

3D Reactive Transport Modeling of Wellfields for In-Situ Leaching Using the FEFLOW Plug-in piChem

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ABSTRACT: UIT investigates the applicability of 3D reactive transport modeling with FEFLOW to optimize well-field design for in-situ leaching (ISL) of technology metals. With the new FEFLOW plug-in piChem chemical processes are modeled by PHREEQC. Alternatively, FEFLOW's reaction kinetics editor allows for modeling chemical processes by coupled kinetic rate equations. Both, a kinetic rate and an equilibrium approach using piChem, in combination with 3D flow and mass transport simulation have been tested for a simplified ISL application. The test case considers acidic uranium leaching in a symmetric 5-spot well-field pattern. In general, both the kinetic and the equilibrium model generate plausible and comparable results regarding the defined ISL operation. Best performance could be obtained by the SAMG solver with automatic time stepping. The kinetic model shows moderate run-times on a common computer that allows diverse variation with manageable effort. It is a promising tool for ISL optimization with the focus on optimization of flow regime and metal extraction. The equilibrium model handles complex chemical processes easily; however, computation times are too extensive for real ISL optimization purposes. Options that improve performance are available but have not been tested so far. Providing an acceptable performance, ISL optimization using piChem is applicable with special focus on varying mineralogical/geochemical conditions. Numerical instabilities have been observed in both models. In particular, (erroneous) negative mineral abundances within the kinetic dissolution process can be addressed by mesh refinement. In conclusion, it is recommended to improve formulation of kinetics rates with respect to numerical stability.

INTRODUCTION

In-situ leaching (ISL), also referred to as in-situ recovery (ISR), is the recovery of metals from underground ore deposits by injecting a chemical leaching solution (leachant) through injection wells into the ore zone to mobilize the metal(s) of interest and by recovering the pregnant solution (leachate) via extraction wells to the surface for further processing. ISL is an alternative mining technology with several advantages over conventional methods including underground and open-pit mining: (i) less environmental impacts (no waste rock dumps, no tailings, marginal surface disturbance), (ii) better economics with regard to CAPEX and OPEX (less equipment, less power consumption, less labor costs), (iii) reduced period of project development and start-up. However, two aspects need to be carefully considered in ISL mining: (i) *hydrologic* and *mineralogical/geochemical* conditions enabling an efficient (economic) operation, and (ii) avoidance/minimization of environmental impacts in line with regulatory requirements.

The development and operation of ISL mines in correspondence with these two basic requirements can be supported by computer simulation on the base of hydrological models and reactive transport models (RTM). The simulation of ISL including the quantification of potential environmental impacts (risk of leachant excursions, post-mining strategies and natural attenuation processes) requires a regional hydrological model that considers the overall stratigraphy (geometry and permeability of both mining aquifer and adjacent sedimentary layers) in general and any irregularities (e.g. tectonic faults) in particular. Especially, stratigraphic irregularities are a major concern and subject to scrutiny by regulatory organizations. The evaluation of potential environmental impacts requires the computer simulation of all relevant time periods including pre-mining conditions, mining operation and post-mining processes in a consistent manner.

On the other side, optimization of ISL well-field operation requires a local RTM that accounts for hydrological dynamics in a very short time scale combined with high chemical complexity. The reactive transport of the leachant from the injection well (screened section) to the extraction well (screened section) has to be optimized in two regards: (i) hydrologically, to realize an optimum pore-volume exchange and to maximize the contact of the leachant to the mineralized zone (ore zone), (ii) geochemically, to maximize the (effective) leaching rate of the metal of interest for economic recovery. The application of a RTM to ISL well-field operation is an ideal case to test the computer simulation of a combined hydraulic/chemical regime and to validate numerics under such challenging conditions.

APPROACHES FOR ISL PROCESS SIMULATIONS

In general, ISL technology for metal recovery is applicable to sedimentary-hosted deposits in *confined* aquifers at sufficient hydraulic *permeability* and appropriate *mineralogy/geochemistry* suitable to leach the metal of interest quantitatively.

