Virtual Upscaling

Combining CFD with Constrained Equilibrium Calculations

Task 2.4: System level studies using process simulation

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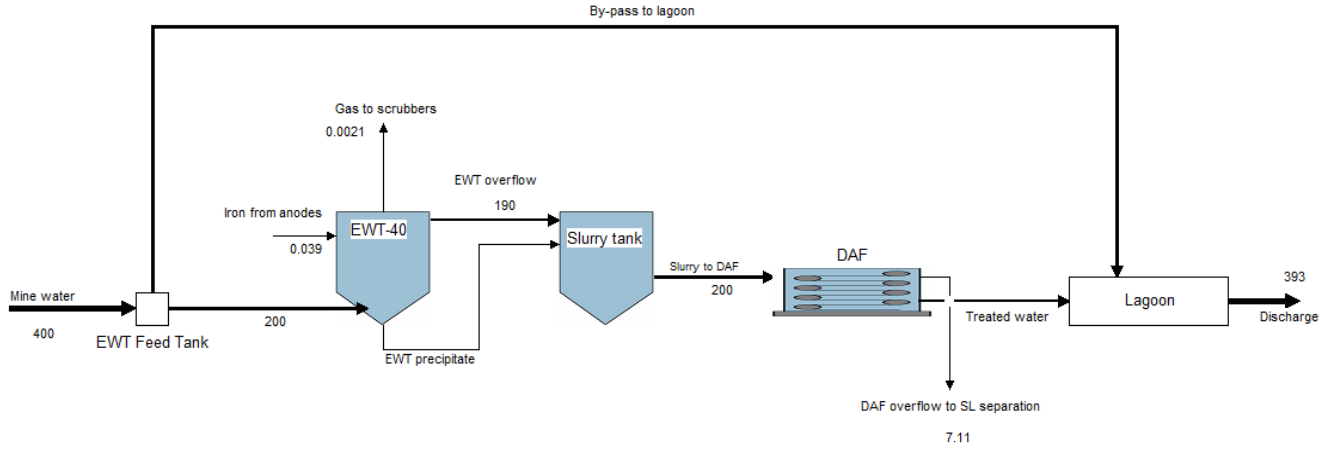
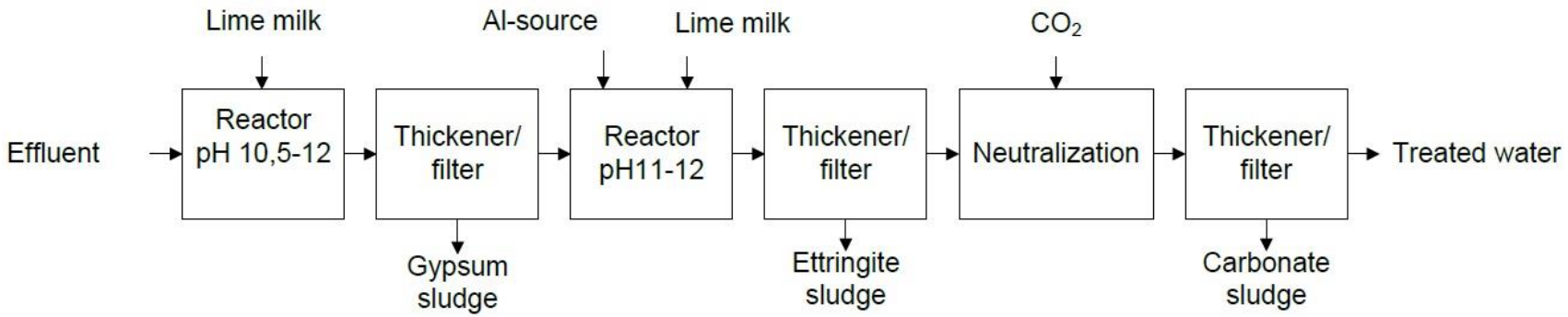
Test Cases

Electrochemical Water Treatment EWT (Outotec)

