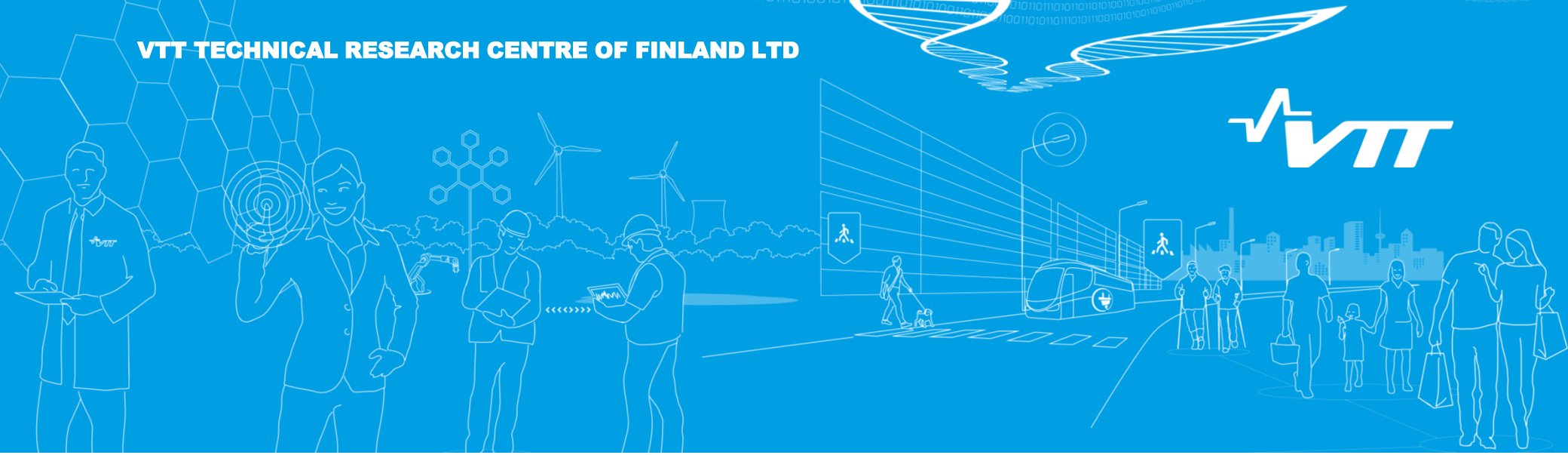

Task 2.3: Creation of CFD model for the EWT process development

20.12.2017

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VTT

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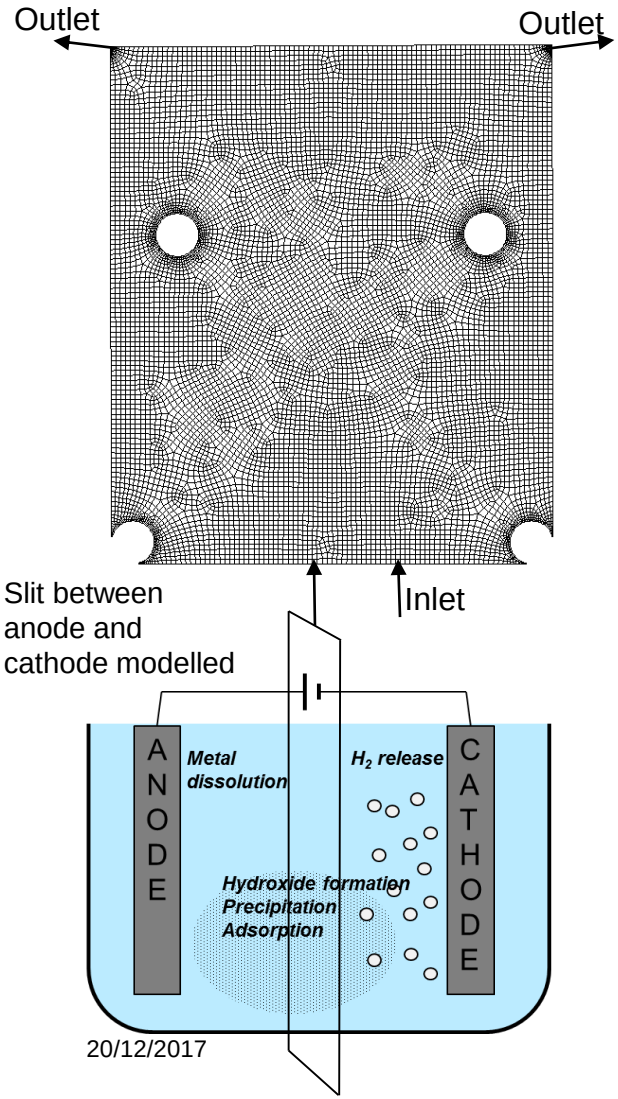