Hydrology

Sedimentary deposits can be classified in several categories including (i) tabular type, (ii) basal channels (distinctive paleodrainage or complexly braided fluvial systems), and (iii) rollfronts (distributed at continental basins, mixed fluvial-marine genesis, or multi-episodic distal rolls) which are applicable to ISL provided the conditions outlined above are fulfilled. In contrast to the more regular shape of tabular deposits, basal (paleo-)channels and rollfront type deposits (and mixed forms of those) show a complicated geomorphology (including multi-horizon, staggered forms) depending on the specific metallogeny of the metal(s) of interest.

The hydrological conditions are met by the well-field design (geometry of injection/extraction well patterns including depth intervals of screened sections) and specification of operational parameters (injection pressures, individual injection/extraction flowrates). The injection/extraction flow regime has to be balanced to avoid/minimize the excursion of mining fluid into the aquifer (in particular, by applying a bleed from the lixiviant cycle in the order of 0.5 to 2 %; in exceptional cases beyond these limits). The achievable flow rate in a well-field pattern is mainly determined by permeability, thickness of the permeable horizon, hydraulic head above the mining horizon, and injector-extractor spacing.

Conventionally, well-fields (i.e. a system of injection and extraction wells with filter sections in the mineralized horizons) have been designed by applying 2D hydrological modeling and by adjusting (balanced) flow pathline patterns to the (2D) grade thickness (GT) contours in [wt.-% m] (criterion: 'coverage' of GT contours by pathline patterns to achieve an optimized contact of the leaching solution with the sedimentary ore). Filter sections of wells are specified in accordance to the depth interval of the mineralized horizon. Obviously, this quasi-2D methodology will not suffice to achieve maximum ISL recovery in the case of massive, irregular and/or stacked rollfront formations. Here 3D effects constraining the coverage of ore zone by the (3D) leachant flow pattern are evident. For this, 3D hydrological modeling on the basis of 3D structural modeling is required.

Hydrology of well-fields is quite dynamic due to the evolution of the well-field along the deposit during leaching operation (including additional optimization measures like change of flow regimes by flow modifications, re-screening of wells, role reversals of wells, infill wells etc.). Matching 3D flow pattern with the deposit geometry is just the first step. The next step, non-reactive mass transport simulation with the 3D hydrologic model would allow first conclusions with regard to the in-situ leaching progress if a constant metal leaching rate is assumed. Complex well-fields can be simulated targeting optimum well-field design and operation. While the task can be very challenging, especially in the case of complex deposit geometry, 3D mass transport simulations can already be considered as state of the art.

However, the ideal, most representative ISL simulation can be achieved by the full-scale reactive transport with 3D flow considering *mineralogical/geochemical* conditions, e.g. metal grade distribution, mineral texture, abundance distribution of interfering matter, and leachant composition.

Mineralogy/Geochemistry

The mineralogical/geochemical conditions are multifold, in particular determining the applicability of possible leaching types: e.g. acidic leaching by sulfuric acid (not exercisable at significant abundance of calcareous minerals like calcite), (bicarbonate) alkaline leaching or leaching by brines. The leaching rate of metals that are present in chemically reduced minerals (e.g. copper sulfides, like chalcocite and covellite, and U(IV) minerals, like uraninite and coffinite) depends on:

- the oxidation potential of the leachant (concentration of e- acceptors, e.g. Fe(III), O₂) required to oxidize the metal-bearing minerals into the soluble form of the metal and its relevant complexes,
- the concentration of the complexing ion (e.g. sulfate, bicarbonate),
- the temperature, and
- the mineral texture (specific form of metal-bearing mineral in particular).

Under such conditions, several minerals as well as organic matter could interfere metal leaching considerably, either due to competing reducing reactions consuming oxidation potential (e. g. sulfidic minerals like pyrite, degradation of organic matter) or – in the case of acid ISL – caused by neutralizing reactions (dissolution of calcareous minerals and silicates in form of clay and feldspar, ferric iron minerals). Appropriate conditioning of the injected leachant is required to achieve quantitative metal leaching in the course of flowing through the formation from injection to extraction points.