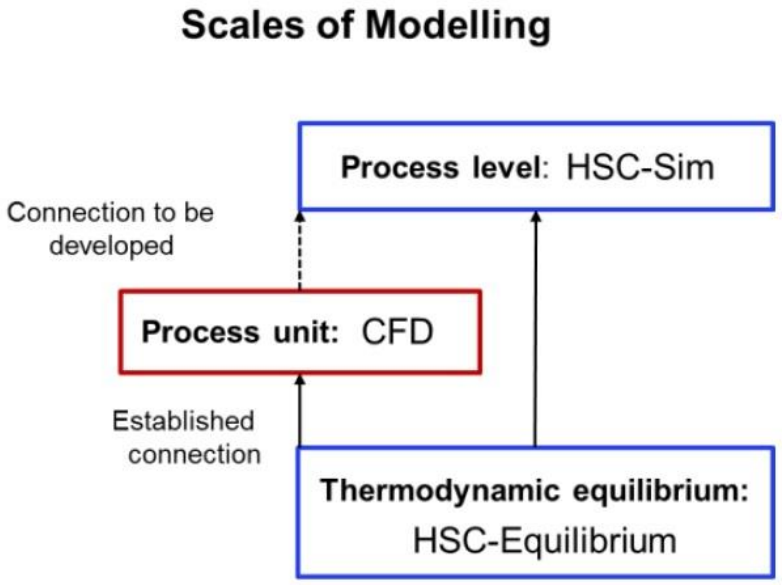


Ettringite Precipitation Process (VTT)



HSC Equilibrium module was coupled with Ansys Fluent

HSC Chemistry utilizes its own proprietary algorithm for Gibbs Energy Minimization. This algorithm uses a combination of method of feasible directions with linear programming (LP) problem. The solution of the LP problem is integrated into the search for the new feasible direction, which improves the overall calculation speed. The equilibrium solver is capable of handling multi-phase chemical systems, and the method is based on Gibbs energy minimization.



The HSC Equilibrium module was coupled with the Fluent CFD software. The link was done by Outotec and it was tested by VTT.

Results: Electrochemical Water Treatment, EWT (VTT)

