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Flow through porous media with applications to heap leaching of copper ores

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Abstract

The classical equations of two-phase flow in a porous media are solved together with two transport equations representing the leaching process. For the two-phase flow we use the pressure-saturation formulation, where the principal variables are the total pressure, the total flux and the saturation of the liquid phase. For the transport equations the variables of interest are the sulfuric acid and the copper concentration. The numerical method combines a mixed finite element method with a finite volume method. The first one is used to approximate the total pressure and flux, while the second is used to calculate the saturation and both concentrations. The advantage of this approach is its capacity to completely characterize the dynamics of the liquid and gaseous phase, and treat with the same model acid and bio-leaching processes. Several examples show the application of the method.

Keywords: Porous Media; Heap leaching; Two-phase flow

1. Introduction

Most companies, as a result of the favorable economics possible in heap leaching, consider heap leaching an alternative to conventional processing (flotation, agitation and vat leaching) [12]. This process is considered an integral part of most copper mining operations and should determine, along with other factors, the cutoff grade of the material sent to the mill.

Leaching is a transfer process of mass between the leaching solution (fluid phase) and the ore bed (solid phase) [6]. The heap leaching process can be considered as a multiphase system in a porous medium, where the multiphase system is formed by two fluids phases: a liquid phase (leach solution) and a gaseous phase [3,11]. We consider the case where the liquid phase transports two component: the sulfuric acid (leaching agent) and the copper as species of interest (cf. [6,9]).

Two distinct phenomena are of interest in the study of heap leaching: fluid flow and the physicochemical reactions. These two phenomena can be studied separately if the extent of leaching of an element of solution that has participated in this process, and the extent of leaching that an element of the heap has undergone, does not influence the solution flow pattern. In other words, the solution flow pattern in a heap depends only on the initial conditions of the heap. In general, researchers in heap leaching have separated the fluid flow problem from the physicochemical problem. We develop a mathematical model, which consists in a system of nonlinear partial differential equations, in the context of multiphase system in a porous medium, that considers simultaneously the fluid flow problem and the physicochemical problem. Our model generalizes previous models which consider only one phase (see for instance [3,9]). For example, our model eliminates the assumption that the gaseous phase pressure is at the atmospheric pressure, i.e., we consider the interaction between both fluids phases.

Respect to the numerical solution, we present a generalization to the nonlinear case, which is very useful for engineering applications [4].

Finally, we report numerical results that illustrates the application of our model to the heap leaching process.

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Nomenclature

c_{a}	volumetric concentration of sulfuric acid in solution (kg/m^3)
c_{c}	volumetric concentration of copper in solution (kg/m^3)
c_{n}	compressibility of gaseous phase
D	capillary diffusion coefficient
$\boldsymbol{D}$	tensor of hydrodynamic dispersion (m^2/s)
g	gravity (m/s^2)
$\boldsymbol{g}$	gravity vector (=0, 0, $-g$)
k	absolute permeability of the porous system (m^2)
k_{d}	equilibrium distribution constant (adsorption coefficient) (m^3/kg)
k_{e}	first-order kinetic constant (extraction coefficient) (m^3/kg s)
$k_{\mathrm{r\alpha}}$	relative permeability of the α-phase (–)
p	global pressure (Pa)
p_{c}	capillary pressure function (Pa)
p_{d}	entry pressure (Pa)
p_{α}	pressure of α-phase (Pa)
q_{α}	fractional flow function (–)
$\Re$	real numbers
s_{wr}	residual water saturation (–)
s_{α}	saturation of α-phase (m^3/m^3)
S_{c}	concentration (mass of copper/mass of solid phase) of copper in solid phase (kg/kg)
t	time (s)
T	total time of simulation (s)
$\boldsymbol{u}_{\boldsymbol{\alpha}}$	flow velocity (m/s)
$\boldsymbol{v}$	total velocity (m/s)
$\boldsymbol{v}_{\alpha}$	volumetric (flux or Darcy's velocity) velocity of α-phase (m/s)

Greek symbols and subscripts

α	phase ($\alpha = \mathrm{w}, \mathrm{n}$)
$\alpha = \mathrm{w}$	liquid phase (leach solution)
$\alpha = \mathrm{n}$	gaseous phase
λ	total mobility (m s/kg)
λ_{α}	phase mobility function (m s/kg)
λ_{BC}	Brooks–Corey parameter (–)
λ_{LF}	Lax–Friedrichs parameter
μ	first-order consumption factor (consumption coefficient) (1/s)
μ_{α}	viscosity of the α-phase (kg/m s)
ρ_{s}	solid bulk (dry) density (kg/m^3)
ρ_{α}	density of α-phase (kg/m^3)
ϕ	porosity of ore bed (volume of void/volume of bed) (m^3/m^3)
ϕ_{s}	volume of solid phase/volume of bed (=1 $-\ \phi$) (m^3/m^3)

2. Multiphase fluid flow

We consider a multiphase system in a porous medium. Let a representative elementary volume (REV) (see [7] for more details) in the porous medium formed by the solid matrix and both fluids phases: liquid and gaseous. The porosity of the porous medium is defined as $\phi = \frac{\text{volume of the pore space within the REV}}{\text{volume of REV}}$, and the saturation of phase α is defined as $s_{\alpha}(\boldsymbol{x}, t) = \frac{\text{volume of fluid } \boldsymbol{\alpha} \text{ within the REV}}{\text{volume of the pore space within the REV}}$, where $\alpha = \mathrm{w}$ is the liquid phase and $\alpha = \mathrm{n}$ is the gaseous phase. We impose the customary property that the fluids fill the volume:

$$s_{\mathrm{w}} + s_{\mathrm{n}} = 1. \tag{1}$$

2.1. Compositional flow/transport equations

A mass balance must be specified for each component. The mass balance equations for the transport of component κ in α-phase can be written as [2,7]:

$$\frac{\partial(\phi s_{\alpha} c_{\kappa}^{\alpha})}{\partial t} + \mathrm{div}(c_{\kappa}^{\alpha} \boldsymbol{v}_{\alpha} - \phi s_{\alpha} \boldsymbol{D} \nabla c_{\kappa}^{\boldsymbol{\alpha}}) + \boldsymbol{\Phi}_{\boldsymbol{\alpha}} = 0, \tag{2}$$

where c_{κ}^{α} is the volumetric concentration defined by $c_{\kappa}^{\alpha} = \frac{\text{mass of component } \kappa \text{ in phase } \alpha}{\text{volume of phase } \alpha}$, $\boldsymbol{v}_{\alpha}$ the *volumetric flux of phase* α, Φ_{α} (kg/m^3 s) the irreversible rate of solute removed (or added) from (to) the liquid solution, $\boldsymbol{D}$ the dispersity-diffusion tensor given by $D_{ij} = \alpha_{\mathrm{T}} |\boldsymbol{u}_{\boldsymbol{\alpha}}| \delta_{ij} + (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \frac{u_i u_j}{|\boldsymbol{u}_{\boldsymbol{\alpha}}|} + D_{\mathrm{m}} \delta_{ij}$, where α_{L} and α_{T} are the longitudinal and transverse dispersivities, respectively, $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$, and D_{m} is the molecular diffusion coefficient (in this paper we set $D_{\mathrm{m}} = 0$) and $\boldsymbol{u}_{\boldsymbol{\alpha}} = \phi s_{\alpha} \boldsymbol{v}_{\alpha}$ is the *flow velocity of phase* α.

In the case of sorption, (2) is modified to include a retardation factor. It is assumed that there is a Freundlich equilibrium isotherm between the liquid phase and the solid phase. The isotherm has the form

$$F_{\kappa}^{\alpha} = \frac{\text{mass of component in solid phase}}{\text{mass solid phase}} = k_{\mathrm{d}} c_{\kappa}^{\alpha},$$

where k_{d} is called the distribution coefficient. Using the assumption that sorption only occurs from the liquid to the solid phase, the equation for the liquid phase can be modified to include adsorption:

$$\frac{\partial(\phi_{\mathrm{s}} \rho_{\mathrm{s}} F_{\kappa}^{\alpha})}{\partial t} + \frac{\partial(\phi s_{\alpha} c_{\kappa}^{\alpha})}{\partial t} + \mathrm{div}(c_{\kappa}^{\alpha} \boldsymbol{v}_{\alpha} - \phi s_{\alpha} \boldsymbol{D} \nabla c_{\kappa}^{\mathrm{w}}) + \Phi_{\alpha} = 0, \tag{3}$$

where $\phi_{\mathrm{s}} = 1 - \phi$, ρ_{s} is ore bulk density.