In general, two opposed approaches can be applied to simulate reactive transport: (i) a pure kinetic rate model and (ii) a chemical equilibrium model. A pure kinetic rate model is independent on the numerical time-step, easy to implement, easy to solve and, thus, allows a comparably short runtime. But, complex chemical systems like interfering leaching require a significant number of species to be considered. Each species is defined by a kinetic rate equation with corresponding kinetic parameters potentially dependent on other species. Thus, a simplification of the chemically complex model to the main reactions would be prudent.

A chemical equilibrium model does not need any additional parameters except the thermodynamic data. Thus, complex chemical systems can be simulated (including activity corrected solution speciation, mineral dissolution/precipitation, ion exchange, ...) with low effort while the numerical effort of transport is limited to the elements present for the reason that the chemical equilibrium state is independent on the initial state of the system. However, chemical equilibrium models may be dependent on the numerical time-step. The chemical equilibrium in every spatial element has to be reachable at every calculated time-step. In general, a chemical conversion introduced by a significant change in elemental concentrations requires more time. Unfortunately, this constraint is contrary to the time-step reduction for numerical stability. Overall, heterogenic reactions like mineral dissolution are slow compared to pure aquatic reactions. Mineral dissolution involving the transfer of electrons between species (redox reactions) is even slower; usually microbial catalysis is required to accelerate the reaction.

Meanwhile FEFLOW (Diersch, 2014) enables computer simulations implementing both kinetic rate model using FEFLOW's reaction kinetics editor and equilibrium model using FEFLOW's plug-in piChem, each in combination with 3D flow and mass transport simulation. Both models have been tested for simplified applications of ISL performance. This test case has been defined for acidic uranium leaching in a hydrologically, mineralogically and geochemically symmetric (homogeneous) 5-spot well-field pattern. The different model approaches have been compared by evaluating required input data, achievable (representative) results and computational effort.

SIMULATION METHODS

FEFLOW's reaction kinetics editor allows the formulation of user-specific chemical equations for complex kinetic applications. Individual reaction rate expressions R_k can be expressed for each species k or be combined with other participating species' concentrations and specific variables (e.g. temperature, porosity or solid fraction).

The development of a quite simplified (practicable) kinetic model requires a basic understanding of the complex chemical system of ISL. The consideration of high-order effects, e.g. speciation or activity, is possible at higher effort. The higher the complexity of the model space the larger the number of free parameters – a major challenge. However, we limit the kinetic model to the main chemical processes in order to optimize ISL operation and therewith restrict the number of kinetic model parameters to a minimum.

The implementation of the *plug-in piChem* allows the coupling of FEFLOW and PHREEQC (Parkhurst, 1999) and, thus, combines the calculation of complex geochemical reactions (e.g. speciation/complexation, mineral dissolution/precipitation, ion exchange, kinetic reactions) with aqueous phase flow and transport (Wissmeier, 2015).

At the beginning of simulation, user-defined PHREEQC input scripts are checked by piChem, and PHREEQC component concentrations are calculated for every node and boundary condition in the model domain. Thereby piChem copies the set of PHREEQC components to the user-defined placeholder species with the result that all PHREEQC components have the same transport properties as the placeholder species. After every time-step (or user-defined time-step) piChem collects the PHREEQC component concentrations from FEFLOW flow and transport simulation and performs

reaction calculations with PHREEQC. Component concentrations are reassigned to the FEFLOW model to continue simulations. This workflow is repeated until the end of simulation.

The use of the piChem plug-in enables the description of complex chemical systems thermodynamically – with all its potentials and limits. The number of free parameters for a pure thermodynamic application (chemical equilibrium) is zero. However, the piChem plug-in requires the basic knowledge of geochemical modeling and practice in using PHREEQC. It is most challenging to select the best database for the problem and to define the right primary and secondary minerals.