HSC Equilibrium module was coupled with Ansys Fluent

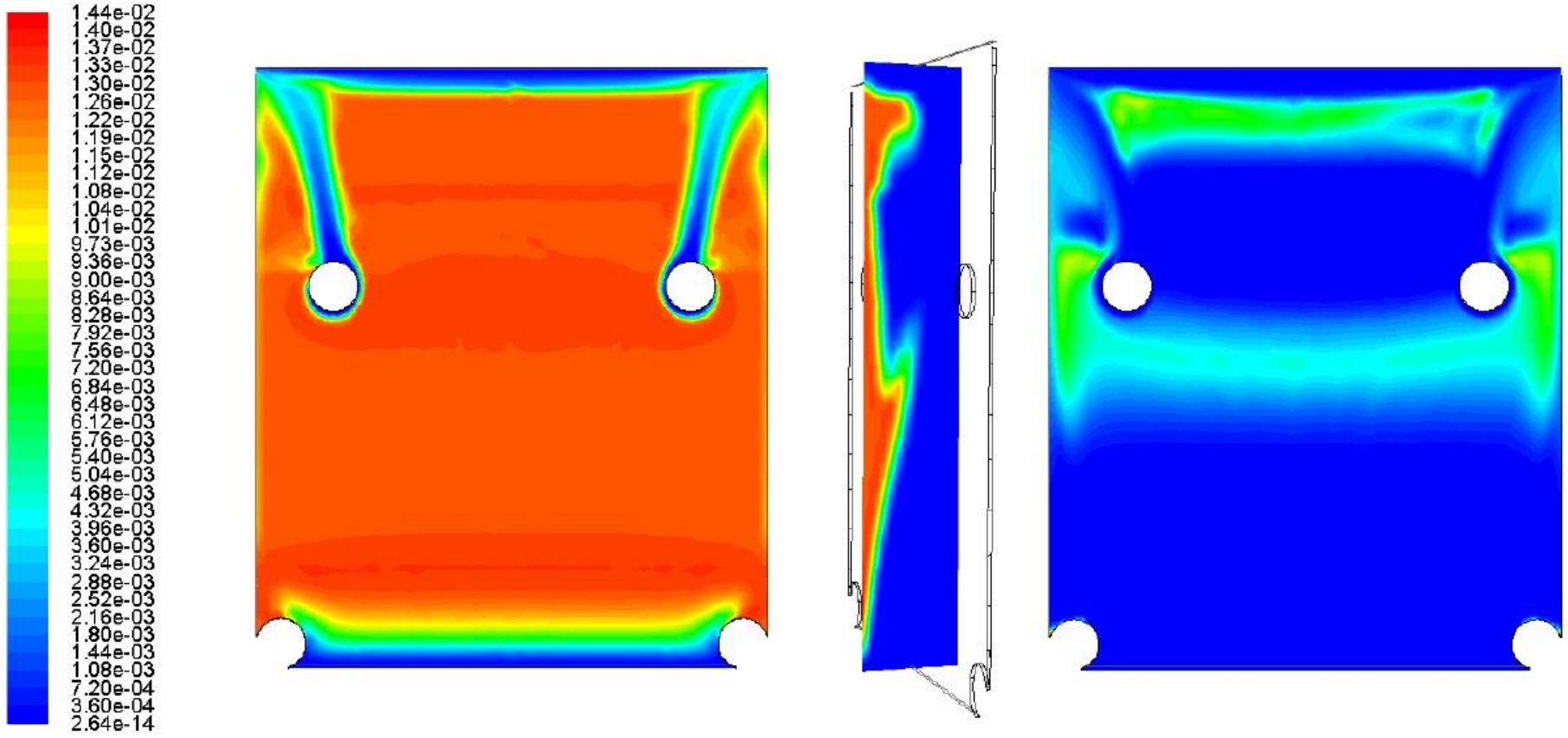


Figure 7. Molar concentration of Fe^{2+}, $kmol/m^3$. From the left: Anode, Between the electrodes, Centre between the plates.

Results: Ettringite Precipitation Process (VTT)

