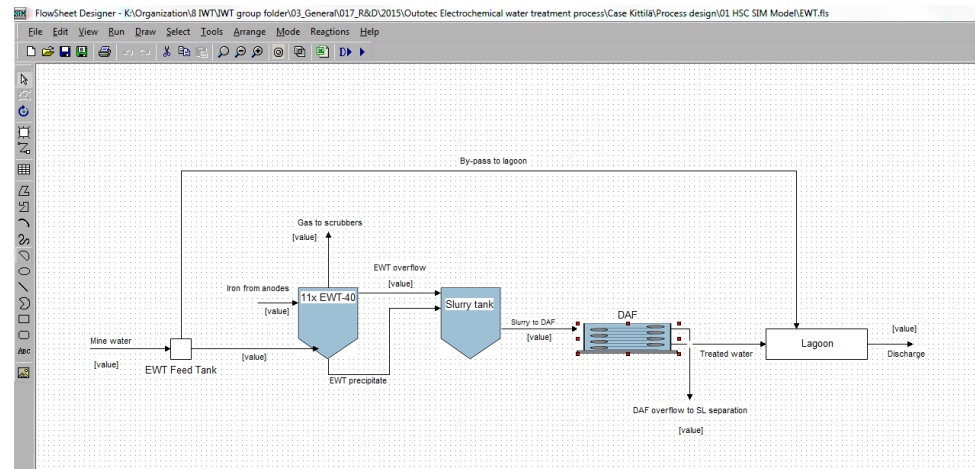
Testing as basis of process modelling

- Testing and verifying done on lab (5 l/h), pilot (50-200 l/h) & demo scale (1-20 m^3/h)
- Modelling results compared with data obtained from different scales
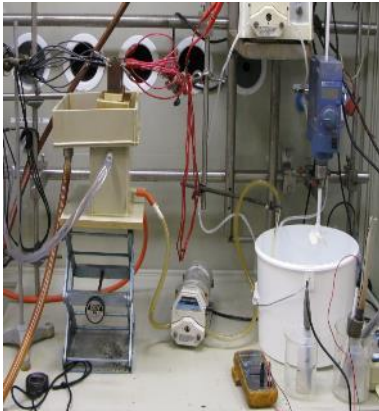
Process level simulation model findings & status Dec 2017

We were able to demonstrate the link between CFD and HSC calculating the local electrochemical reaction mass balances

However, when comparing experimental concentrations with predictions, we concluded that:

- The system is not in steady state equilibrium but the electrochemical reactions are strongly kinetically restricted; thus the reaction model using Gibbs free energy minimization is not adequate

- In order to take kinetic factors into account, relevant constraint functions need to be developed

(In current modelling process this is handled by manually set macro scale reaction rates that are based on experience and empirical data)