MODEL DESCRIPTION

Hydrologic Model

The performance of 3D reactive transport simulation of a well-field has been investigated by a simplified hydrological model consisting of a 3D homogenous aquifer of $L \times D \times B = 300 \text{ m} \times 300 \text{ m} \times 19 \text{ m}$ and a symmetrical 5-spot well-field pattern including one extraction and four surrounding injection wells. The wells were simulated by a multi-layer well (MLW) boundary condition with the following dimensions: well radii of 0.1 m each, screening lengths of 3 m each, spacing of 30 m between injection and extraction wells. Further, a triangle-generated mesh of 9,549 nodes was chosen, consisting of 34 layers á 18,902 triangle prism elements. For the temporal discretization an automated time-stepping was defined with a total simulation time of 50 days. A summary of model parameters, initial conditions (IC) and boundary conditions (BC) for the aquifer model is presented in table 1.

Parameter	Value	Unit
<i>Domain and Mesh:</i>		
Confined aquifer, saturated, steady flow/transient transport		
Width; height; depth	300; 300; 19	m
Number of dimensions	3	
Element type	Triangle prism	
Mesh elements/nodes	642,668/334,215	
<i>Fluid Flow Properties:</i>		
Hydraulic conductivity (horizontal/vertical)	2.0e-05 / 1.0e-06	m s ⁻¹
Specific storage	1.0e-04	m ⁻¹
<i>Mass Transport Properties:</i>		
Porosity	0.3	-
Dispersivity (longitudinal/ transversal)	0.1/0.01	m
Molecular diffusion	0	m ² s ⁻¹
<i>IC's and BC's:</i>		
<i>Fluid Flow</i>		
Dirichlet-type BC (western and eastern border)	1000	m
5 MLW's (1 extractor and 4 injectors)	202 / 4 x -50	m ³ d ⁻¹
<i>Mass Transport</i>		
IC of species	see Table 2	
Dirichlet-type BC of species at injection sites	see Table 2	
<i>FEM:</i>		
Automated time stepping mechanism, equation-system solver SAMG, no upwinding (GFEM)		
Initial time step size	10 ⁻⁷	d
RMS error tolerance (AB/TR)	10 ⁻⁴	-
Simulation time period	50	d

Table 1: Parameters, initial conditions (IC) and boundary conditions (BC) used for the 3D multispecies mass transport aquifer models

Geochemical Model

The simplified test case was defined for the in-situ leach of uranium from a permeable ore body containing uraninite (UO₂) at a quite low abundance of calcite (CaCO₃). The acidic leachant contains ferric sulfate (ferric acting as oxidant). Initially, both minerals were equally distributed over the whole model domain. Continuous injection of the acidic leachant of pH 1.8 results in the dissolution of calcite by consumption of hydrogen ions resulting in an increase of pH value. Uraninite is oxidized by ferric

(Fe(III)) to aqueous uranyl (UO_2^{2+}) that is complexed by sulfate ions. In order to keep the problem simple no additional competing minerals or elements were considered. The composition of the leachant was considered to be constant over time. The leachant enters the model via a constant concentration boundary at the lowest node of the injection MLW's. Initial and boundary concentrations are listed in table 2.

Kinetic Model Using FEFLOW's Reaction Kinetics Editor

The defined kinetic model simplifies the ISL chemistry to two mineral dissolution reactions neglecting effects of speciation or activity:



Both dissolution reactions are described by a 1st order kinetics with respect to the mineral:

$$R_k = -r_k \cdot c_k \quad for \ k = UO_2, CaCO_3 \quad (3)$$

Therewith, the model considers two solid species, namely uraninite (UO_2) and calcite ($CaCO_3$) and two reactive fluid species, particularly hydrogen (H^+) and ferric (Fe^{3+}) ions. The dependence of the dissolution on the reactive fluid species was defined by the kinetic rate r_k constrained with respect to pH value.