HSC Equilibrium module was coupled with Ansys Fluent

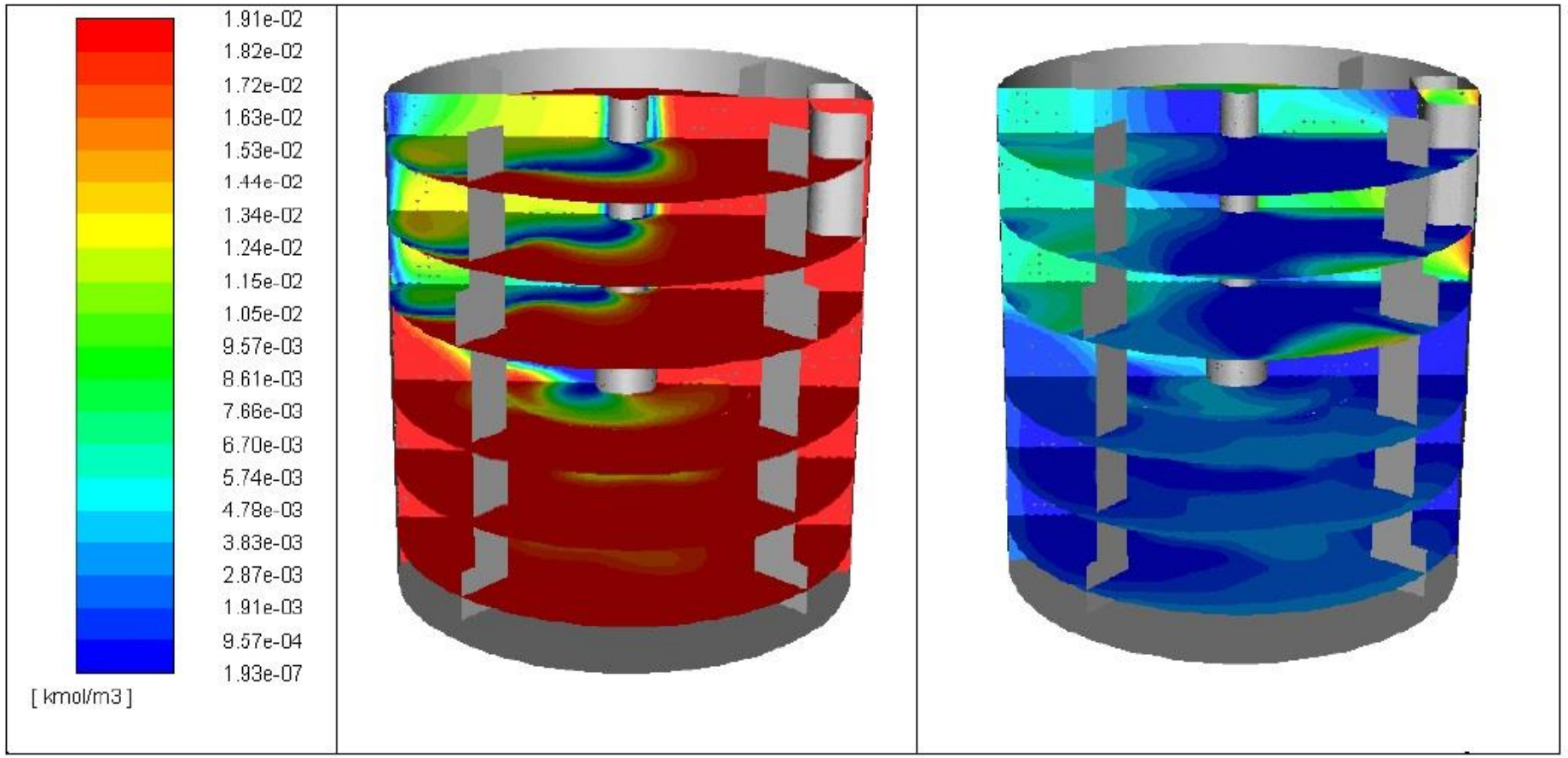


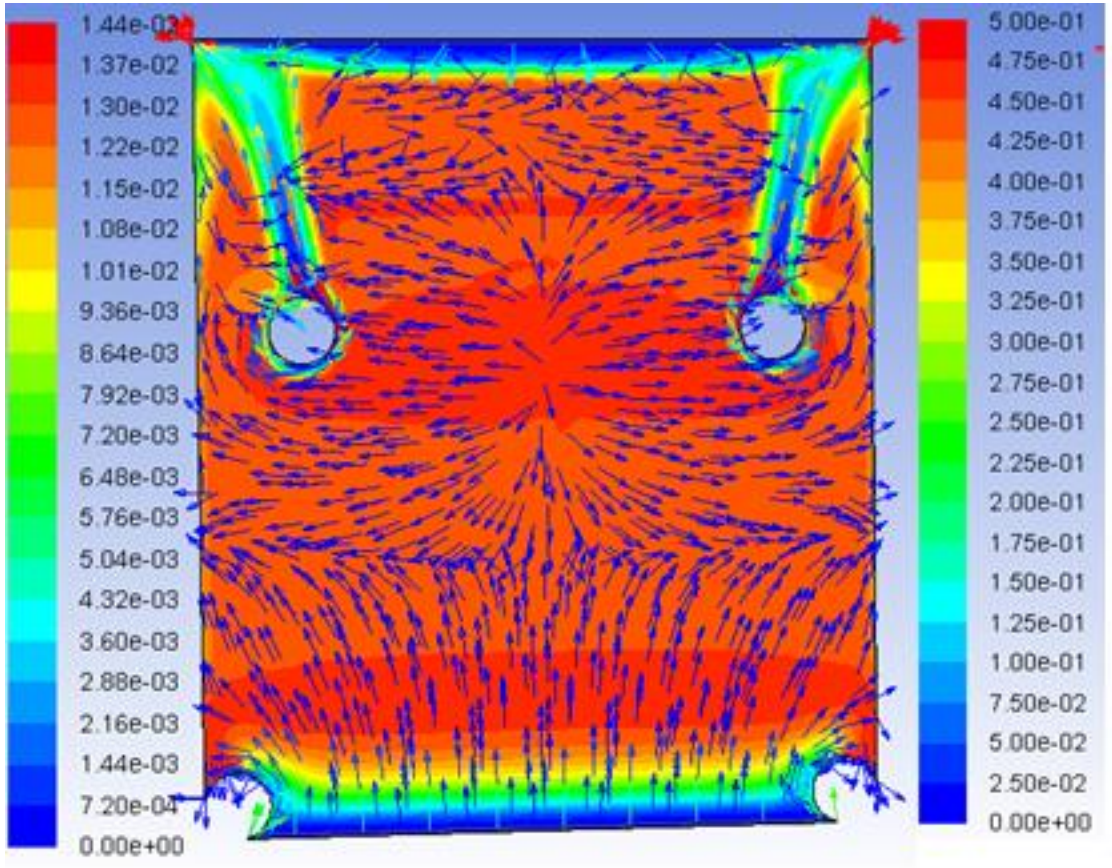
Figure 10. Sulphate ion, SO_4^{2-} distribution at the time instant 1.25 seconds a) 150 rpm, b) 650 rpm.

HSC Equilibrium - Ansys Fluent – Link Testing (Outotec, Jiliang Xia)