Electrochemical Water Treatment (EWT):

Computational Fluid Dynamics (CFD) modeling coupled with HSC Chemical equilibrium calculation for simulating precipitation process.

- A simplified CFD model for EWT process developed (Ansys Fluent 18.1)
- Time dependent simulation with species transport
- Thermodynamic equilibrium calculated with HSC 9.1 at the end of the time step within every computational cell
- Interface for coupling CFD and HSC developed (HSC 9.1)

- Geometry:
  - Width 0.924 m
  - Depth 0.006 m
  - Height 1.085 m
- Grid size: 165 000 cells
- Temperature 288.15 K

Anode: dissolution of metal ions by oxidation

Cathode: reduction of water into hydrogen (gas)

Bulk liquid: hydroxide formation, reactions with pollutants, precipitation, settling (or flotation) of particles

Coupling CFD with HSC for calculating thermodynamic equilibrium

- The coupling has been made using the AddIn-functionality of the HSC Chemistry.
  - The functionality allows to call the chemical equilibrium solver using a COM-interface from C or C++ code.
  - As COM interfaces are relatively complicated to use with pure C, a separate C++ wrapper has been created which makes it easier to use the interface from UDFs written in C.
  - The wrapper is called using C-style conventions and no knowledge of C++ is required to use the coupling from UDFs

Function	Description
int openInterface()	Opens the COM-interface to the HSC. This has to be called at least once before calling any HSC-specific functions. Nonzero return value indicates an error.
void closeInterface()	Can be called to close the interface, optional.
int loadSpecies(const char* fileName)	Load species from the given filename. The file must have UTF-8 encoding with one line per phase or specie. Returns the number of species (including phases) that were loaded.
int streamEQAqua (const double* amounts, const double* ACs, double T, double p, double* results, int rounds)	Call the streamEQAqua-function from the HSC solver. The amounts, ACs and results are assumed to be arrays with a length equal to the value returned from loadSpecies. If the call is successful, results-array will contain the results returned from HSC. Nonzero return value indicates an error.

