

Relevance of hydro-geomechanical-geochemical processes in the design and management of copper heap leach pads

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Abstract

Heap leach pads are common in the mining industry. In their design and management, criteria based on coupled hydro-geomechanical-geochemical processes are not commonly taken into account. However, these are of paramount importance for two main reasons: (1) they could play an important role in the physical stability of the pad; and (2) they are critical for metallurgical efficiency, especially in the mid to long term.

As an example of the relevance of complex coupled phenomena, it may be mentioned that the geotechnical stability of the heap is related to the distribution of liquid pressures which, at the same time, is related to the permeability through Darcy's law. In its turn, permeability will be affected by porosity changes, which depend on the consolidation state and the dissolution/precipitation of minerals. Obviously, the hydrometallurgical performance of the heap ore is also strongly linked with the abovementioned coupled processes.

In this work, we present a numerical model to solve the hydro-geomechanical-geochemical coupled processes, developed with COMSOL-PHREEQC, a Java interface developed for combining COMSOL Multiphysics—a well-known commercial FEM platform—with PHREEQC, the open-software geochemical simulator developed at USGS and used worldwide. The resulting numerical tool is able to solve simultaneously unsaturated liquid flow, soil effective stress, and geochemical dissolution and

precipitation. Geochemical changes affecting porosity and permeability are coupled explicitly in the hydraulic and geomechanical calculations.

Introduction

Heap leach facilities are complex systems involving processes related to hydrology, mechanics, and geochemistry. Although these processes from different disciplines can be treated separately, it is obvious that they are related to each other. An example of the coupling between processes from different disciplines is the relationship between the geotechnical stability and the distribution of liquid pressures within the heap, which, at the same time, is related to the permeability through Darcy's law. In its turn, permeability will be affected by porosity changes, which depend on the consolidation state and the dissolution/precipitation of minerals. Obviously, the hydrometallurgical performance of the heap ore is also strongly linked with the abovementioned coupled processes. However, the prediction or even the interpretation of the behavior of the heap is a complex issue that should be addressed with the help of modeling tools.

There are several models in the literature related to geotechnical, hydrogeological, and geochemical disciplines, but it is not common that these models are coupled in an actual engineering problem. The usual approaches for heap leaching models solve the different phenomena in an uncoupled or just partially coupled way, due to their resolution complexity. Some of the existing approaches were formulated to calculate hydrodynamics and solute transport (Decker and Tyler, 1999), or soil mechanics and hydrodynamics (Pacheco et al., 2011).

In the last decade some efforts about incorporating the chemistry in Hydro-Mechanical (HM) problems (Liu and Brady, 2004; Mata et al., 2005; Mohajeri et al., 2011) have been made, but most of them only considered simple geochemical models regarding synthetic cases. Also some attempts to solve the Thermal-Hydro-Mechanical-Chemical (THMC) equations in the context of the design of radioactive waste facilities have been reported as well (Guimarães et al., 2002). Also, there is a clear demand for numerical simulators that can help in the design, planning, and predicting of leaching operations at industrial scale (Cross et al., 2006; Bennett et al., 2012; McBride, Gebhart and Cross, 2012; McBride et al., 2013). In this context, McBride, Cross & Gebhart (2012) developed a mathematical model based on CFD technology that considered operational aspects of a leaching process, such as active 3D leached and unleached heap areas. Nevertheless, the flow through the heap is modeled in 1-D, which can lead to substantial errors in the prediction of metal recovery as the lateral flow is disregarded. In addition, mechanical phenomena were not considered.

Improving the design of heap leach pads requires performing an integrated analysis of the HMC phenomena. Key aspects of the construction and operation, such as mechanical stability and mineral recovery efficiency, cannot be estimated accurately without taking into account multiple coupling of

complex chemistry, soil mechanics, and hydrodynamics. To our knowledge, there is no numerical simulation of a coupled HMC model that accounts for the kinetics of several mineral species and the evolution of a multilift heap. In this paper, we present a model that considers all the above-mentioned coupled phenomena and a numerical tool for the simulation of copper heap leaching.

Methodology

In this work we provide a simulation of a synthetic copper heap leach pad to demonstrate the relevance of the HMC coupling, as well as the capabilities of the numerical tool utilized. In brief, the methodology followed in this study consists of: (i) development of a numerical tool for the simulation of HMC problems; (ii) application of the numerical tool for simulating copper heap leaching; and (iii) demonstration of the potential of the tool for the design, planning, and prediction of industrial heap leaching operations.

Hydro-mechanical-chemical model

Several coupled HMC processes are involved during the construction and operation of a heap leach pad. In this section we describe the governing equations assumed in the modeling of the heap leaching process. First, the mass balance equation of liquid under isothermal conditions is expressed as follows:

$$\rho_l (C_m + S_l S) \partial_t p_l = \rho_l \nabla \cdot \mathbf{q}_l + \rho_l \partial_t \varepsilon_{vol} + f_{ext}^w \quad (1)$$

where ρ_l the liquid density, S_l is the liquid saturation, C_m is the specific moisture capacity, p_l is the liquid pressure, S is the storage term, \mathbf{q}_l is the liquid flow velocity, ε_{vol} is the volumetric deformation and f_{ext}^w is an external source term. The liquid flow velocity equation is given by Darcy's law (Bear, 1988):

$$\mathbf{q}_l = -\frac{\mathbf{k}k_r}{\mu} (\nabla p_l - \rho_l \mathbf{g}) \quad (2)$$

where \mathbf{k} is the intrinsic permeability tensor, k_r is the relative permeability, μ is the dynamic viscosity of the liquid and \mathbf{g} is the gravity tensor. The van Genuchten's retention function (van Genuchten, 1980) was considered to account for the relationship between liquid saturation and pressure. Also, the relative permeability was calculated according to the model of van Genuchten (1980).