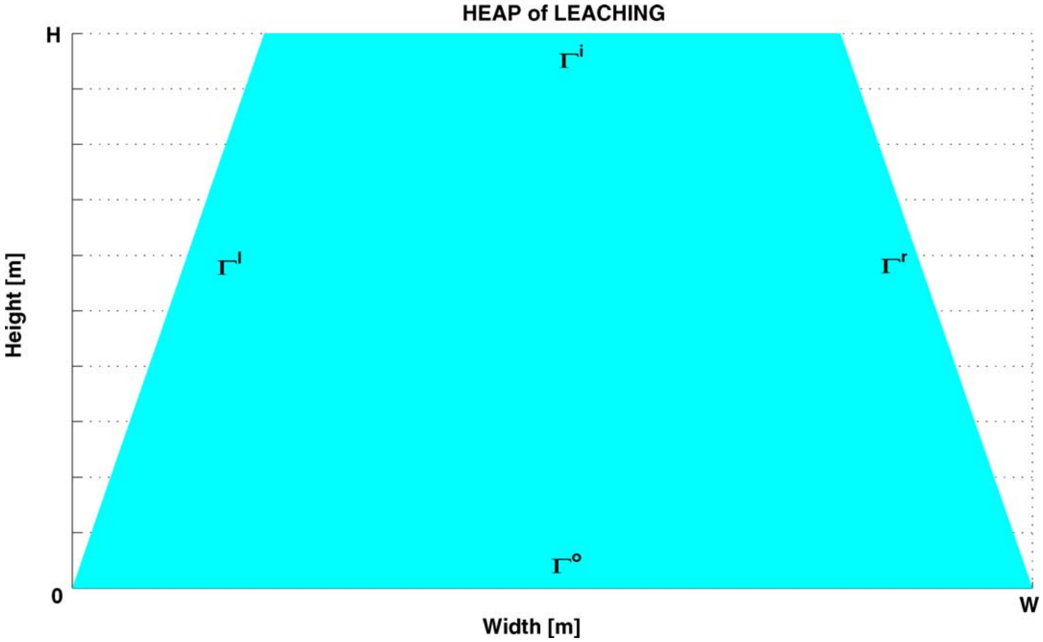

Fig. 1. Plot of the mathematical domain Ω.

3. Model development

3.1. Mathematical domain and assumptions

In this paper we consider 2D geometry (Fig. 1, transversal cut of the heap). The boundary of $\Omega \subset \Re^2$, i.e., $\partial\Omega$ is expressed as $\partial\Omega = \Gamma^i \cup \Gamma^o \cup \Gamma^l \cup \Gamma^r$, where Γ^i is the input boundary (zone of irrigation), Γ^o is the output boundary (zone of drainage), Γ^l is the left boundary, Γ^r is the right boundary.

In this article we consider a heap of leaching of width $W = 25$ m and height $H = 5$ m.

In order to simplify our model, we consider a two phase flow through a porous medium with the following assumptions (see [9] for specific details): flow occurs in a vertical plane 2D, generalized Darcy's law for multiphase flow is valid, the porosity and the absolute permeability are uniform in space and constant with time, the porous medium is non-compressible, homogeneous and isotropic with respect to the transversal and longitudinal dispersivity coefficients, in the void space there are only two fluids phases: the liquid phase (leach solution) and the gaseous phase, the reaction between the acid and the particles of copper minerals proceeds in an instantaneous fashion and is irreversible, the system is isothermal, the regime of flow is laminar, the physical properties of liquid phase are constants, the effect of the transport of solutes on the transport of fluid is weak, and not exist mass exchange between both fluids phases.

3.2. Two-phase flow equations

Thus, the continuity equations [7] for each phase $\alpha = \mathrm{w}, \mathrm{n}$ are derived from the mass balance in the REV:

$$\frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \mathrm{div}(\rho_\alpha \boldsymbol{v}_{\boldsymbol{\alpha}}) = r_{\boldsymbol{\alpha}}, \tag{4}$$

where ϕ is the porosity of the porous medium, ρ_α, s_α, $\boldsymbol{v}_{\boldsymbol{\alpha}}$, are the density, saturation, pressure, volumetric velocity of the α-phase, and r_α is the source term (by assumption: $r_\alpha = 0$, $\alpha = \mathrm{w}, \mathrm{n}$). As in the single-phase case, it can be shown by volume averaging or homogenization techniques that the macroscopic phase velocity can be expressed in terms of the macroscopic phase pressure by the generalized Darcy's law [7]

$$\boldsymbol{v}_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \boldsymbol{g}), \tag{5}$$

where k is the absolute permeability of the porous systems, p_α, μ_α, $k_{r\alpha}$ are the pressure, viscosity and the relative permeability of the α-phase, and $\boldsymbol{g}$ is the gravitational, downward-pointing, constant vector. Therefore, (4) and (5) are the two-phase flow equations (see [1,2,5]).

The pressure at the microscopic level has a jump discontinuity when passing from one fluid phase to the other. The jump is called the *capillary pressure*. This fact is reflected by a macroscopic capillary pressure at the macroscopic level: $p_c(\boldsymbol{x}, t) = p_n(\boldsymbol{x}, t) - p_w(\boldsymbol{x}, t)$. The macroscopic consideration of the capillarity results in the following capillary pressure-saturation relation: $p_c(\boldsymbol{x}, t) = f(s_w, s_n)$, but $s_w + s_n = 1$, therefore p_c is given by:

$$p_c(s_w) = p_n - p_w. \tag{6}$$

The usual correlations for a two-phase gas-liquid system are the Brooks–Corey (BC) and Van Genuchten (VG) parameterizations [7]. In this work we use BC, which is defined by

$$p_{\mathrm{c}}(s_{\mathrm{w}}) = p_{\mathrm{d}} \left(\frac{s_{\mathrm{w}} - s_{\mathrm{wr}}}{1 - s_{\mathrm{wr}}} \right)^{-1/\lambda_{\mathrm{BC}}}, \quad p_{\mathrm{c}} \geq p_{\mathrm{d}},$$

where $0.2 \leq \lambda_{\mathrm{BC}} \leq 3.0$ is a BC-parameter (*a very small* λ_{BC}*-parameter describes a single grain size material, while a very large value indicates a highly non-uniform material*) and p_{d} is the entry pressure (*capillary pressure required to displace the wetting phase from the occurring pore*). In this paper $\lambda_{\mathrm{BC}} = 1$, and $p_{\mathrm{d}} = 101{,}325\,\mathrm{Pa}$, i.e., the atmospheric pressure.

In conjunction with constrains (1) and (6), Eqs. (4) and (5), represent a coupled dynamic system of differential equations, which describes the simultaneous flow of two or more immiscible fluids in a variable saturation porous medium. The behavior of the system of equations is strongly nonlinear because there is a nonlinear dependence of the saturation on the capillary pressures and on the relative permeabilities.

Alternative formulations for system (4)–(5)–(6)–(1) have been developed which depend on the individual problem and on the efficiency of the chosen numerical methods [7]:

- (**P–P**) pressure formulation: with phase pressures as unknowns (primary variables).
- (**P–S**) pressure–saturation formulation: with the pressure of the fluid with the highest affinity and the saturations of the other phases as unknowns.
- (**S–S**) saturation formulation: with phase saturations as unknowns.

In petroleum reservoir simulation the governing equations that describe fluid flow are usually written in a fractional flow formulation, i.e., in term of a saturation and a global pressure. The main reason for this fractional flow approach is that efficient numerical methods can be devised to take advantage of many physical properties inherent in the flow equations. Therefore, the systems (4)–(5)–(6)–(1), can also be written in our case as [5]:

$$c(s_{\mathrm{w}}, p) \frac{\mathrm{d}p}{\mathrm{d}t} + \operatorname{div} \boldsymbol{v} = q(s_{\mathrm{w}}, p), \tag{7}$$

$$-\lambda(s_{\mathrm{w}}) k (\nabla p - \boldsymbol{G}_{\lambda}(s_{\mathrm{w}}, p)) = \boldsymbol{v}, \tag{8}$$

$$\phi \frac{\partial s_{\mathrm{w}}}{\partial t} + \operatorname{div}(q_{\mathrm{w}}(s_{\mathrm{w}}) \boldsymbol{v} - \boldsymbol{G}_1(s_{\mathrm{w}}, p) - D(s_{\mathrm{w}}) \nabla s_{\mathrm{w}}) = 0, \tag{9}$$

with unknowns: p, $\boldsymbol{v}$, s_{w}, where: $\lambda = \lambda_{\mathrm{w}} + \lambda_{\mathrm{n}}$ is the total mobility with: $\lambda_\alpha = \frac{k_{\mathrm{r}\alpha}}{\mu_\alpha}$ is the mobility of α-phase, p is the total pressure given by

$$p = p_{\mathrm{n}} - \int_0^s q_{\mathrm{w}} \frac{\mathrm{d}p_{\mathrm{c}}}{\mathrm{d}\xi} \, \mathrm{d}\xi, \tag{10}$$

with $q_\alpha = \frac{\lambda_\alpha}{\lambda}$, $\alpha = \mathrm{w}, \mathrm{n}$ is the fractional flow function, $c(s_{\mathrm{w}}, p) = (1 - s_{\mathrm{w}}) c_{\mathrm{n}}(p)$ with: $c_{\mathrm{n}}(p) = \frac{1}{\rho_{\mathrm{n}}} \frac{\mathrm{d}\rho_{\mathrm{n}}}{\mathrm{d}p_{\mathrm{n}}}$ is the compressibility of the gaseous phase, $q(s_{\mathrm{w}}, p) = -s_{\mathrm{n}} c_{\mathrm{n}}(p) q_{\mathrm{w}} (\mathrm{d}p_{\mathrm{c}}/\mathrm{d}t)$, $\boldsymbol{G}_{\lambda}(s_{\mathrm{w}}, p) = \frac{\lambda_{\mathrm{w}} \rho_{\mathrm{w}} + \lambda_{\mathrm{a}} \rho_{\mathrm{n}}}{\lambda} \boldsymbol{g}$, $\boldsymbol{G}_1(s_{\mathrm{w}}, p) = k \lambda_{\mathrm{n}} q_{\mathrm{w}} (\rho_{\mathrm{n}} - \rho_{\mathrm{w}}) \boldsymbol{g}$, and $D(s_{\mathrm{w}}) = -k \lambda_{\mathrm{n}} q_{\mathrm{w}} \frac{\mathrm{d}p_{\mathrm{c}}}{\mathrm{d}s}$ is the capillary diffusion coefficient. Finally, $\boldsymbol{v}$ is the total velocity, given by