The functions defined in the C^{++}-wrapper

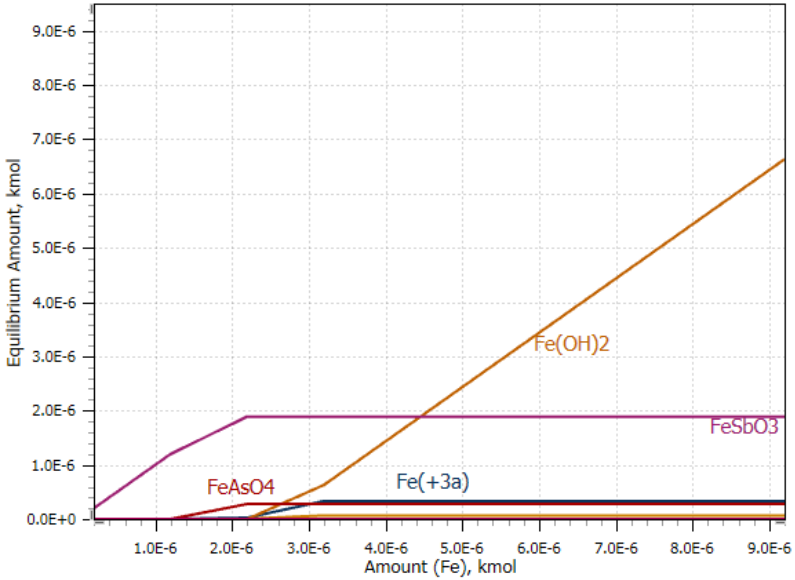
Studied chemical system

- The liquid and gas phase chemical and ionic species included in the (simplified) model are
  - $Fe^{2+},\ Fe^{3+},\ Ni^{2+},\ MnO_2^{2-}, H^+,\ OH^-,\ O_2,\ H_2$
  - $HAsO_4^{2-},\ H_2AsO_4^-,\ H_3AsO_4,\ Sb(OH)_4^-,\ Sb(OH)_3$
- The precipitating compounds are
  - $FeSbO_3,\ FeAsO_4,\ Mn(OH)_2,\ Ni(OH)_2,\ Fe(OH)_2$
- The effect of electric forces on the ionic species transport with user defined functions (UDF).

$$\bar{J}_e = -\frac{DzF}{RT} \cdot c\nabla\Phi$$

where D is the diffusion constant, z is valence of the ion, e is elementary charge, R is gas constant, T is temperature, c is the species concentration and Φ is the electric potential. As a first approximation the electric field ($\bar{E} = -\nabla\Phi$) can be approximated by a constant.

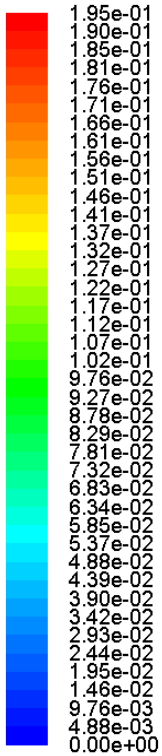
Equilibrium with HSC

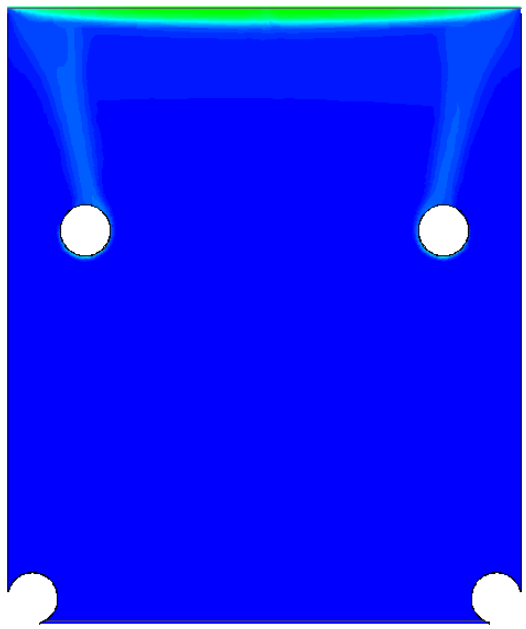


Simplifications applied

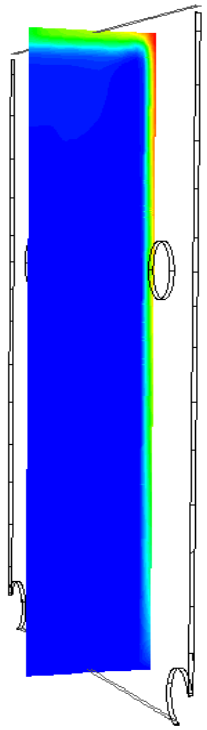
- The main focus was in coupling of different modeling tools. Therefore the CFD-model of the process has been kept simple.
  - Single phase approach is used, because it allows the use of ANSYS Fluent's electrochemical model. Precipitating particles and gas bubbles are modeled as species component. Slip velocity is then ignored, but the buoyant flow due to hydrogen gas concentration is accounted for.
  - Electric potential is solved from the Laplace equation, but the conductivity due to ion concentration is not correctly taken into account, because all ion species present in the feed are not included in the chemical model. Effect of gas on the conductivity is taken into account.
  - Chemistry is based solely on thermodynamic equilibrium. Kinetic reaction rates for liquid phase reactions or precipitation are not implemented. In particular, the solid formation is based on chemical compounds, attachment of metal ions to iron hydroxides through adhesion is not considered.