On the other hand, we used the so-called nonconservative formulation for reactive transport of a chemical species (Bea et al., 2009):

$$\omega \partial_t \mathbf{c} = L_t(\mathbf{c}_a) + f_{ext}^w \mathbf{c}_a^* \rho_l + \omega \mathbf{r}_{eq} + \omega \mathbf{r}_{kin} \quad (3)$$

$$\omega = \phi S_l \rho_l \quad (4)$$

where \mathbf{c} is the concentration vector of species, \mathbf{c}_a is the concentration vector of aqueous species, \mathbf{c}_a^* is the vector of external concentrations of species, ϕ is porosity, \mathbf{r}_{eq} and \mathbf{r}_{kin} are the vectors of equilibrium and

kinetics reactions, respectively. In (3) we have introduced the linear operator accounting for advection, dispersion, diffusion, and nonchemical sink-source terms:

$$L_t(\cdot) = -\rho_l \mathbf{q}_l \cdot \nabla(\cdot) + \nabla(\rho_l \mathbf{D} \cdot \nabla(\cdot)) - f_{ext}^w(\cdot) \quad (5)$$

where \mathbf{D} is the tensor of dispersion and diffusion coefficients. The equation (3) consists of a system of N_s equations, where N_s is the number of chemical species. However, it can be reduced to a system of size N_c , the number of chemical components, by eliminating the equilibrium reactions. Chemical components are defined as linear combination of species whose mass is not affected by equilibrium reactions (Steefel and MacQuarrie, 1996; Saaltink, Ayora and Carrera, 1998):

$$\omega \partial_t \mathbf{m} = L_t(\mathbf{m}_a) + f_{ext}^w \mathbf{m}_a^* + \omega \mathbf{M} \mathbf{r}_{kin} \quad (6)$$

where \mathbf{m} is the vector of components, which can be decomposed in subcomponents containing the chemical species of the component present in the aqueous (\mathbf{m}_a), gaseous (\mathbf{m}_g), mineral (\mathbf{m}_m) and sorbed (\mathbf{m}_d) phases; \mathbf{M} is a component matrix, which is defined as a matrix that eliminates the equilibrium reactive term, i.e., $\mathbf{M} \mathbf{r}_{eq} = \mathbf{0}$ (Saaltink, Ayora and Carrera, 1998); and \mathbf{m}_a^* is the vector of external aqueous component concentration.

Finally, the soil mechanics of a heap leach pad were assumed to be governed by the equilibrium equations (Zienkiewicz and Taylor, 1989):

$$\nabla \cdot \boldsymbol{\sigma} + ((1 - \varphi) \rho_s + \varphi S_l \rho_l) \mathbf{g} = \mathbf{0} \quad (7)$$

where $\boldsymbol{\sigma}$ is the total stress tensor and ρ_s is the soil density. In a variable saturated porous medium the effective stress, $\boldsymbol{\sigma}'$, controls the mechanical behavior. We adopted a simple approach, in which:

$$\boldsymbol{\sigma}' = (\boldsymbol{\sigma} - p_a \mathbf{I}) + ((S_l - S_{lr}) / (1 - S_{lr})) (p_a - p_l) \mathbf{I} \quad (8)$$

where p_a is the air pressure, \mathbf{I} is the identity matrix and S_{lr} is the residual liquid saturation. The Cam-Clay elasto-plastic constitutive law (Wood, 1990) and plane strain conditions were assumed to close the problem.

The initial suction and composition of the ore material layers are represented by p_l^0 and \mathbf{m}_a^0 , respectively. Initial mechanical conditions assumed are zero strains and stresses for each layer. No flow conditions are assumed at the boundaries of the bedrock. Also, no flow conditions are imposed at the lateral boundaries of the ore layers and the free surface of those layers beneath the current layer under irrigation. Atmospheric pressure and mass outflow conditions are imposed at the lateral boundaries of the drainage system. An inflow condition (q_{in}) is considered at the surface of every layer to reproduce the irrigation process. Horizontal displacement (u_x) at the lateral boundaries of the rock foundation is set at zero. Also

zero vertical (u_y) and horizontal displacements are considered at the bottom boundary of the bedrock. No mechanical constraints and no loads are considered at the remaining boundaries.

Numerical implementation in COMSOL-PHREEQC

The governing equations (1 to 8) have been solved with the numerical interface COMSOL-PHREEQC (iCP) (Nardi et al., 2014). iCP is a Java interface that couples the general purpose finite element framework COMSOL Multiphysics and the geochemical simulator PHREEQC (Parkhurst and Appelo, 2013). In brief, the tool is based on implementing an operator splitting technique for solving the hydro-mechanical problem (a coupled or uncoupled system of partial/ordinary equations and algebraic differential equations) on COMSOL and the chemical system of algebraic and differential equations on PHREEQC. A problem is set in iCP through three types of input files: (i) a COMSOL file for solving the hydro-mechanical phenomena, (ii) a set of PHREEQC files defining the chemical system, including initial and boundary conditions; and (iii) a XML file that establishes the link between COMSOL and PHREEQC, sets the time discretization and specifies the outputs.