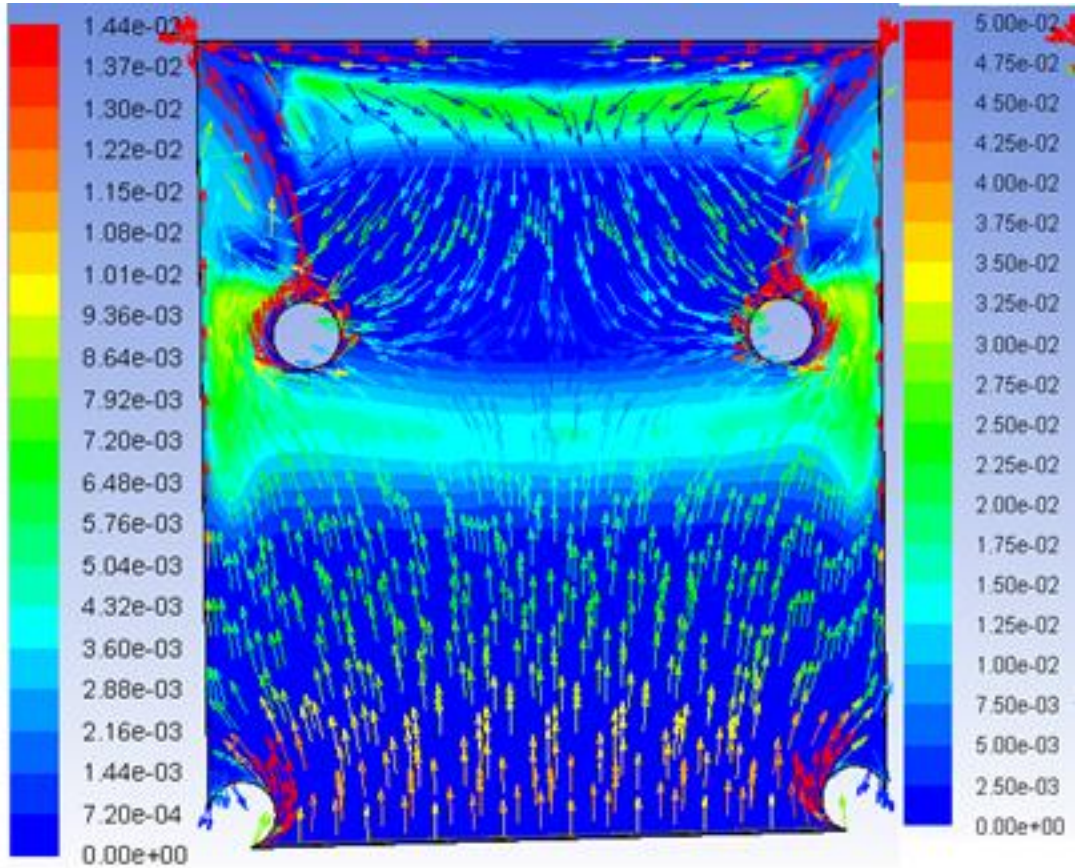
- Outotec developed the communication interface link from HSC Equilibrium module to the Fluent CFD software.
- VTT tested and validated the operation of the HSC-CFD coupling to utilize chemical equilibriums in CFD calculations.
- This kind of HSC-CFD coupling is especially valuable when the drastic change of flow and thermal fields in a process is involved.
- Outotec tested this new interface using the Electrochemical Water Treatment model.

- RESULT: The interface for HSC-CFD coupling developed by Outotec works well and offers a promising way for digital solution of engineering processes.

HSC Equilibrium - Ansys Fluent – Link Testing (Outotec, Jiliang Xia)



Molar concentration of Fe^{2+} ($kmol/m^3$) and velocity magnitude (m/s) at anode



Molar concentration of Fe^{2+} ($kmol/m^3$) and velocity magnitude (m/s) at middle plane