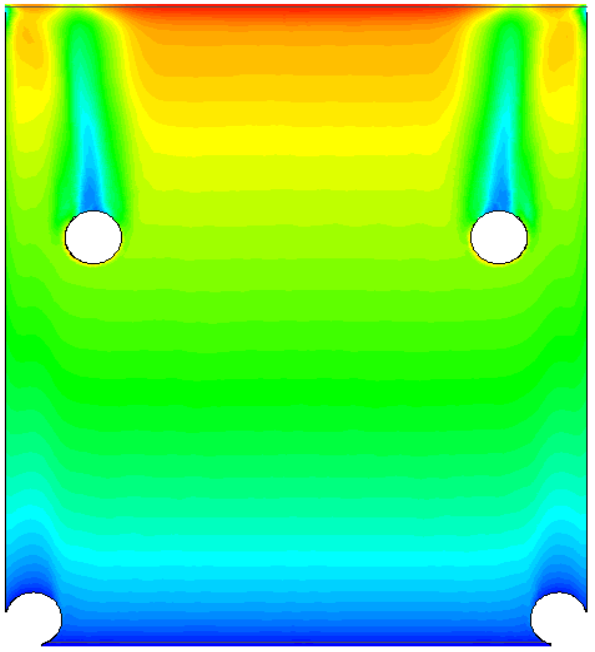
Effective volume fraction of H_2 bubbles