In addition, to deal with the large computational requirements of THMC models, iCP automatically divides the model domain into subdomains where geochemical reactions are solved in parallel by balancing the computational load over multiple threads. In particular, the simulation of this work comprised of 14,641 elements simulating a 500 day leach operation and employing a transport time step of 86,400 s, required 1 GB of storage and 1 day of CPU time on a 3.8 GHz processor with 4 cores and 16 GB RAM. These numbers are in the range of other codes and computational methods that only solve flow and reactive transport (e.g., McBride, Gebhart and Cross, 2012; McBride, Cross and Gebhart, 2012).

Application example: Simulation of a multilift heap leach pad

The present HMC model was applied to simulate the construction and operation of a synthetic copper heap leach pad consisting of five ore layers settled on a terrain with a slight slope (2%). Each layer (stacking level) is simulated sequentially, mimicking the sequence of construction and operation of a real heap leach pad as schematized in Figure 1. In this sequential simulation approach the results obtained during the calculation of the previous layers (u_{n-1} , p_{n-1} , c_{n-1}) are used to define the initial (u_0 , p_0 , c_0) and boundary conditions of the next layer.

We have considered that the construction of each layer is performed over 10 days, followed by an irrigation period of 90 days at a constant irrigation rate of $q_{in} = 7.5 \text{ l h}^{-1} \text{ m}^{-2}$ applied on the top surface of each layer. The initial liquid pressure in the ore layer (p_l^0) is considered equal to -30 kPa . The temperature of the system is assumed to be 25°C . The rock and ore densities were set at $3,000 \text{ kg/m}^3$ and $2,600 \text{ kg/m}^3$, respectively. An initial porosity of 30% was assumed both for the liner system and ore bed, while the initial intrinsic permeabilities were set at $5 \times 10^{-10} \text{ m}^2$ and $4 \times 10^{-11} \text{ m}^2$, respectively. The longitudinal dispersivities

of the liner system and ore bed were assumed to be equal to 50 m and 10 m, respectively. The respective transversal dispersivities were set at 10 m and 2 m. These values were chosen to ensure numerical stability of the simulation, but they may be representative of industrial heap leaching, where the total heap height can be up to 200 m and the area under leach can be in the order of 106 m² (Schlesinger et al., 2011).

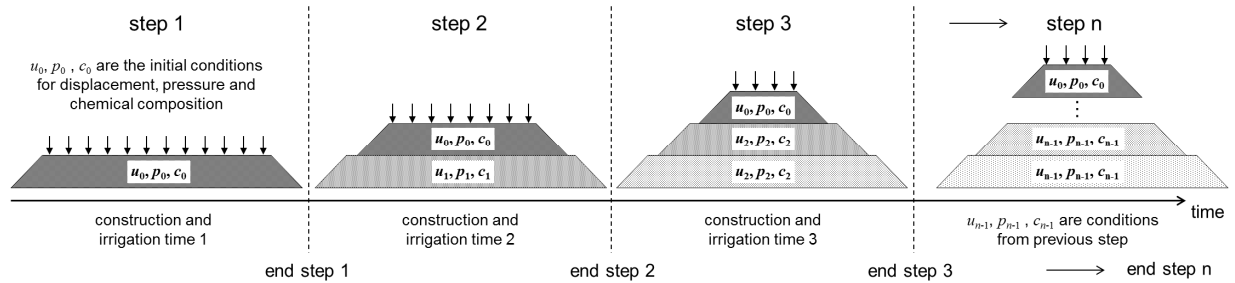


Figure 1: Sequence of construction of a heap leach pad layer by layer. The layer “n” is represented by “step n”. State variables of the problem are displacement (u), liquid pressure (p) and concentration (c)

Table 1: Chemical reactions considered in the geochemical model

Mineral	Kinetic reactions
Chrysocolla	$\text{CuSiH}_4\text{O}_5 + 2\text{H}^+ = \text{Cu}^{+2} + \text{H}_2\text{O} + \text{H}_4\text{SiO}_4$
Chalcopyrite	$\text{CuFeS}_2 + 2\text{H}^+ = \text{Cu}^{+2} + \text{Fe}^{+2} + 2\text{HS}^-$
Pyrite	$\text{FeS}_2 + 2\text{H}^+ + 2\text{e}^- = \text{Fe}^{+2} + 2\text{HS}^-$
Albite	$\text{NaAlSi}_3\text{O}_8 + 2\text{H}_2\text{O} = \text{Na}^+ + \text{Al}(\text{OH})_4^- + 3\text{H}_4\text{SiO}_4$
K-Feldspar	$\text{KAlSi}_3\text{O}_8 + 8\text{H}_2\text{O} = \text{K}^+ + \text{Al}(\text{OH})_4^- + 3\text{H}_4\text{SiO}_4$
Mineral	Equilibrium reactions
Jarosite-K	$\text{KFe}_3(\text{SO}_4)_2(\text{OH})_6 + 6\text{H}^+ = \text{Fe}^{+3} + 6\text{H}_2\text{O} + \text{K}^+ + 2\text{SO}_4^{-2}$
Jurbanite	$\text{AlOHSO}_4 + \text{H}^+ = \text{Al}^{+3} + \text{SO}_4^{-2} + \text{H}_2\text{O}$
Basaluminite	$\text{Al}_4(\text{OH})_{10}\text{SO}_4 + 10\text{H}^+ = 4\text{Al}^{+3} + \text{SO}_4^{-2} + 10\text{H}_2\text{O}$
$\text{Fe}(\text{OH})_3(\text{a})$	$\text{Fe}(\text{OH})_3 + 3\text{H}^+ = \text{Fe}^{+3} + 3\text{H}_2\text{O}$
Schwertmannite	$\text{Fe}_8\text{O}_8(\text{OH})_{4.5}(\text{SO}_4)_{1.75} + 20.5\text{H}^+ = 1.75\text{SO}_4^{-2} + 8\text{Fe}^{+3} + 12.5\text{H}_2\text{O}$