$$\boldsymbol{v} = \boldsymbol{v}_{\mathrm{w}} + \boldsymbol{v}_{\mathrm{n}}, \tag{11}$$

where the volumetric velocity of leaching solution is given by

$$\boldsymbol{v}_{\mathrm{w}} = q_{\mathrm{w}} \boldsymbol{v} + k \lambda_{\mathrm{n}} q_{\mathrm{w}} \nabla p_{\mathrm{c}} - k \lambda_{\mathrm{n}} q_{\mathrm{w}} (\rho_{\mathrm{n}} - \rho_{\mathrm{w}}) \boldsymbol{g}, \tag{12}$$

and the volumetric velocity of gaseous phase is given by

$$\boldsymbol{v}_{\mathrm{n}} = q_{\mathrm{n}} \boldsymbol{v} + k \lambda_{\mathrm{w}} q_{\mathrm{n}} \nabla p_{\mathrm{c}} - k \lambda_{\mathrm{w}} q_{\mathrm{n}} (\rho_{\mathrm{n}} - \rho_{\mathrm{w}}) \boldsymbol{g}. \tag{13}$$

3.3. *Transport equations*

The sulfuric acid and the copper ions are transported by the leach solution. The presented equations conform the classical transport equations in the context of biphasic/bicomponent flow [1,7] and this formulation generalizes the saturated flow in a porous medium [9] to a biphasic flow.

In Eq. (2) we consider $\alpha = \mathrm{w}$, $\kappa = \mathrm{a}$ for the sulfuric acid and $\kappa = \mathrm{c}$ for the copper. About the notation for the volumetric concentration: $c_{\mathrm{a}}^{\mathrm{w}} \equiv c_{\mathrm{a}}$ and $c_{\mathrm{c}}^{\mathrm{w}} \equiv c_{\mathrm{c}}$, i.e., we omit w.

3.3.1. *Sulfuric acid transport equation*

During migration through the porous media (heap) sulfuric acid reacts with the copper. Acid consumption is assumed to be proportional to its concentration (μc_{a} in (14)), therefore, from (2) with $\Phi_\alpha = \phi s_{\mathrm{w}} \mu c_{\mathrm{a}}$, the transport equation of sulfuric acid in leach solution is given by

$$\frac{\partial(\phi s_{\mathrm{w}} c_{\mathrm{a}})}{\partial t} + \operatorname{div}(c_{\mathrm{a}} \boldsymbol{v}_{\mathrm{w}} - \phi s_{\mathrm{w}} \boldsymbol{D} \nabla c_{\mathrm{a}}) + \phi s_{\mathrm{w}} \mu c_{\mathrm{a}} = 0, \tag{14}$$

where μ is a first-order reaction constant (consumption factor) and c_{a} the volumetric concentration of acid in leach solution.

3.3.2. *Copper transport equation in liquid phase*

The transport of copper ions through the heap is mainly governed by two processes. The first process consists of a chemical reaction that occurs between the leaching agent and the mineral particles. The copper present in the ore is solubilized passing from the solid to the liquid phase. The kinetic involved is a the first order ($\rho_{\mathrm{s}} k_{\mathrm{e}} c_{\mathrm{a}} S_{\mathrm{c}}$ in (15)) heterogeneous reaction. Therefore, the first process is extraction of copper from the solid phase to the liquid phase. The second process in the copper adsorption/desorption phenomenon, which is modeled using a linear equilibrium isotherm ($F_{\mathrm{c}}^{\mathrm{w}} = k_{\mathrm{d}} c_{\mathrm{c}}$ in (15)). Therefore, from (3) with $\Phi_\alpha = \phi_{\mathrm{s}} \rho_{\mathrm{s}} k_{\mathrm{e}} c_{\mathrm{a}} S_{\mathrm{c}}$, the transport equation of copper in leach solution is given by

$$\begin{aligned} &\frac{\partial(\phi_{\mathrm{s}} \rho_{\mathrm{s}} k_{\mathrm{d}} c_{\mathrm{c}})}{\partial t} + \frac{\partial(\phi s_{\mathrm{w}} c_{\mathrm{c}})}{\partial t} + \operatorname{div}(c_{\mathrm{c}} \boldsymbol{v}_{\mathrm{w}} - \phi s_{\mathrm{w}} \boldsymbol{D} \nabla c_{\mathrm{c}}) \\ &\quad + \phi_{\mathrm{s}} \rho_{\mathrm{s}} k_{\mathrm{e}} c_{\mathrm{a}} S_{\mathrm{c}} = 0, \end{aligned} \tag{15}$$

where k_e is a first-order kinetic constant, S_c the concentration of copper associated with the solid phase (cf. (16)) and c_c the volumetric concentration of copper in leach solution.

3.3.3. Copper transport equation in solid phase

The change in the concentration of copper in the solid phase follows the mass balance [9]:

$$\frac{\partial S_c(\cdot,t)}{\partial t} + \phi_s k_e c_a S_c(\cdot,t) = \frac{\partial(\phi_s k_d c_c)}{\partial t}, \tag{16}$$

where S_c is the concentration of copper in solid phase, i.e., $S_c = \frac{\text{mass of copper in solid phase}}{\text{mass of solid phase}}$.

3.4. Mathematical model

The heap leaching of copper ore model is described by Eqs. (7)–(9) and (14)–(16), i.e.,

$$c(s_w, p)\frac{\mathrm{d}p}{\mathrm{d}t} + \operatorname{div} \boldsymbol{v} = q(s_w, p), \tag{17}$$

$$-\lambda(s_w)\boldsymbol{K}(\nabla p - \boldsymbol{G}_\lambda(s_w, p)) = \boldsymbol{v}, \tag{18}$$

$$\phi\frac{\partial s_w}{\partial t} + \operatorname{div}(q_w(s_w)\boldsymbol{v} - \boldsymbol{G}_1(s_w, p) - D(s_w)\nabla s_w) = 0, \tag{19}$$

$$\phi\frac{\partial(s_w c_a)}{\partial t} + \operatorname{div}(c_a \boldsymbol{v}_w - \phi s_w \boldsymbol{D}\nabla c_a) + \phi s_w \mu c_a = 0, \tag{20}$$

$$\phi_s\frac{\partial(\rho_s k_d c_c)}{\partial t} + \phi\frac{\partial(s_w c_c)}{\partial t} + \operatorname{div}(c_c \boldsymbol{v}_w - \phi s_w \boldsymbol{D}\nabla c_c) + \phi_s \rho_s k_e c_a S_c = 0, \tag{21}$$

$$\frac{\partial S_c}{\partial t} + \phi_s k_e c_a S_c = \phi_s\frac{\partial(k_d c_c)}{\partial t}, \tag{22}$$

where the total pressure p, the saturation of leach solution s_w, the volumetric concentration of sulfuric acid c_a, the volumetric concentration of copper in leach solution c_c and the concentration of copper in solid phase S_c, are the unknowns, which are function of the physical point $\boldsymbol{x} \in \bar{\Omega}$ and the time $t \in [0, T]$. Note that the unknowns c_a, c_c and S_c are not in Eqs. (17)–(19) because the effect of the transport of solutes on the transport of fluid is weak. This hypothesis allows to relax the level of coupling between the equations that form the system.

3.5. Initial and boundary conditions

To complete the definition of our model, the initial and boundary conditions are indicated for each of the unknowns. In effect, for p, by (6) and (10), is sufficient to specify an initial and boundary condition for the pressure of the gaseous phase, i.e., p_n:

$$p_n(\boldsymbol{x}, t=0) = p_{atm}, \quad \boldsymbol{x} \in \bar{\Omega}, \qquad p_n(\boldsymbol{x}, t) = p_{atm}, \quad \boldsymbol{x} \in \partial\Omega, t \in [0, T],$$

with p_{atm} atmospheric pressure. For $\boldsymbol{v}$, by (11), is sufficient to specify boundary conditions for $\boldsymbol{v}_w$ and $\boldsymbol{v}_n$:

$$\boldsymbol{v}_w(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\boldsymbol{x}) = d_w(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial\Omega, t \in [0, T],$$
$$\boldsymbol{v}_n(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\boldsymbol{x}) = d_n(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial\Omega, t \in [0, T],$$

with $\boldsymbol{n}(\boldsymbol{x})$ outward normal to $\partial\Omega$. For s_w, by (19), the initial and boundary conditions are given by:

$$s_w(\boldsymbol{x}, t=0) = s_{wo}, \quad \boldsymbol{x} \in \bar{\Omega},$$
$$(q_w(s_w)\boldsymbol{v} - \boldsymbol{G}_1(s_w, p) - D(s_w)\nabla s_w)(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\boldsymbol{x}) = d_s(t),$$
$$\boldsymbol{x} \in \Gamma^i, t \in [0, T], \qquad \frac{\partial s_w}{\partial \boldsymbol{n}}(\boldsymbol{x}, t) = 0,$$
$$\boldsymbol{x} \in \partial\Omega/\Gamma^i, t \in [0, T],$$