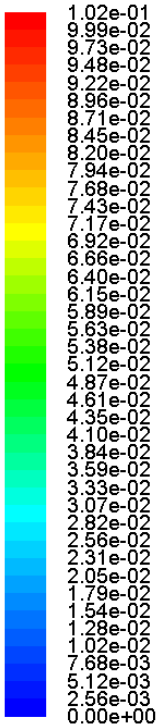
Anode

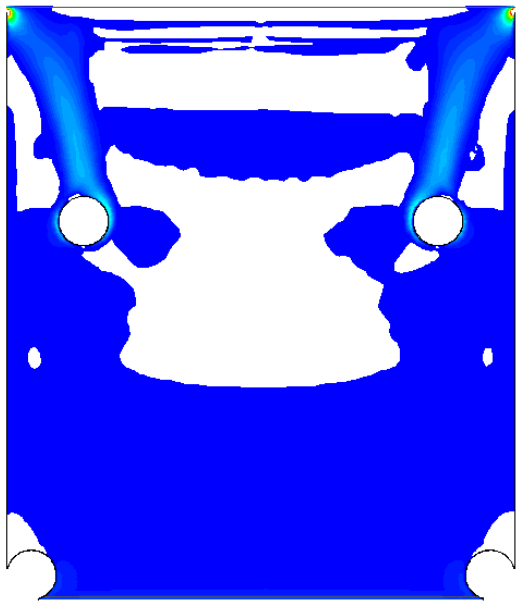




Cathode

Positive z-velocity, m/s





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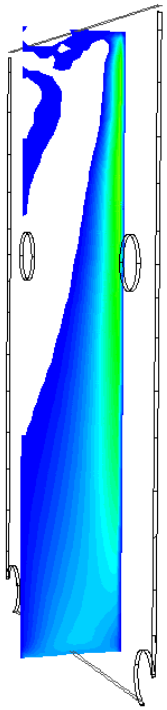
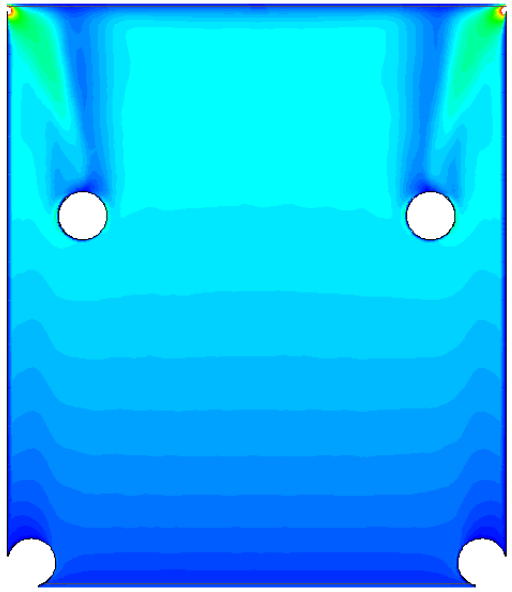
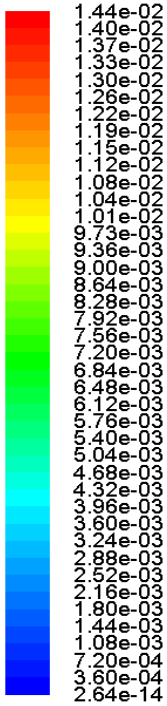
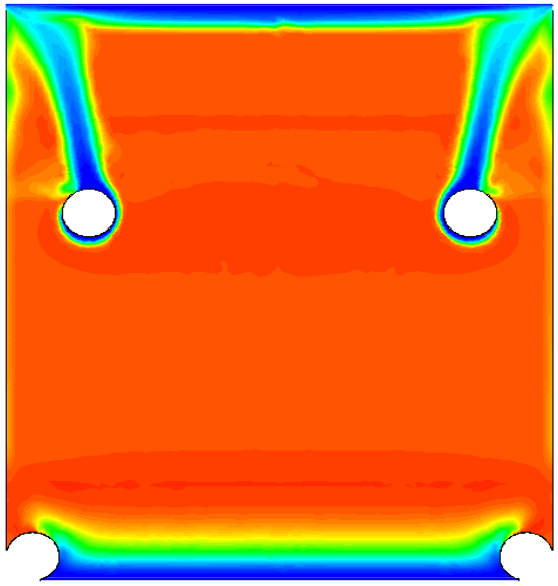




Cathode

Molar concentration of Fe_2^+ , mol/L





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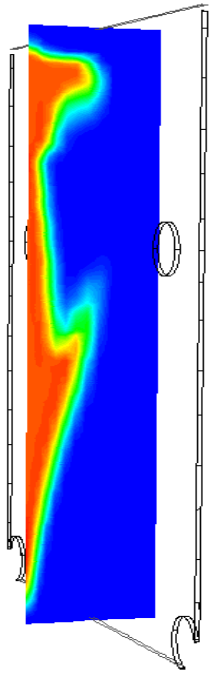
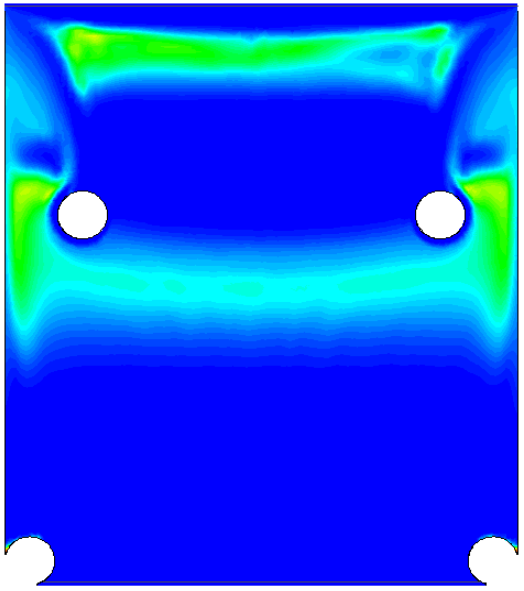
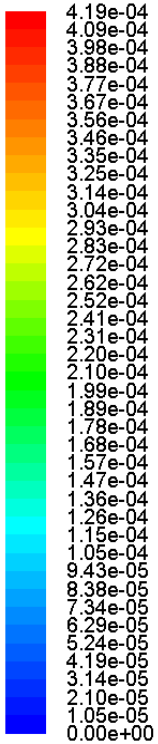
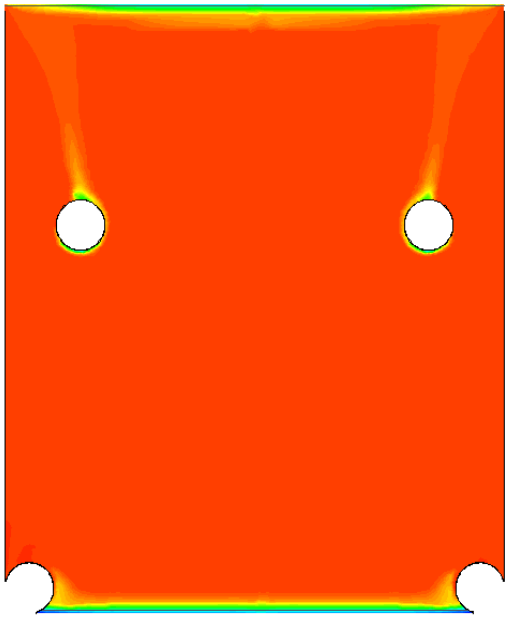