The assumed rock composition is as follows: chrysocolla (20 wt%), chalcopyrite (10 wt%), pyrite (8 wt%), albite (30 wt%), and K-feldspar (32 wt%), and a Cu grade of 0.48%. This composition may be representative of a zone of increased fracturing with a low pyrite/chalcopyrite ratio. The chemical evolution

of the above minerals is assumed to be governed by kinetic reactions (Dreier, 1999; Kimball et al., 2010; Williamson and Rimstidt, 1994; Chou and Wollast, 1985; Schweda, 1989) (see Table 1). Equilibrium precipitation-dissolution reactions of Jarosite-K, Jurbanite, Basaluminite, $\text{Fe}(\text{OH})_3(\text{a})$ and Schwertmannite are also taken into account (Table 1). To simplify the problem, bioleaching of chalcopyrite was not considered in the model. The chemical compositions of the initial pore water and irrigation solution are shown in Table 2.

Table 2: Chemical compositions of the initial pore water and irrigation solution

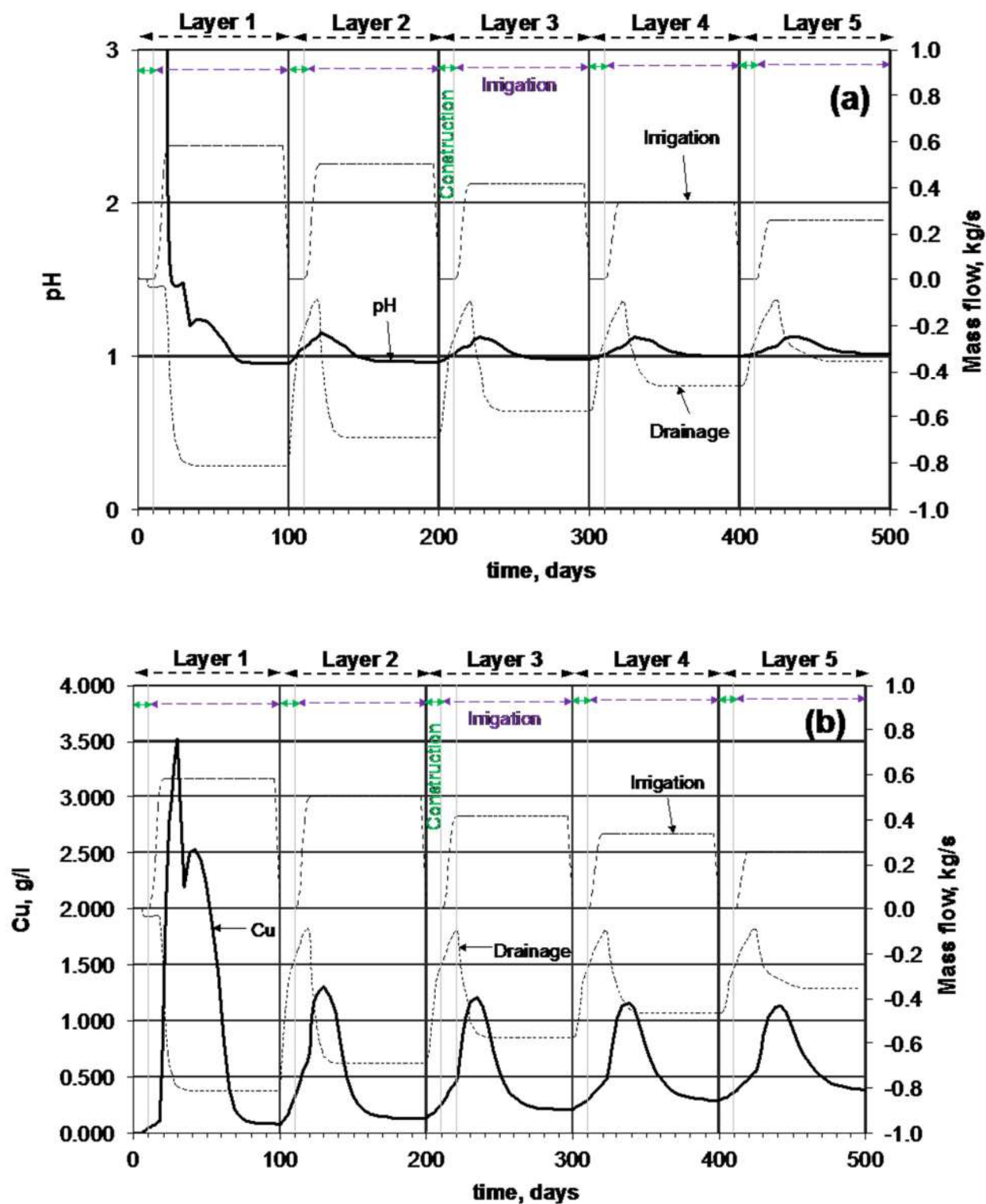
	Initial pore water, m_a^0	Irrigation solution, m_a^*
pH	5.95	0.94
Eh, mV	738	1161
Al, mol/l	2.56×10^{-10}	10^{-22}
C, mol/l	3.49×10^{-2}	1.04×10^{-5}
Ca, mol/l	3.49×10^{-2}	2.70×10^{-3}
Cl, mol/l	1.30×10^{-6}	9.63×10^{-2}
K, mol/l	1.89×10^{-2}	6.30×10^{-4}
Fe, mol/l	2.50×10^{-7}	7.50×10^{-6}
Mg, mol/l	3.99×10^{-8}	1.30×10^{-5}
Na, mol/l	10^{-14}	6.10×10^{-4}
S, mol/l	3.79×10^{-2}	4.50×10^{-2}
Si, mol/l	9.25×10^{-17}	3.20×10^{-4}