Challenges 2017

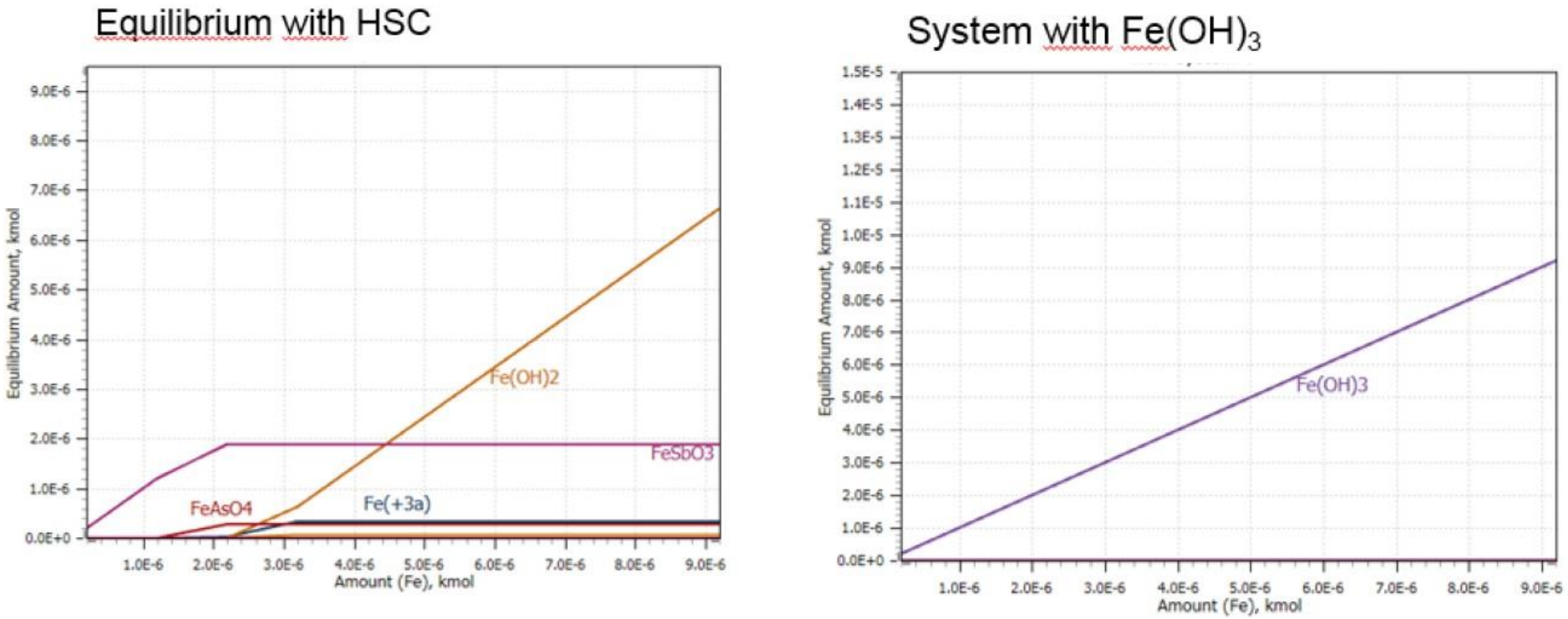
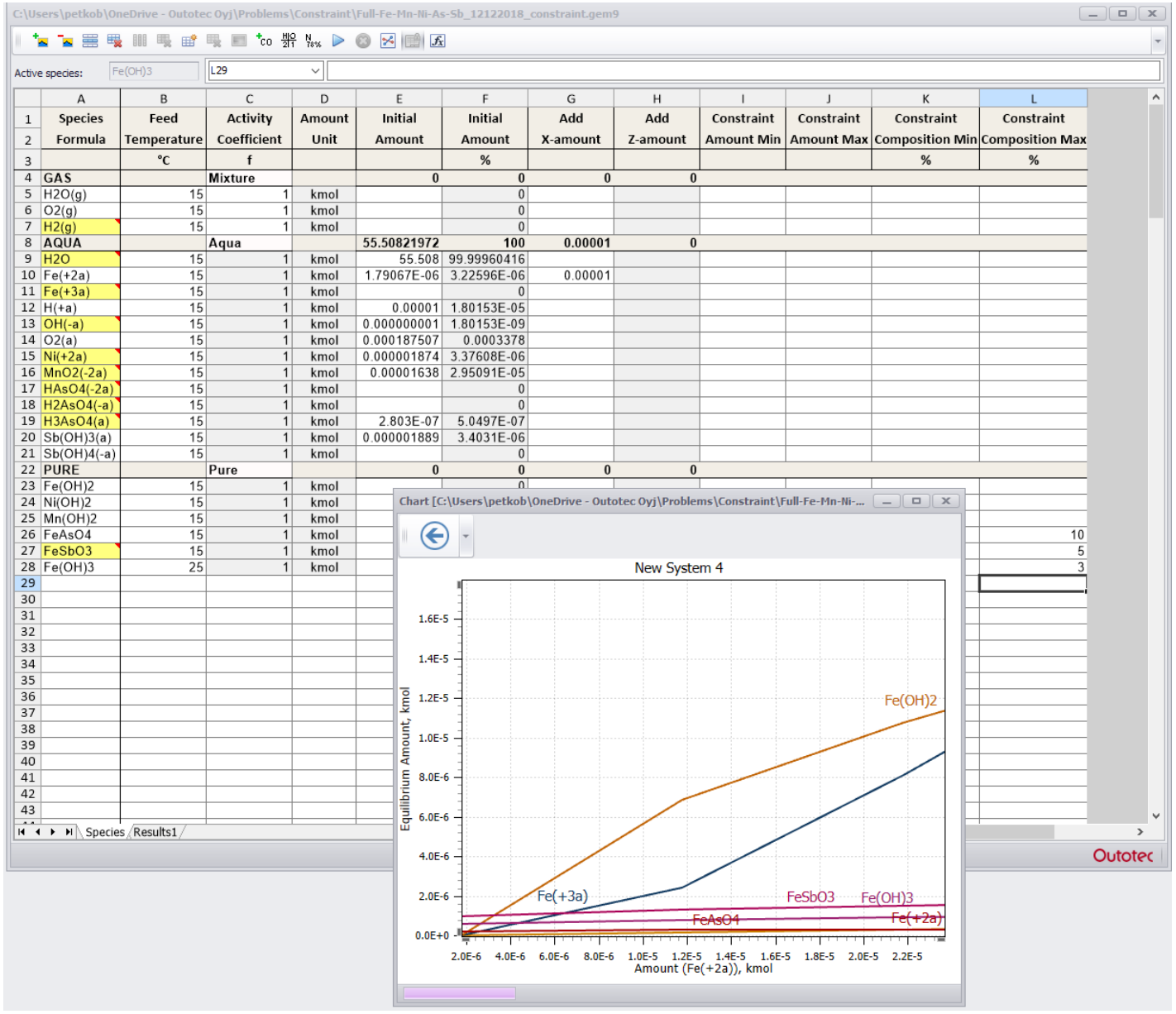