Cathode

Molar concentration of $Fe(OH)_2$, mol/L





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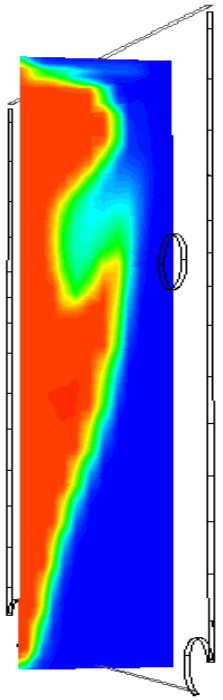

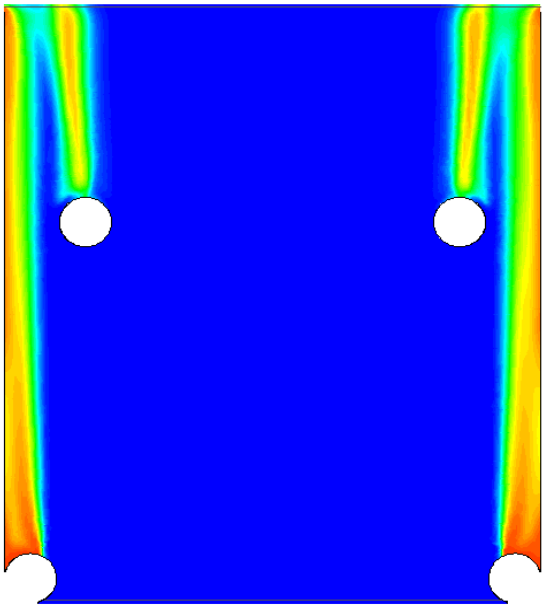

Cathode

Conclusions

- The thermodynamic equilibrium solver of HSC Chemistry, based on Gibbs energy minimization, was successfully coupled to ANSYS Fluent.
  - The HSC module is called in every computational cell in every time step (transient simulation) or iteration (steady state simulation). Therefore, the coupling must be fast.
- The first test case for the HSC-CFD coupling was the electrochemical water treatment process of Outotec. The model developed for the quite complex process is simplified, but nevertheless contains the most important elements needed to describe the process.
- The EWT process is not the best application for the chemical equilibrium model, because it is known that the system does not reach full equilibrium.
  - The methods for refining the model to include the kinetics of the process are studied further.
  - The present model already proves the value of the coupled modeling. This is the first time the EWT process is modelled with detailed local information of flow, species and gas distribution.
- The first test case of HSC-CFD coupling shows that this type of modelling approach is promising and can be applied in many types of chemical processes.