Results and discussion

Figure 2 shows the evolution of concentrations of selected dissolved species at the output of the drainage system. The evolution of pH shows the arrival of the acidic solution at the liner system in a time of around 60 days (Figure 2a). Kinetic dissolution of chrysocolla and chalcopyrite is triggered by the infiltration of the acidic solution and, as a result, an increase of Cu concentrations is observed in the outlet flow (Figure 2b). The chemical evolution of Si and Al concentrations (Figure 2c) clearly shows that under these low pH conditions kinetic dissolution of aluminosilicates is also favored. This process is highly dependent on the pH and, over a long period of time, porosity can be significantly modified.

Figure 3 shows the temporal evolution of chalcopyrite and chrysocolla concentrations. The concentration of chalcopyrite hardly changes, while the chrysocolla is almost completely dissolved at the

end of the leaching of each layer. This is due to the combination of three factors: the slow dissolution rate of chalcopyrite, the fast dissolution rate of chrysocolla, and the initial amounts of both minerals, which are very similar.



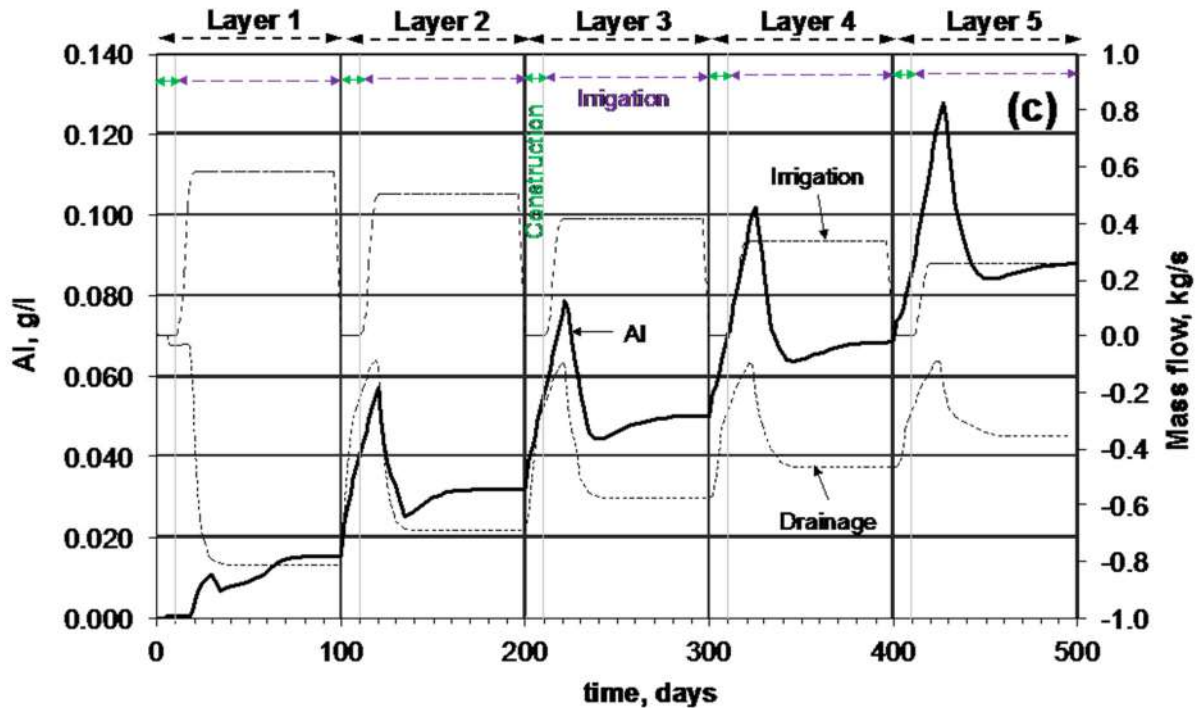


Figure 2: Evolution of pH (a) and concentrations of Cu (b) and Al (c) in the pregnant leach solution. Irrigation and drainage mass flows during each stage are also included