Figure Z. Equilibrium data obtained without and with $Fe(OH)_3$ as potential product from the EWT process.

Kinetics have a great impact on behavior of some species in the water solutions !

Solution: Constrained Equilibrium Calculations 2018

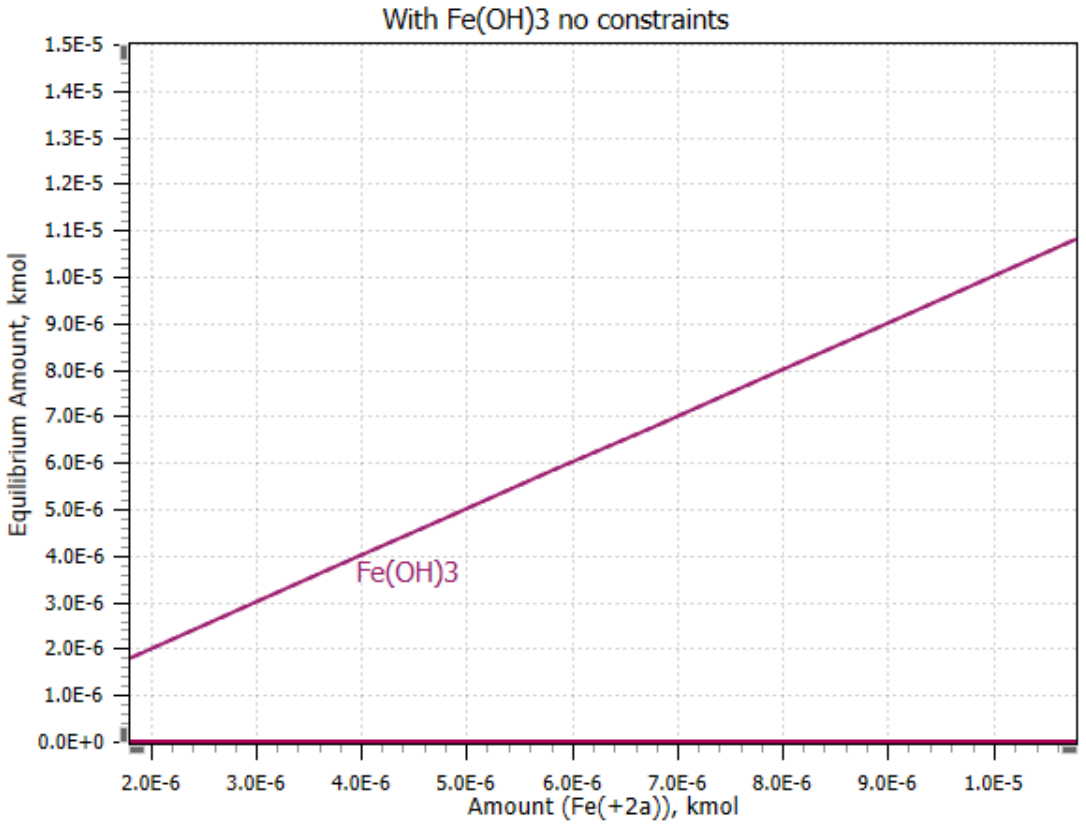


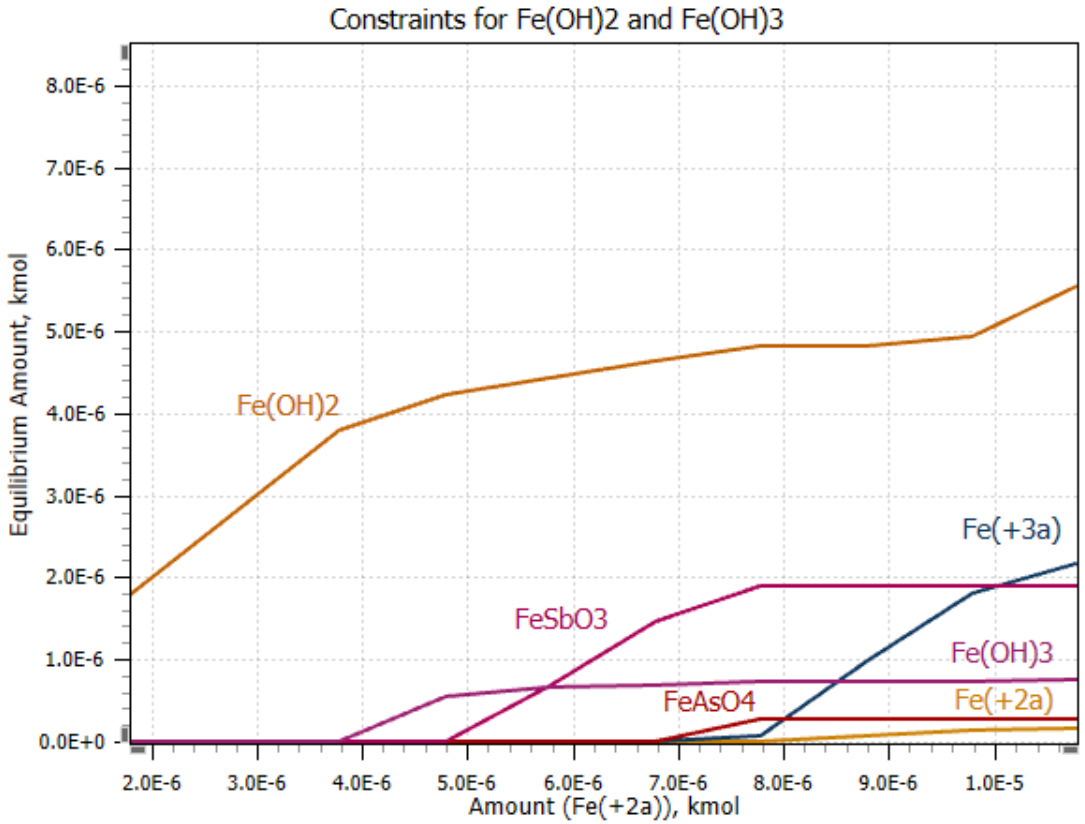
	A	B	C	D	E	F	G	H	I	J	K	L
1	Species	Feed	Activity	Amount	Initial	Initial	Add	Add	Constraint	Constraint	Constraint	Constraint
2	Formula	Temperature	Coefficient	Unit	Amount	Amount	X-amount	Z-amount	Amount Min	Amount Max	Composition Min	Composition Max
3		°C	f			%					%	%
4	GAS		Mixture		0	0	0	0				
5	H2O(g)	15	1	kmol		0						
6	O2(g)	15	1	kmol		0						
7	H2(g)	15	1	kmol		0						
8	AQUA		Aqua		55.50821972	100	0.00001	0				
9	H2O	15	1	kmol	55.508	99.99960416						
10	Fe(+2a)	15	1	kmol	1.79067E-06	3.22596E-06	0.00001					
11	Fe(+3a)	15	1	kmol		0						
12	H(+a)	15	1	kmol	0.00001	1.80153E-05						
13	OH(-a)	15	1	kmol	0.000000001	1.80153E-09						