In detail, the kinetic rate of uraninite leaching was assumed in accordance with Torrero et al. (1997) depending on concentration of hydrogen ion (H^+) and electron acceptors $[A^e] = [Fe^{3+}]$ as shown in equation 4. The mineral specific rate coefficient (free parameter) for uraninite dissolution was estimated according to Mårten et al. (2015) to $r_{0UO_2} = 0.048 \text{ d}^{-1}$. Calcite dissolution kinetic rate was described dependent on concentration of hydrogen ion (H^+) for strong acid conditions with $pH < 4$ according to (Compton et al., 1989) as shown in equation 5. The free parameter $r_{0CaCO_3} = 8.64 \text{ d}^{-1}$ was taken from Peng et al. (2015).

$$r_{UO_2} = -r_{0UO_2} \cdot [H^+]^{0.37} \cdot [Fe^{3+}]^{0.31} \quad for \ pH < 2.5 \quad (4)$$

$$r_{CaCO_3} = -r_{0CaCO_3} \cdot [H^+] \quad for \ pH < 4.0 \quad (5)$$

Additionally three resulting fluid species were defined, calcium (Ca^{2+}), uranyl (UO_2^{2+}) and ferrous (Fe^{2+}) ions, in order to describe the leachate properly. The reaction rate equations for each fluid species, reactive and resulting species, were derived in dependence on the rate of the respective solid according to eq. 3 to 5 and considering stoichiometric values (eq. 1 and 2).

Equilibrium Model Using FEFLOW's piChem plug-in

The equilibrium model software includes PHREEQC for the calculation of mineral dissolution of uraninite and calcite assuming chemical equilibrium. It uses the thermodynamic database wateq4f.dat (Ball et al., 1991). Within FEFLOW chemical equilibrium is calculated after each transport time-step. The chemistry of our simplified problem can be described by PHREEQC by considering the components DIC, S(VI) (SO_4^{2-}) in addition to pH (H), U, Fe, and Ca, which are already present in the kinetic model. The pe value results from the redox pairs of U(IV)/U(VI) and Fe(II)/(III). The pH value is defined as charge balance component. The initial concentrations of U, Ca, DIC in the model domain are in equilibrium with the minerals uraninite and calcite. Small background concentrations are defined for Fe and SO_4^{2-} (see Tab. 2). Additionally, the minerals ferrihydrite ($Fe(OH)_3(a)$) and gypsum are considered in PHREEQC calculations as potential precipitating and re-dissolving phases. The injected solution is charged by SO_4^{2-} . Its composition is presented in Tab. 2, too.

	pH/pe	Ca^{2+}	DIC	SO_4^{2-}	Fe^{2+}	Fe^{3+}	U^{4+}	U^{6+}	UO_2	$CaCO_3$
IC	7.6/ -3.7	1.4e-03	2.0e-03	4.1e-04	1.8e-06	4.5e-13	5.0e-14	1.1e-15	2e-04	3.6e-05
BC	1.8/ 14.5	1.4e-03	2.0e-03	3.1e-02	1.2e-05	1.0e-02	-	-	-	-

Table 2: Initial and boundary concentrations of components in [mol/kgw] for kinetic and equilibrium model (values in bold are only considered in equilibrium model)

MODEL RESULTS

In general, both the kinetic and the equilibrium model generate plausible and comparable results regarding the defined ISL problem. With the beginning of injection of acid leachant, calcite is dissolved followed by uraninite within the well-field along the streamlines. Fig. 1 shows the progress of the mineral dissolution fronts between injector and extractor at 6 different times. Comparing results from the kinetic model to the ones from the equilibrium model, the dissolution is slower and the gradients are smoother due to first order kinetics. Further, high mineral dissolution rates in combination with low mineral abundances result in negative mineral concentrations which are chemically meaningless. The effect is more pronounced for calcite than for uraninite.