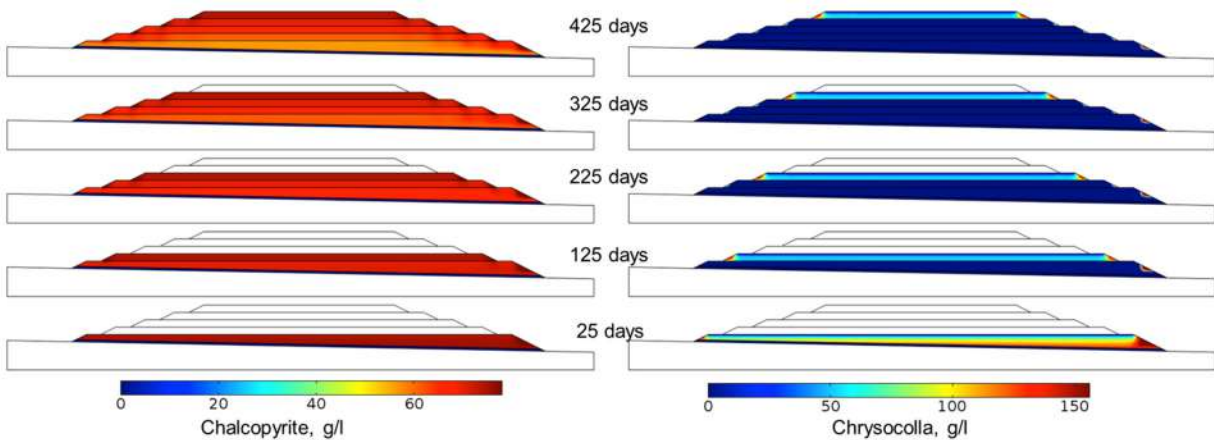
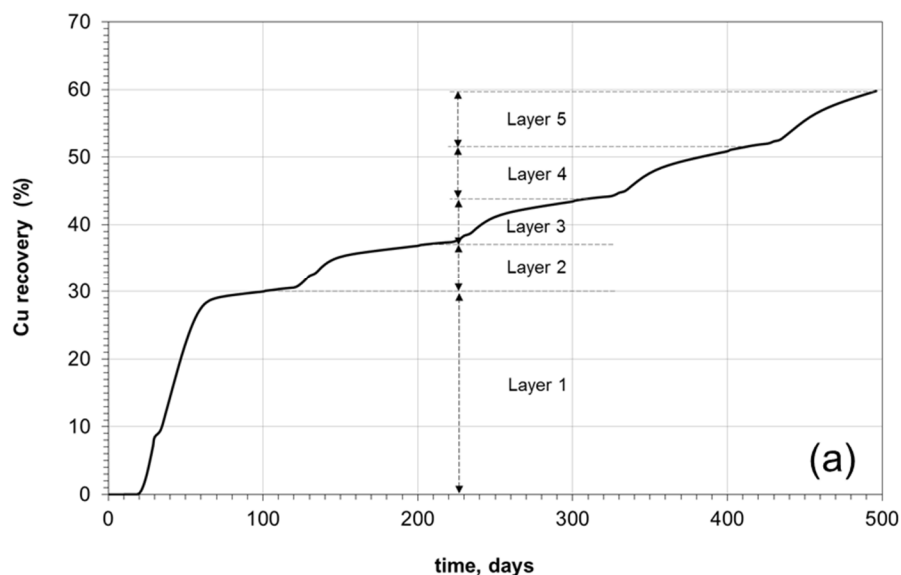


Figure 3: Evolution of the chalcopyrite (left) and chrysocolla (right) concentrations in the leach pad

The copper recovery is presented in Figure 4a. Note that the copper recovery associated with the leaching of each layer displays a common pattern that reflects the difference in the leaching rates of chrysocolla and chalcopyrite. During the first days of leaching of a new layer, the copper is recovered mainly from chrysocolla. The fast dissolution rate of chrysocolla is associated with a higher slope of the recovery curve. Once chrysocolla has been spent, the copper recovery continues from chalcopyrite at a

lower rate (lower slope of the copper recovery curve). This pattern is more evident during the leaching of the first layer, which provides a copper recovery of about 30%. The copper recovered from the leaching of subsequent layers is about 8%. At the end of the operation (500 days), approximately 60% of the copper has been recovered. The recovered copper increases due to the leaching of residual mineral from previous layers, depending on the thickness of the loaded layers and the irrigation times.

The competition between chrysocolla and chalcopyrite is more evident when looking at the acid sulfuric consumption, which is shown in Figure 4b. During a given irrigation period, the consumed acid increases at an almost constant rate until reaching a plateau coinciding with the construction of a new layer. After 25 days from the start of a new irrigation period, the acid consumption experiences a small decrease, due to the complete dissolution of chrysocolla. Note that this time coincides with the time at which the copper recovery changes its rate (see Figure 4a). These changes in copper recovery and acid consumption last about five days, after which the acid consumption increases again at the initial rate of the current leaching stage. That is, the copper recovery and acid consumption curves directly reflect the different dissolution rates of the mineral species considered in the model, especially the chrysocolla (fast dissolution rate) and the chalcopyrite (slow dissolution rate). Also, the plateau of acid consumption is clearly associated with the behavior of the irrigation and drainage flow rates (see Figure 2). In addition, acid consumption during the leaching of a new layer is progressively lower than the acid consumption of previous leaching stages. This is because the mass of mineral of the new layer is lower, and the impact of acid consumption from previous leached layers is minor.