14	O2(a)	15	1	kmol	0.000187507	0.0003378						
15	Ni(+2a)	15	1	kmol	0.000001874	3.37608E-06						
16	MnO2(-2a)	15	1	kmol	0.00001638	2.95091E-05						
17	HAsO4(-2a)	15	1	kmol		0						
18	H2AsO4(-a)	15	1	kmol		0						
19	H3AsO4(a)	15	1	kmol	2.803E-07	5.0497E-07						
20	Sb(OH)3(a)	15	1	kmol	0.000001889	3.4031E-06						
21	Sb(OH)4(-a)	15	1	kmol		0						
22	PURE		Pure		0	0	0	0				
23	Fe(OH)2	15	1	kmol		0						
24	Ni(OH)2	15	1	kmol								
25	Mn(OH)2	15	1	kmol								
26	FeAsO4	15	1	kmol								10
27	FeSbO3	15	1	kmol								5
28	Fe(OH)3	25	1	kmol								3

Generic Constrains features was developed into HSC Equilibrium module within 2018.

This new constrains feature was also added to the HSC-Fluent communication interface.

Solution: Constrained Equilibrium Calculations - Example





With HSC Gem new constrains features the kinetics may be taken into account

Constrains are generic and may be applied to any equilibrium calculation system


Outotec
Sustainable use of
Earth's natural resources