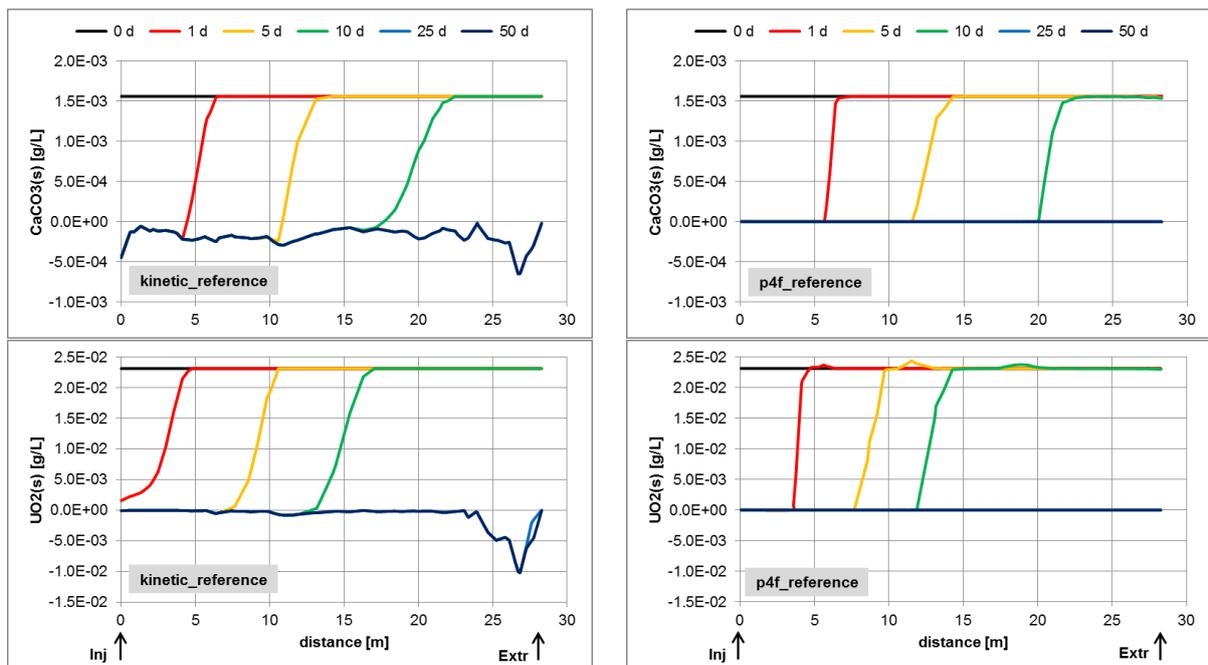


Figure 1: Uraninite and calcite concentration as function of distance from injector (Inj) for kin_reference (left) and eq_reference (right) models for different time steps

In Fig. 2 the (integral) leachate composition at the extractor is presented as function of leaching time for both model approaches. In the kinetic model the pH value decreases slowly and with fulfilling the constraint of $\text{pH} < 2.5$, uraninite is dissolved. The dissolution kinetics results in constant U extraction, whereas the ferric concentration is dominated by leachant transport.

In contrary, in the equilibrium model pH value is buffered by calcite dissolution and drops down immediately if calcite is dissolved completely. The same process happens for uraninite with ferric. The ferric ions oxidize the uraninite by completely transforming to ferrous ions. If uraninite is dissolved completely, concentration of ferric ions increases in leachate and uranium concentration drops, followed by a smooth decrease, whereas the uranium from longer streamlines is transported to the extractor.

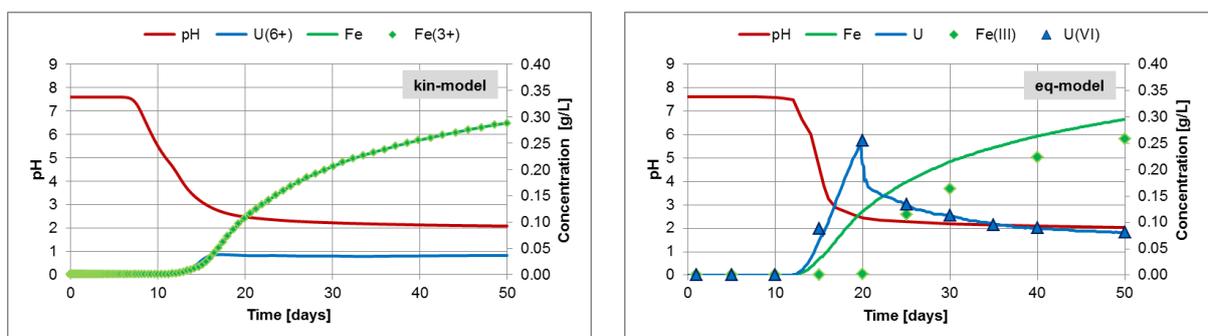


Figure 2: Leachate composition over time for kinetic (left) and equilibrium model (right)