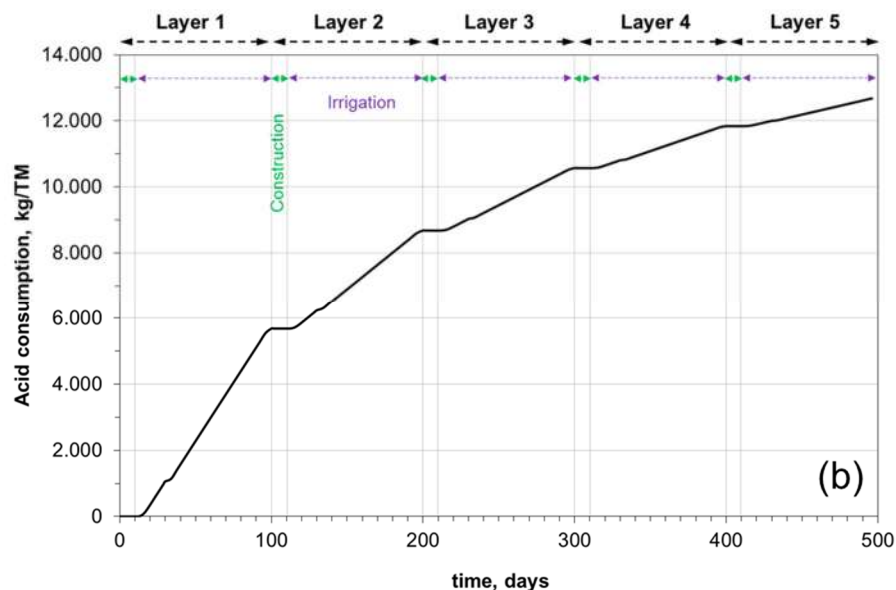


Figure 4: Predicted copper recovery (a) and acid consumption (b)

The hydrodynamic behavior of the system is conditioned by the time required for the irrigation solution to saturate the heap as it flows to the drainage system. The evolution of the liquid saturation is shown in Figure 5a. After a short period of time, a quasi-steady state is achieved for every layer. In the present case it takes about 40 days from the layer construction. We have set an observation point to understand the evolution of the liquid pressure (red spot on Figure 5a). As shown in Figure 5b, two stages are found for every leaching step: the construction and the irrigation periods. The effect of construction does not generate pore water pressure (as occurs in undrained conditions), as the ore is mainly unsaturated and the construction has been simulated in a progressive manner. The increase of liquid pressure at the beginning of each leaching step is caused by irrigation. Nevertheless, as shown in Figure 5b, this increase is progressively lower because the irrigation decreases in the next leaching step. The irrigation time plays an important role in the system behavior. This is due to the influence of irrigation on the liquid pressure and the mass of recovered minerals. Some amount of copper remains in the pad close to the slope limits, because irrigation is not very effective in those zones. Ideally, those zones could be exploited as well.