with $\boldsymbol{n}(\boldsymbol{x})$ outward normal to $\partial\Omega$. For c_a, by (20), the initial and boundary conditions are given by:

$$c_a(\boldsymbol{x}, t) = c_{ao}, \quad \boldsymbol{x} \in \bar{\Omega},$$
$$(c_a \boldsymbol{v}_w - \phi s_w \boldsymbol{D}\nabla c_a)(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\boldsymbol{x}, t) = c_a^i(t),$$
$$\boldsymbol{x} \in \Gamma^i, t \in [0, T], \qquad \frac{\partial c_a}{\partial \boldsymbol{n}}(\boldsymbol{x}, t) = 0,$$
$$\boldsymbol{x} \in \partial\Omega/\Gamma^i, t \in [0, T],$$

with $\boldsymbol{n}(\boldsymbol{x})$ outward normal to $\partial\Omega$. For c_c, by (21) the initial and boundary conditions are given by:

$$c_c(\boldsymbol{x}, t=0) = 0, \quad \boldsymbol{x} \in \bar{\Omega},$$
$$(c_c \boldsymbol{v}_w - \phi s_w \boldsymbol{D}\nabla c_c)(\boldsymbol{x}, t)\cdot\boldsymbol{n}(\boldsymbol{x}, t) = c_c^i(t),$$
$$\boldsymbol{x} \in \Gamma^i, t \in [0, T], \qquad \frac{\partial c_c}{\partial \boldsymbol{n}}(\boldsymbol{x}, t) = 0,$$
$$\boldsymbol{x} \in \partial\Omega/\Gamma^i, t \in [0, T],$$

with $\boldsymbol{n}(\boldsymbol{x})$ outward normal to $\partial\Omega$. For S_c, the initial condition is given by

$$S_c(x, t=0) = S_{co}, \quad \boldsymbol{x} \in \bar{\Omega}.$$

4. Numerical method

In this paper we will use the finite element approximations, which combines the mixed finite element methods for pressure and velocity [4,5], and the finite volume method for the saturation and the concentrations [10].

4.1. Main features of the mathematical model

Eqs. (17) and (18) form a parabolic–elliptic equation. In effect, if $c(s_w, p) = 0$ the equation is elliptic (non-liquid phase is incompressible, for example, oil), and if $c(s_w, p) \neq 0$ the equation is parabolic (non-liquid phase is compressible, for example, gas). Eq. (19) is parabolic, but it can be degenerate when $D(s_w) = 0$. The total mobility λ in (18) satisfies

$\lambda > 0$, while $k_{\mathrm{r}\alpha} \geq 0$ in (5). This is one reason because the systems (7)–(9) is better that (4)–(5)–(1)–(6). While the phase mobilities λ_α can be zero, the total mobility λ is always positive.

4.2. Discretization of the flow equations

The discretization of Eqs. (17)–(19) is done in two stages. The first stage is related to (17) and (18), which generalizes [4] to the nonlinear case. The second stage is about (19) where we apply [10].

4.2.1. Discretization of systems (17) and (18)

Assume that p and $\boldsymbol{v}$, are functions of the space variable $\boldsymbol{x}$, have the usual degree of regularity of the variational solutions of elliptic or parabolic problems: $p \in \{p \in L^2(\Omega);\ \frac{\partial p}{\partial x_i} \in L^2(\Omega), i = 1, 2\}$ and $\boldsymbol{v} \in \{\boldsymbol{v} \in L^2(\Omega) \times L^2(\Omega);\ \operatorname{div} \boldsymbol{v} \in L^2(\Omega)\}$, where $L^2(\Omega) = \{f : \Omega \longrightarrow \Re$, such that $\int_\Omega |f(x)|^2\,\mathrm{d}x < +\infty\}$. Let $\mathcal{T}_h = \{K : K$ be a triangle, $A \subset \partial K\}$ a mesh defined on the domain Ω. The (lowest order) Raviart–Thomas [4] space of vector functions over K is a finite dimensional subspace $\boldsymbol{X}_K$ of $\{\boldsymbol{v} \in (L^2(K))^2;\ \operatorname{div} \boldsymbol{v} \in L^2(K)\}$, having the following properties: for all $\boldsymbol{v} \in \boldsymbol{X}_K$: $\operatorname{div} \boldsymbol{v}$ is constant over K, for all $i = 1, 2, 3$: $\boldsymbol{v} \cdot \boldsymbol{n}_K$ is constant over the edge A_i, with $\boldsymbol{n}_K$ outward unitary normal to K and any vector $\boldsymbol{v} \in \boldsymbol{X}_K$ is perfectly determined by the knowledge of its flux v_i through the edges A_i, $i = 1, 2, 3$. It is then natural to use as basis functions for $\boldsymbol{X}_K$ the vector fields $\boldsymbol{w}_1$, $\boldsymbol{w}_2$ and $\boldsymbol{w}_3$ defined by $\int_{A_i} \boldsymbol{w}_j \cdot \boldsymbol{n}_K = \delta_{ij}$, $i, j = 1, 2, 3$. Hence $\boldsymbol{w}_j$ is a vector field having a flux of one through the edge A_j and a zero flux through all the remaining edges. For all $\boldsymbol{v}_K \in \boldsymbol{X}_K$ there are scalars $v_{K,1}$, $v_{K,2}$, $v_{K,3} \in \Re$, such that $\boldsymbol{v}_K = v_{K,1}\boldsymbol{w}_1 + v_{K,2}\boldsymbol{w}_2 + v_{K,3}\boldsymbol{w}_3$. By definition $\int_K \operatorname{div} \boldsymbol{w}_j = \int_{\partial K} \boldsymbol{w}_j \cdot \boldsymbol{n}_k = 1$ and $\int_K \operatorname{div} \boldsymbol{v} = v_{K,1} + v_{K,2} + v_{K,3}$. The basic mixed idea consists in approximating simultaneously the pressure p and the velocity field $\boldsymbol{v}$. On each element K we approximate p and $\boldsymbol{v}$ by the approximation of the mean p on K, i.e., $P_K \in \Re$, by the approximation of the mean of p on A_i, $i = 1, 2, 3$, i.e., $TP_{K,i} \in \Re$, $i = 1, 2, 3$, and by the approximation of $\boldsymbol{v}$ on K, i.e., $\boldsymbol{v}_K \in \boldsymbol{X}_K$. As we have seen, $\boldsymbol{v}_K$ is perfectly known once its fluxes through the three edges of K are know. Therefore, the approximation p and $\boldsymbol{v}$ on K is completely determined when one knows the 7 degrees of freedom: $P_K \in \Re$, $TP_{K,i} \in \Re$, $i = 1, 2, 3$, and $v_{K,i} \in \Re$, $i = 1, 2, 3$. These numbers cannot be chosen completely arbitrary, i.e., additional conditions are necessary. In effect, taking the scalar product of (18) with a test function $\boldsymbol{s} \in \{\boldsymbol{v} \in (L^2(\Omega))^2; \operatorname{div} \boldsymbol{v} \in L^2(\Omega)\}$, integrating over K and using a Green's formula we obtain

$$\int_K (\lambda(s)k)^{-1} \boldsymbol{v} \cdot \boldsymbol{s} = \int_K p \operatorname{div} \boldsymbol{s} - \sum_{j=1}^{3} \int_{A_j} p\boldsymbol{s} \cdot \boldsymbol{n}_{A_j} + \int_K \boldsymbol{G}_\lambda(s, p) \cdot \boldsymbol{s}, \tag{23}$$

with $\partial K = A_1 \cup A_2 \cup A_3$. The sought consistency equation for the approximate quantities $\boldsymbol{v}_K$, P_K (over K) and TP_K (over ∂K) will then be obtained by requiring that they satisfy a relation similar to (23), namely

$$(\lambda(s_K)k)^{-1} \int_K \boldsymbol{v}_K \cdot \boldsymbol{s}_K = P_K \int_K \operatorname{div} \boldsymbol{s}_K - \sum_{j=1}^{3} TP_{K,j} \int_{A_j} \boldsymbol{s}_K \cdot \boldsymbol{n}_{A_j} + \int_K \boldsymbol{G}_\lambda(s_K, P_K) \cdot \boldsymbol{s}_K,$$

for all $\boldsymbol{s}_K \in \boldsymbol{X}_K$. Taking as a test function $\boldsymbol{s}_K$ successively the three basis functions $\boldsymbol{w}_K \in \boldsymbol{X}_K$:

$$(\lambda(s_K)k)^{-1} \sum_{j=1}^{3} v_{K,j} \int_K \boldsymbol{w}_j \cdot \boldsymbol{w}_i = P_K \int_K \operatorname{div} \boldsymbol{w}_i - \sum_{j=1}^{3} TP_{K,j} \int_{A_j} \boldsymbol{w}_i \cdot \boldsymbol{n}_{A_j} + \int_K \boldsymbol{G}_\lambda(s_K, P_K) \cdot \boldsymbol{w}_i,$$

for $i = 1, 2, 3$. Because $\int_K \operatorname{div} \boldsymbol{w}_i = 1$, $\sum_{j=1}^{3} TP_{K,j} \int_{A_j} \boldsymbol{w}_i \cdot \boldsymbol{n}_K = TP_{K,i}$, $i = 1, 2, 3$, and $A_{K,i,j} = \int_K \boldsymbol{w}_j \cdot \boldsymbol{w}_i$, $i, j = 1, 2, 3$, we have equivalently for $i = 1, 2, 3$:

$$(\lambda(s_K)k)^{-1} \sum_{j=1}^{3} v_{K,j} A_{K,j,i} = P_K - TP_{K,i} + \int_K \boldsymbol{G}_\lambda(s_K, P_K) \cdot \boldsymbol{w}_i,$$

or in matrix notation:

$$\boldsymbol{A}_K[\boldsymbol{v}_K^n] = a_K^n(s_K^n)[P_K^n \mathrm{DIV}_K^{\mathrm{T}} - TP_K^n + \boldsymbol{G}_{\lambda,K}^n(s_K^n, P_K^{n-1})], \tag{24}$$

where $\boldsymbol{A}_K = (A_{K,i,j})_{3\times 3}$, $[\boldsymbol{v}_K^n] = (v_{K,i}^{n-1})_{3\times 1}$, $\mathrm{DIV}_K = [1, 1, 1]$, $TP_K^n = (TP_{K,i}^n)_{3\times 1}$, $G_{K,i}^n \approx \int_K \boldsymbol{G}_\lambda(s_K^n, P_K^{n-1}) \cdot \boldsymbol{w}_i$, $\boldsymbol{G}_{\lambda,K}^n = (G_{K,i}^n)_{3\times 1}$, and $a_K^n(s_K^n) = \lambda(s_K^n)k$. Eq. (24) is called consistency equation. In order to obtain the balance equation, we multiply (17) by $\varphi \in L^2(K)$ and integrating over K:

$$\int_K (1 - s)c_{\mathrm{a}}(s, p)\frac{\mathrm{d}p}{\mathrm{d}t}\varphi + \int_K (\operatorname{div} \boldsymbol{v})\varphi = \int_K q(s, p)\varphi. \tag{25}$$

The consistency equation has to be completed by another equation expressing the fact that P_K and $\boldsymbol{v}_K$ satisfy (25) in some approximate sense. As the chosen approximations P_K and $\boldsymbol{v}_K$ satisfy: P_K constant over K and $\operatorname{div} \boldsymbol{v}_K = \frac{1}{|K|}\sum_{A\subset\partial K} v_{K,A}$, constant over K, it will be natural to require of P_K and $\boldsymbol{v}_K$ that they satisfy an equation analogous to (25):

$$|K|(1 - s_K^n)c_{\mathrm{a}}(s_K^n, P_K^{n-1})\frac{P_K^n - P_K^{n-1}}{\Delta t}\varphi_K + |K|\varphi_K\left(\frac{1}{|K|}\sum_{A\subset\partial K} v_{K,A}^n\right) = \varphi_K F_K^n(s_K^n, P_K^{n-1}),$$

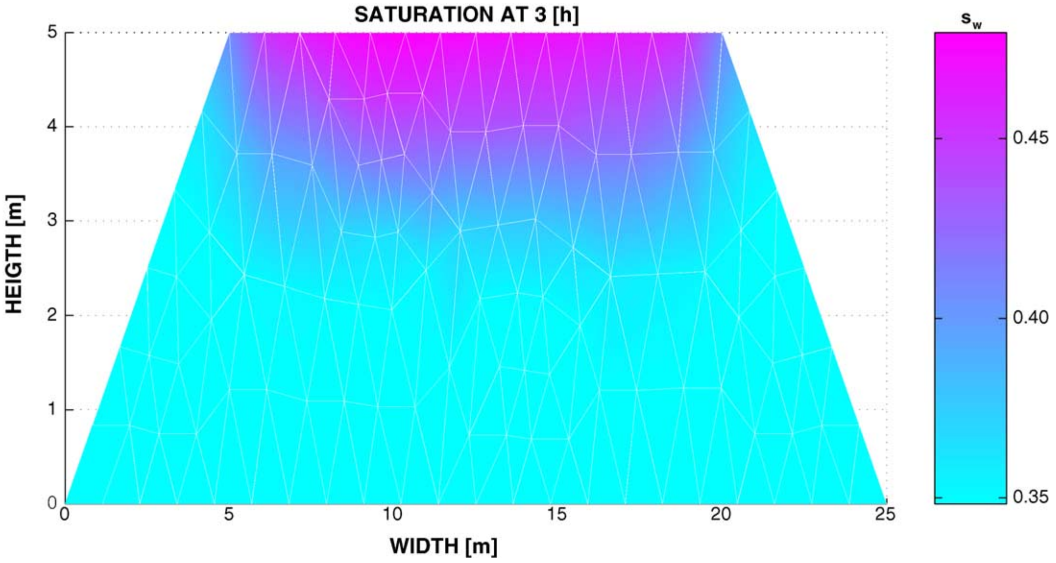

Fig. 2. Plot of saturation of leach solution at 3 h.

after division by φ_K:

$$|K|(1-s_K^{n-1})c_{\mathrm{a}}(s_K^n, P_K^{n-1})\frac{P_K^n - P_K^{n-1}}{\Delta t} + \sum_{A\subset\partial K} v_{K,A}^n = F_K^n(s_K^n, P_K^{n-1}),$$

where $F_K(s_K^n, P_K^{n-1}) \approx \int_K q(s,p)$. In matrix notation the balance equation is given by

$$c_K^n(s_K^n, P_K^{n-1})\frac{P_K^n - P_K^{n-1}}{\Delta t} + \mathrm{DIV}_K[\boldsymbol{v}_K^n] = F_K^n(s_K^n, P_K^{n-1}), \tag{26}$$

with $c_K^n(s_K^n, P_K^{n-1}) = |K|(1-s_K^n)c_{\mathrm{a}}(s_K^n, P_K^{n-1})$. Now, we need five additional conditions to close our system. First, we consider, the continuity of pressures, i.e., for each edge A such that $A \subset K$ and $A \subset K'$: $TP_{K,A}^n = TP_{K',A}^n$. Next, we consider the continuity of normal components of velocities across interior edges, i.e., for each edge A such that $A \subset K$ and $A \subset K'$: $v_{K,A}^n + v_{K',A}^n = 0$. The 3rd condition is the Dirichlet condition of the total pressure on each boundary edge, i.e., for all edge $A \subset \partial\Omega$, $n = \overline{0, N}$:$TP_{K,A}^n = P_D(x, t_{\mathrm{n}})$, $x \in A$. The 4th condition is the boundary condition for the total velocity, i.e., for all edge $A \subset \partial\Omega$, $n = \overline{0, N}$: $v_{K,A}^n = v_D(x, t_{\mathrm{n}})$, $x \in A$. Finally, the 5th condition is the initial condition for the total pressure, i.e., for all $K \in \mathcal{T}_h$, $P(x, t=0) = P_0(x)$, $x \in K$. Depending on the choice of the principal unknowns and the

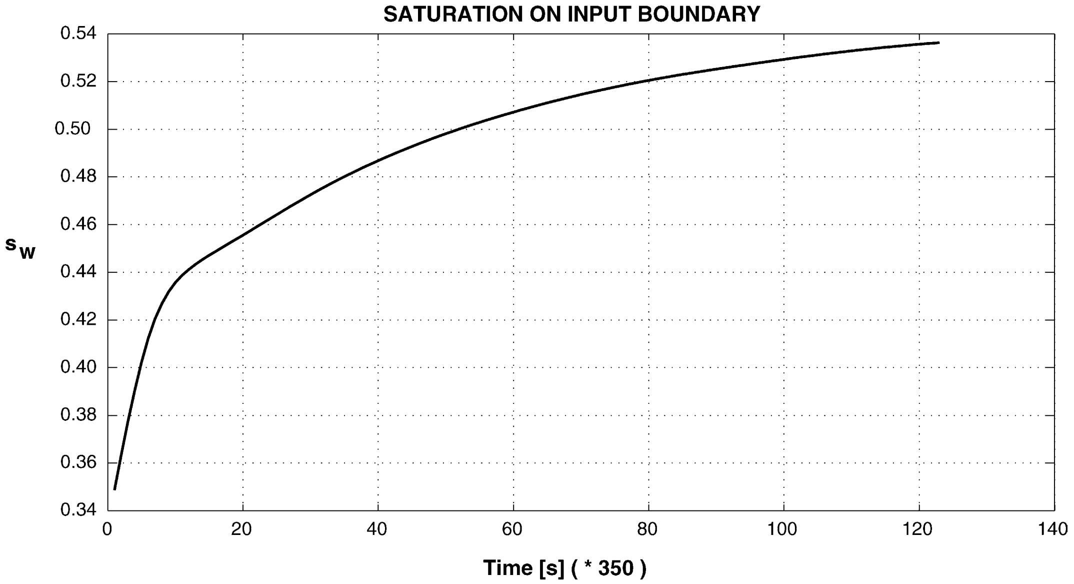

Fig. 3. Plot of saturation of leach solution vs. time on the irrigation boundary.