In conclusion, both models describe the main reactive processes, whereas the equilibrium model is more informative from chemical point of view. However, both model softwares generate numerical instabilities. As already mentioned above, kinetic mineral dissolution results in negative abundances which are balanced mathematically by an increased formation of dissolved species. The equilibrium model develops numerical artefacts in zones with significant pH/pe gradients, e.g. at the flow boundary between groundwater and leachant and at the extractor. In these zones pH values increase extremely up to pH 12 (and, thus, pe values decrease) resulting in a precipitation of uraninite and calcite. These numerical effects are presented in Fig. 3 for calcite at 50 days leaching as an example.

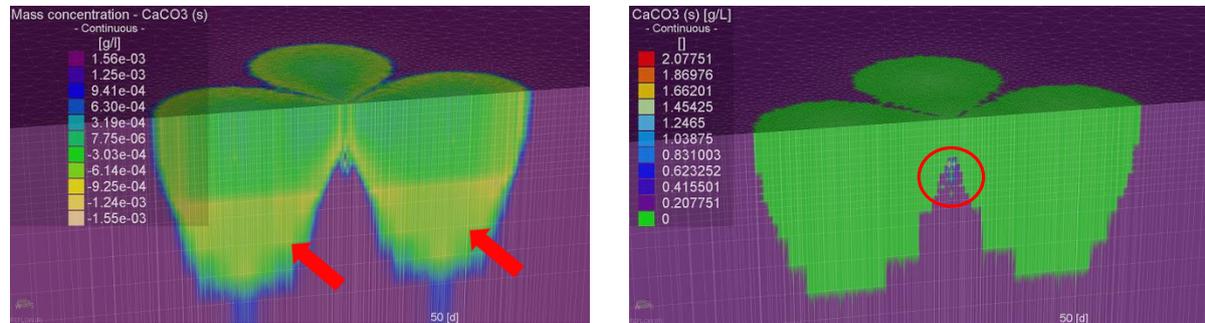


Figure 3: CaCO₃(s) rest abundances at 50 d from the kinetic (left) and the equilibrium (right) models (3D image of the intersected 5-spot wellfield). Numerical instabilities are marked in red.

MODEL PERFORMANCE

Numerical instabilities are typically addressed by mesh refinements which do mainly increase the calculation time and, thus, the model performance. The model performance was tested for different scenarios varying equation-system solver and mesh size for both kinetic and equilibrium models. The kinetic rates of mineral dissolution were varied by factors of 10 and 100 for the kinetic model (cf. Tab. 3). All calculations were executed on a common desktop PC with Intel Xeon E3-1225 V2 processor (4 x 3.2Ghz, 12 GB RAM) using the operating system Windows 7.

Nr.	Scenario	Model designation	No. of elements
(1)	Reference case (see table 1)	eq_reference kin_reference	642,668
(2)	Refinement of mesh	eq_refined kin_refined	2,205,376
(3)	Solver PCG & BiCGSTABP (default)	eq_solver kin_solver	642,668
(4)	Full upwinding	- kin_upwinding	642,668
(5)	Increase kinetic rate by factor 10	- kin_rate10	642,668
(6)	Increase kinetic rate by factor 100	- kin_rate100	642,668

Table 3: Definition of model scenarios

The mesh refinement within the leaching area has reduced the occurrence of negative mineral abundances in the kinetic model significantly, but the numerical instability is still present in the whole leaching domain (not shown here). The effect of less overshooting has also resulted in slightly smaller concentrations of the dissolved components in the leachate (cf. Fig. 4). Further mesh size refinement (including vertical scale) is recommended for future model studies. Unfortunately, the effect of mesh refinement on the results of the equilibrium model could not be studied due to the long run-time.