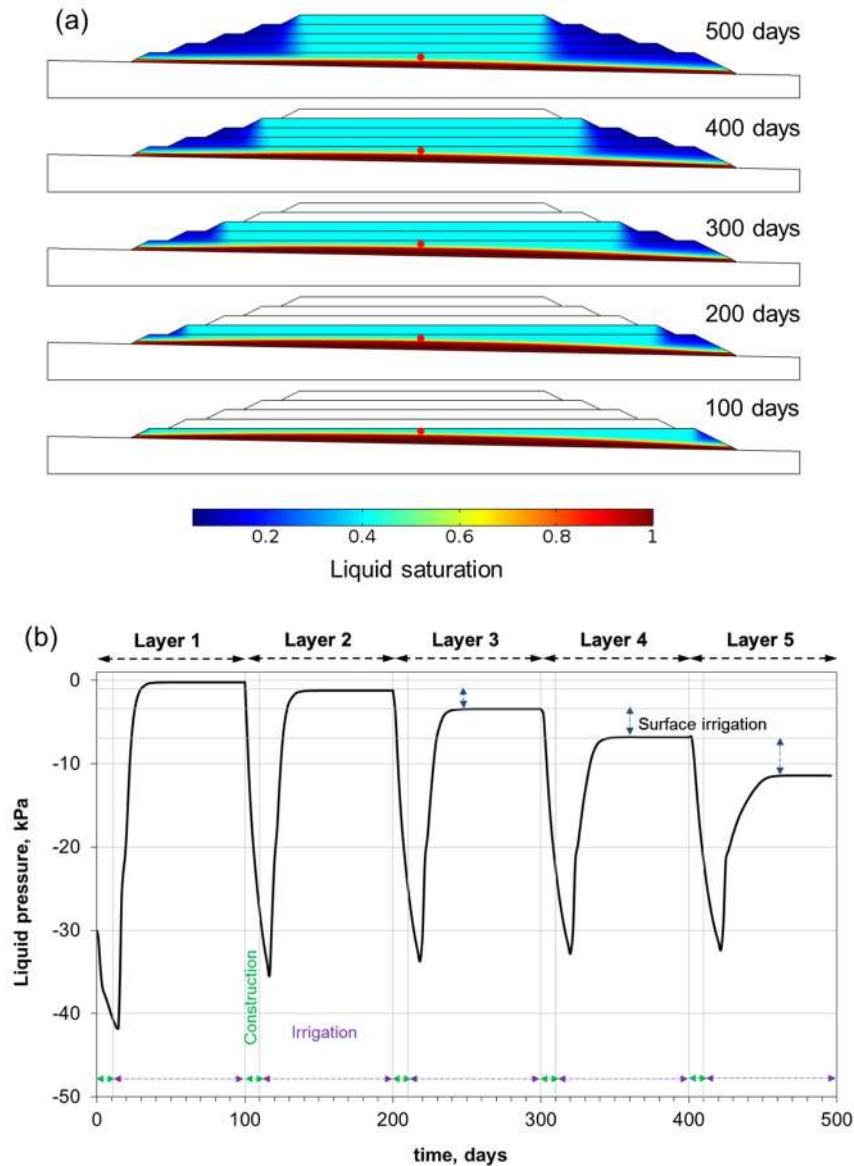


Figure 5: Evolution of the liquid saturation in the leach pad. The red circle on the upper figure (a) denotes the observation point for pressure evolution shown in (b)

Changes in porosity and permeability due to mineral dissolution/precipitation and irrigation time can affect significantly the hydromechanical behavior of the heap leach pad. Figure 6a shows the evolution of the global porosity due to the combined hydromechanical and chemical effects. We found that there are zones of the ore where the porosity increases due to the mineral dissolution, and other zones where the consolidation of the layers leads to a porosity decrease. In turn, the mechanical effects consist in an increase in the vertical stress developed mainly on the rock foundation as the layers are progressively loaded. This

vertical stress increase also reaches the top of the third layer, where the vertical displacement reaches a maximum.

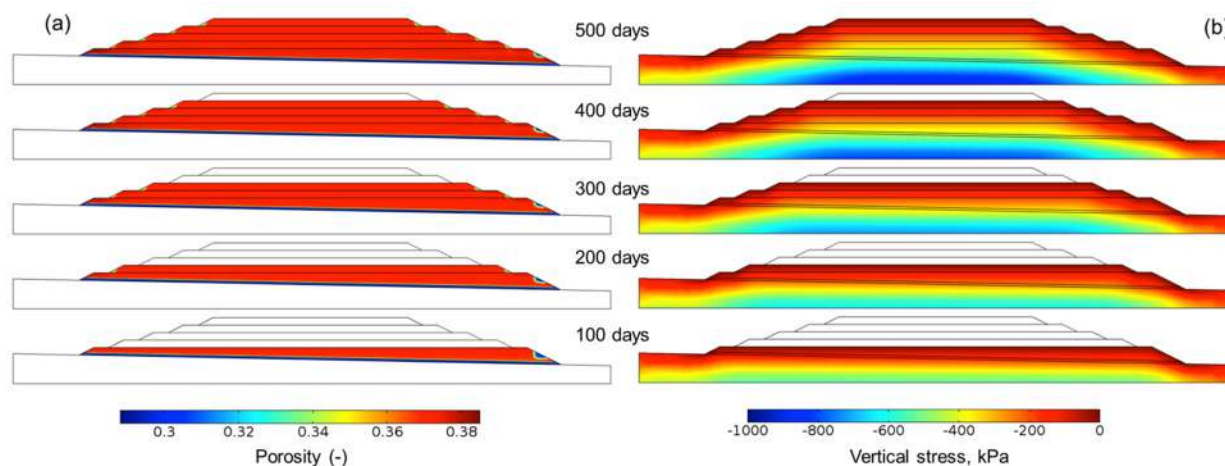


Figure 6: Evolution of global porosity (a) and vertical stress in the leach pad (b)

Conclusions

This paper presented iCP, a numerical tool that is able to solve simultaneously unsaturated flow, soil mechanics, and reactive transport in porous media. This tool allows integrating in a single framework hydromechanical and geochemical coupled phenomena and the processes involved in the construction and operation of heap leach pads. Geochemical changes affecting porosity and permeability are coupled explicitly in the hydraulic and geomechanical calculations. The model calibration may be conducted in a two-stage optimization process based on (i) experimental data from batch tests and kinetics test columns for reaction rate parameters optimization in PHREEQC; and (ii) field scale measurements and operational indicators (e.g., pressures, flow rates, copper recovery, and acid consumption) for inverse modeling of hydro-mechanical-solute transport parameters in COMSOL.

The simulation results show that changes in porosity due to mineral dissolution/precipitation and irrigation time affect significantly the hydromechanical behavior of the heap leach pad, and vice versa. For the synthetic case of a multilift heap considered in the study, the simulated copper recovery and acid consumption responds directly to the dissolution rates of the copper bearing minerals considered in the model. A strong advantage of the present model is that it can treat multiple chemical species simultaneously, providing solutions that are best for interpreting all the chemical interactions within a leaching system. In addition, the stability of the pad and the ore recovery efficiency can be predicted with more accuracy because the model considers the interaction between variable saturated flow, mechanical deformation, and chemical reactions during the construction and irrigation of the different layers of the heap. Finally, the

modeling methodology presented in this work can help to improve the stability of the heap pad and optimize mineral recovery efficiency.

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