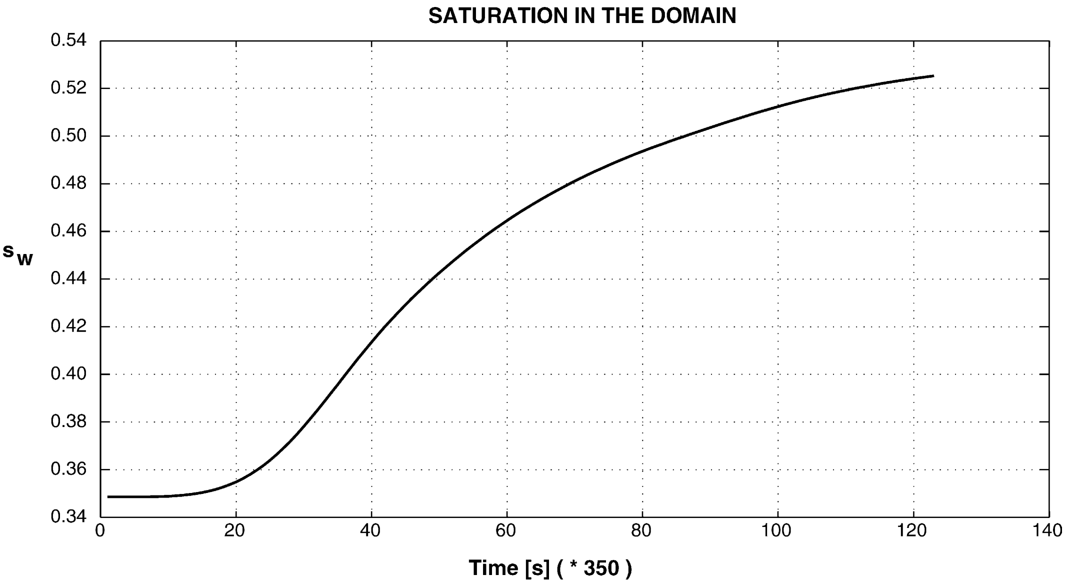

Fig. 4. Plot of saturation of leach solution vs. time in the domain.

unknowns which will be eliminated, we obtain either the *mixed* approximation of (17) and (18) or its *mixed-hybrid* approximation. Hence the mixed-hybrid formulation has to be preferred to the mixed formulation especially for problems which have both elliptic and parabolic regions. Here we choose as principal unknowns for the solution of equations defined by the previous conditions the pressures TP_A, for each $A \subset \Omega$, i.e., the mixed-hybrid approximation.

4.2.2. Discretization of (19)

For a finite index set $I \subset N$, let $\mathcal{T} = \{T_k / k \in I\}$ be an admissible triangulation of Ω. For a finite index set $J \subset N$, $\{p_j / j \in J\}$ denote the set of vertices of the triangulation $\mathcal{T}$. The shared edge joining two neighbouring vertices p_j and p_l will de denoted by Γ_{jl}. Define for each vertex p_j, $j \in J$, the corresponding dual cell Ω_j by connecting the centres of gravity of the surrounding triangles with the centres of gravity of the edges Γ_{jl}. The resulting curve is the contour line of the dual volume Ω_j. The mesh of dual cells $\{\Omega_j / j \in J\}$ is a partition of our domain Ω. The elements of which serve as the finite volumes in our numerical method. Let $N(j) \subset J$ indicate the indices of neighbouring cells of the dual cell Ω_j. Let us indicate values above the edge Γ_{jl} by an upper index a and values below Γ_{jl} by an upper index b and let $\mathcal{A} = \{a, b\}$. Thus, the joint edges of Ω_j and Ω_l will be denoted by S^a_{jl}, S^b_{jl}. The unit outer normal vector to S^a_{jl}, S^b_{jl} with respect to Ω_j will be denoted by $\boldsymbol{n}^a_{jl}$, $\boldsymbol{n}^b_{jl}$ [10].

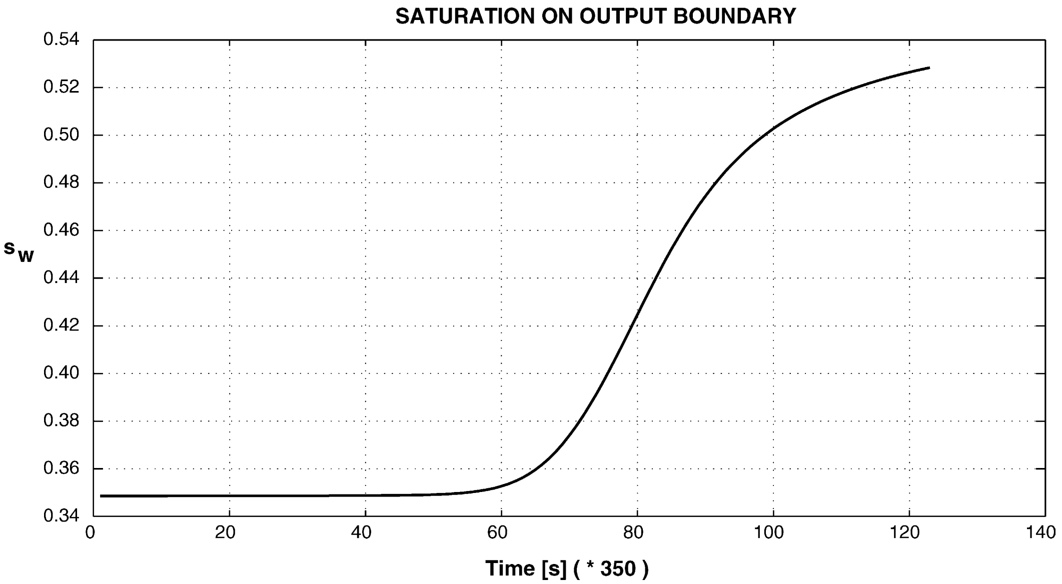

Fig. 5. Plot of saturation of leach solution vs. time on the drainage boundary.

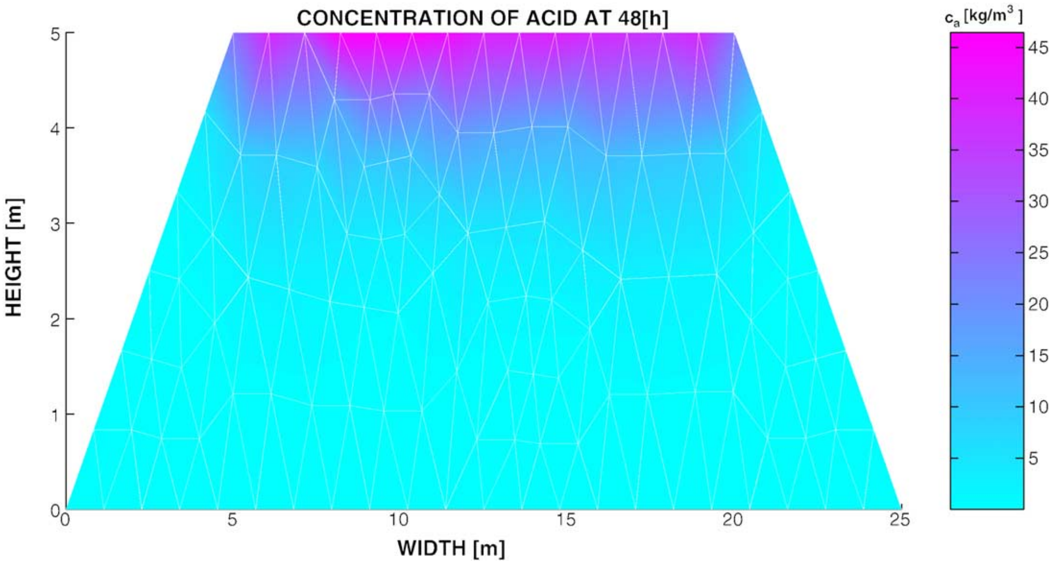

Fig. 6. Plot of concentration of acid at 48 h.

In this section we define an implicit vertex-centred finite volume approximation of (19). In order to do so we first define numerical fluxes for the convective and diffusive part of the problem. For any $j, l \in I, a \in \mathcal{A}$, and $t^n \in \Re^+$, let $g_{lj}^{a,n} \in C^1(\Re^2, \Re)$ be a numerical convective flux, satisfying the following conditions for all $w, v, w', v' \in [A, B]$, where $A, B \in \Re$ are chosen such that $A \le c \le B$:

$$\partial_{\mathrm{w}} g_{jl}^{a,n}(w, v) \ge 0, \qquad \partial_{\mathrm{v}} g_{jl}^{a,n}(w, v) \le 0.$$

Furthermore, there exists a constant $L_g > 0$ independent of j, l, n, and h, such that for all w, v, w', v':

$$g_{jl}^{a,n}(w, v) = -g_{lj}^{b,n}(v, w),$$

$$|g_{jl}^{a,n}(w, v) - g_{jl}^{a,n}(w', v')| \le L_g |S_{jl}^a| (|w - w'| + |v - v'|),$$

$$g_{jl}^{a,n}(u, u) = \left(\frac{1}{\Delta t^n} \int_{t^n}^{t^{n+1}} \int_{S_{jl}^a} \boldsymbol{v}(x, t) \cdot \boldsymbol{n}_{jl}^a \, \mathrm{d}x \, \mathrm{d}t \right) q_{\mathrm{w}}(u), \tag{27}$$

where n_{jl}^a denotes the outer unit normal to S_{jl}^a with respect to Ω_j. The corresponding conditions should hold for $g_{jl}^{b,n} : \Re^2 \longrightarrow \Re$ as well. This class of convective fluxes are called monotone upwind fluxes in conservation form. Examples are the Lax–Friedrichs or Enquist–Osher fluxes.