Kinetic Model				Equilibrium Model			
Scenario	Time steps	dac-file [GB]	CPU time [h]	Scenario	Time steps	dac-file [GB]	CPU time [h]
reference	143	4.2	1.46	reference	449	38.9	23.98
refined	172	17.1	5.68	refined	-	-	-
solver	143	4.3	1.62	solver	449	39.1	24.35
upwinding	118	3.4	1.16				
rate10	224	6.6	2.28				
rate100	276	8.2	2.70				

Table 4: CPU time [h] for different model scenarios

The run-times of both models differ significantly. Whereas the run-time of the kinetic model without mesh refinement is less than 2 hours, running the equilibrium model takes about a day. The number of time-steps and the size of output file are significantly larger in the latter case, too (cf. Tab. 4). For comparison, the run-time of the pure flow model and the transport model without reactions (neither kinetics nor equilibrium) is about 10 seconds and a half hour, respectively. The long run-time of the equilibrium model makes the opportunity of skipping PHREEQC calculation for several time-steps favorable. In future ISL studies the effect of numerical stability and run-time reduction should be investigated further. The mesh size refinement of the kinetic model by an increase of element number by a factor of 3.4 leads to a considerable increase of CPU time by factor 3.9. The number of time steps increases by 20 % only, whereas the data volumes increase by a factor of 4.

The standard iterative solver PCG & BiCGSTABP, compared to the SAMG solver, needs the same number of time-steps at slightly increased run-time and data space. The third solver PARDISO was only tested in a short run. As expected the run-time is significantly longer and the output file larger than for the other two solvers. The calculation performance could be considerably improved by the use of full upwinding. However, the numerical dispersion is still significant as shown in Fig. 4 for U(VI) in the leachate. Fig. 4 presents the effect of the increase of kinetic rates by a factor of 10. The concentration of U(VI) (and also Ca) in the leachate increases, however, the steep front of the equilibrium model could not be simulated. The further increase of the kinetic rates by a factor of 100 generated numerical instabilities and chemically implausible results. This effect is also observed by changing the number of time-steps and run-time

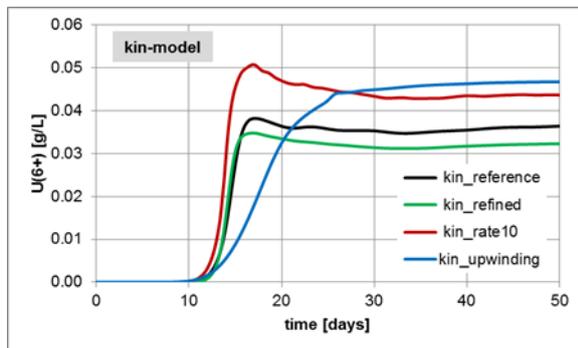


Figure 4: Different kinetic model scenarios represented by the simulated U(6+) concentration at the extractor as function of leaching time

CONCLUSIONS

Two contrary modeling approaches: (i) a kinetic rate model and (ii) a chemical equilibrium model were evaluated and tested to perform 3D reactive transport simulation with regard to the optimization of ISL well-field design. The kinetic model, applying user-defined 1st order kinetic equations via FEFLOW's reaction kinetics editor, as well as the chemical equilibrium model, using the capabilities of FEFLOW's piChem plug-in, produced reasonable results considering the dissolution of major minerals. The kinetic rate parameters affect the numerical model stability strongly, thus, demonstrating the challenge to set up appropriate input data. The further refinement of mesh size is recommended for the kinetic approach. Although piChem has proven to be a valuable tool for simulating ISL performance, very high computation times may limit its application to more complex 3D modeling (real-case scenarios). The feature of skipping time-steps for PHREEQC calculation seems to be promising with respect to improve performance.

The kinetic model presented here is promising as a tool for ISL optimization, but still needs to be improved regarding the formulation of kinetics rates for numerical stability. The focus of this model is the optimization of flow regime and extraction. In contrary, the equilibrium model is highly valuable for the further understanding of the chemical processes. However, a significant improvement of the calculation performance is required either by variations in the model as mentioned above or by applying parallel computing and/or using more powerful, higher-performance computers.

Finally, the simulation of reactive transport for ISL enhances the informative value of the model significantly compared to pure flow or pure transport model. ISL optimization will definitively benefit from adding further reactions, provided that reliable input data is available. Using an ISL optimization scheme that increases the complexity step by step, starting from flow only via transport only to reactive transport, will exploit the available software tools effectively and with manageable effort.

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