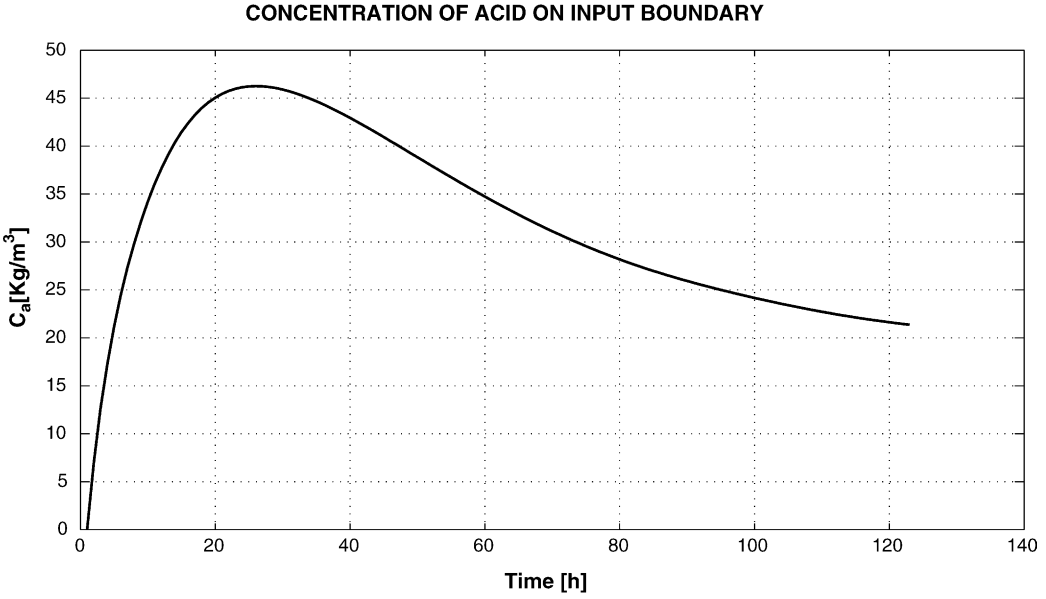

Fig. 7. Plot of concentration of acid vs. time on the irrigation boundary.

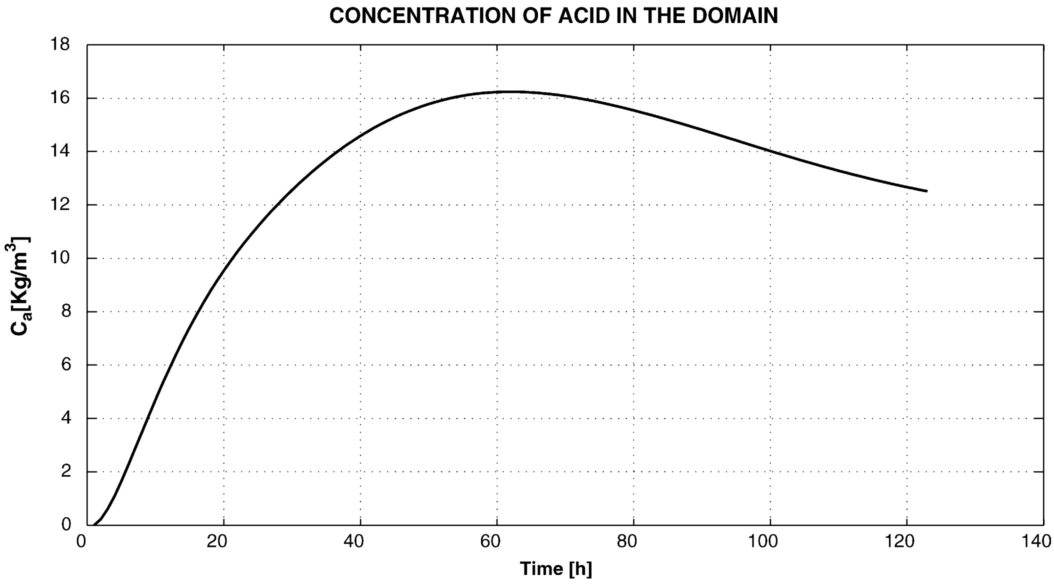

Fig. 8. Plot of concentration of acid vs. time in the domain.

Let V_h be the space of piecewise linear functions on $\mathcal{T}$ which are globally continuous. For any $j, l \in I, * \in PM$ and $t^n \in \Re^+$ let the diffusive numerical fluxes $d_{jl}^{*,n} : V_h \longrightarrow \Re$ be defined as

$$d_{jl}^{*,n}(w_h) = \int_{S_{jl}^*} D\nabla w_h^n \cdot \boldsymbol{n}_{jl}^* \,\mathrm{d}x\,\mathrm{d}t, \tag{28}$$

for any $w_h^n \in V_h$. Let some grid $\mathcal{T}$ and an arbitrary partition $0 = t^0 < t^1 < \cdots < t^n < t^{n+1} < \cdots < t^m = T$, with step size $\Delta t^n = t^{n+1} - t^n, n = 0, 1, \ldots$. For each $n \in \{0, \ldots, N\}$ the approximate solution $s_{\mathrm{w},h}^n \in V_h$ is given by the nodal basis coefficients $s_{\mathrm{w},j}^n$, $j \in I$, defined as:

$$s_{\mathrm{w},j}^{n+1} + \frac{\Delta t^n}{|\Omega_j|\phi} \sum_{l,*} \{ g_{jl}^{*,n+1}(s_{\mathrm{w},j}^{n+1}, s_{\mathrm{w},l}^{n+1}) - G_1^{*,n+1}(s_{\mathrm{w},h}^{n+1}) - d_{jl}^{*,n+1}(s_{\mathrm{w},h}^{n+1}) \} = s_{\mathrm{w},j}^n, \tag{29}$$

where $G_1^{*,n+1}$ (%) is an approximation of $\boldsymbol{G}_1(s_\mathrm{w}, p)$, and $j, l \in I$. With this definition we further define the space-time function $s_{\mathrm{w},h}$ by

$$s_{\mathrm{w},h}(\cdot, 0) = s_{\mathrm{wo}}, s_{\mathrm{w},h}(\cdot, t) = s_{\mathrm{w},h}^{n+1}, \quad \text{for all } t \in (t^n, t^{n+1}].$$

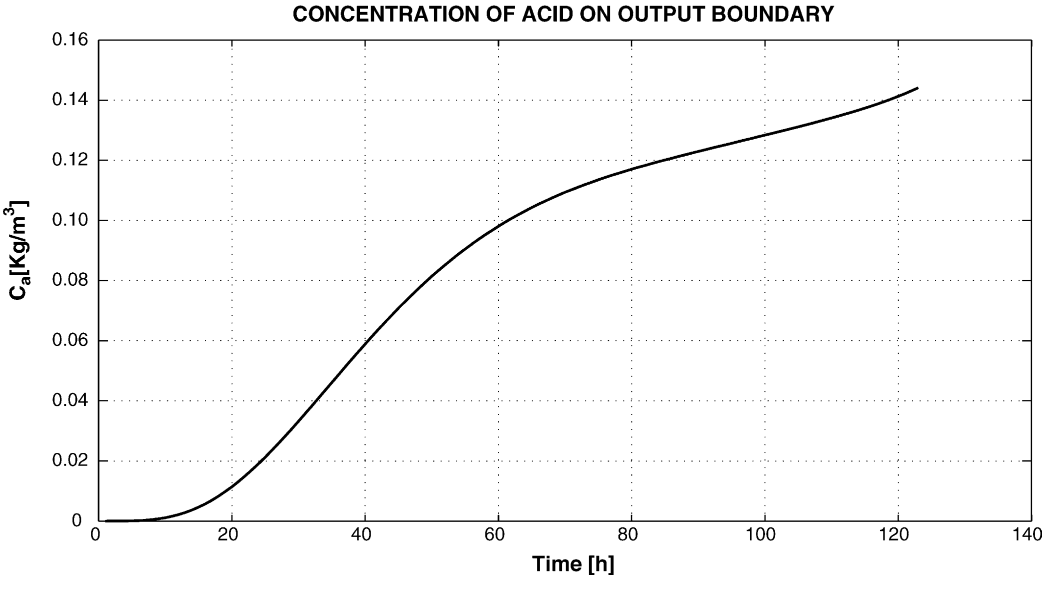

Fig. 9. Plot of concentration of acid vs. time on the drainage boundary.

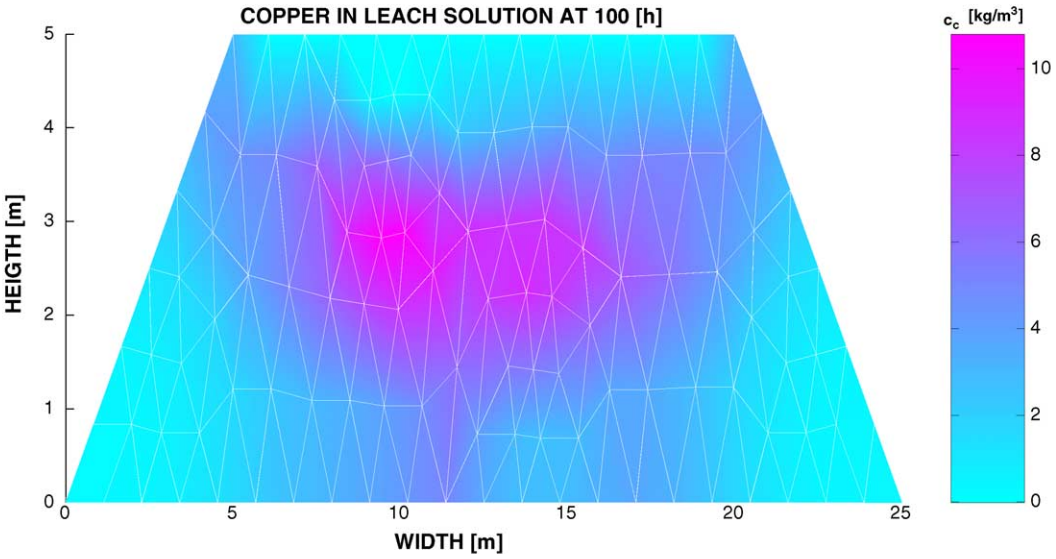

Fig. 10. Plot of concentration of copper in liquid phase at 100 h.

4.3. Discretization of the sulfuric acid transport equation

The same method used for (19) is used for (20). Therefore, the approximate solution $c^n_{a,h}$ is given by

$$\phi s^{n+1}_{w,j} c^{n+1}_{a,j} + \frac{\Delta t^n}{|\Omega_j|} \sum_{l,*} \{ g^{*,n+1}_{jl}(c^{n+1}_{a,j}, c^{n+1}_{a,l}) - d^{*,n+1}_{jl}(c^{n+1}_{a,h}) \} + \mu \Delta t^n \phi s^{n+1}_{w,j} c^{n+1}_{a,j} = \phi s^n_{w,j} c^n_{a,j}, \qquad (30)$$

where

$$g^{a,n}_{jl}(u,u) = \left(\frac{1}{\Delta t^n} \int_{t^n}^{t^{n+1}} \int_{S^a_{jl}} \boldsymbol{v}(x,t) \cdot \boldsymbol{n}^a_{jl} \, \mathrm{d}x \, \mathrm{d}t \right) u \quad \text{and}$$

$$d^{*,n}_{jl}(w_h) = \int_{S^*_{jl}} \phi s^n_{w,h} \boldsymbol{D} \nabla w^n_h \cdot \boldsymbol{n}^*_{jl} \, \mathrm{d}x \, \mathrm{d}t.$$

4.4. Discretization of the copper transport equation in liquid phase

The same method used for (19) is used for (21). Therefore, the approximate solution $c^n_{c,h}$ is given by:

$$(\phi_s \rho_s k_d + \phi s^{n+1}_{w,j}) c^{n+1}_{c,j} + \frac{\Delta t^n}{|\Omega_j|} \sum_{l,*} \{ g^{*,n+1}_{jl}(c^{n+1}_{c,j}, c^{n+1}_{c,l}) - d^{*,n+1}_{jl}(c^{n+1}_{c,h}) \} + \rho_s \phi_s k_e \Delta t^n c^{n+1}_{a,j} S^{n+1}_{c,j} = (\phi_s \rho_s k_d + \phi s^n_{w,j}) c^n_{c,j}, \qquad (31)$$

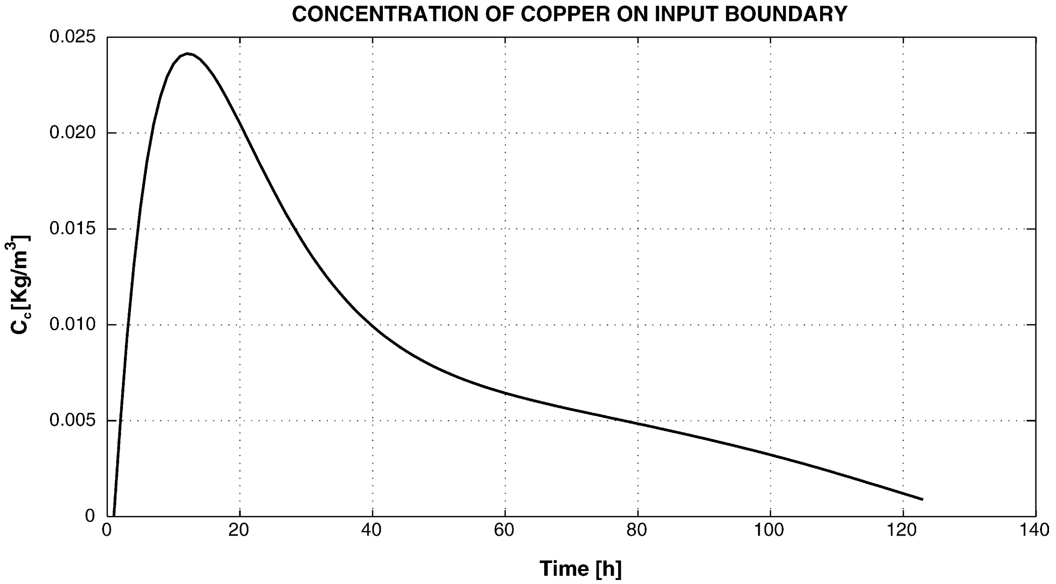

Fig. 11. Plot of concentration of copper in liquid phase vs. time on the irrigation boundary.

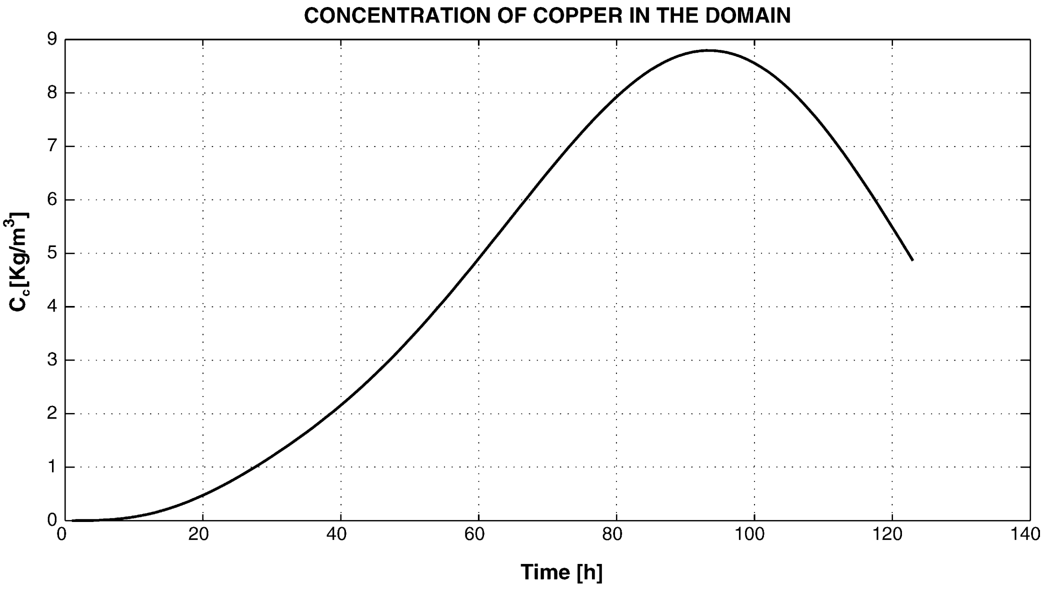

Fig. 12. Plot of concentration of copper in liquid phase vs. time in the domain.

where

$$g_{jl}^{a,n}(u,u) = \left(\frac{1}{\Delta t^n}\int_{t^n}^{t^{n+1}}\int_{S_{jl}^a} \boldsymbol{v}(x,t)\cdot \boldsymbol{n}_{jl}^a \,\mathrm{d}x\,\mathrm{d}t\right) u \quad \text{and}$$

$$d_{jl}^{*,n}(w_h) = \int_{S_{jl}^*} \phi s_{\mathrm{w},h}^n \boldsymbol{D}\nabla w_h^n \cdot \boldsymbol{n}_{jl}^* \,\mathrm{d}x\,\mathrm{d}t.$$

4.5. Discretization of the copper transport equation in solid phase

To Eq. (22) we apply $\int_{\Delta t^n}$ (%):

$$S_{\mathrm{c},j}^{n+1} - S_{\mathrm{c},j}^{n} + \phi_{\mathrm{s}} k_{\mathrm{e}} \int_{\Delta t^n} (c_{\mathrm{a}} S_{\mathrm{c}})(\boldsymbol{x},t)\,\mathrm{d}t = k_{\mathrm{d}}\phi_{\mathrm{s}}(c_{\mathrm{c},j}^{n+1} - c_{\mathrm{c},j}^{n}), \tag{32}$$

where the integral term is approximate with numerical integration.

5. Computer algorithm

A computer program was written to simulate the flow of liquid phase and the concentrations of acid and copper. This program consists in the following subroutines:

1. To obtain the approximations: TP_A^{n+1}, P_K, $v_{K,A1}^{n+1}$, $v_{K,A2}^{n+1}$ and $v_{K,A3}^{n+1}$, for each point $\boldsymbol{x}$ in the triangle K with edges $A1$, $A2$ and $A3$.
2. The approximations P_K^{n+1} and $\boldsymbol{v}^{n+1}(\boldsymbol{x},\cdot)$ are replaced in (29) to obtain the approximation $s_{\mathrm{w},j}^{n+1}$.

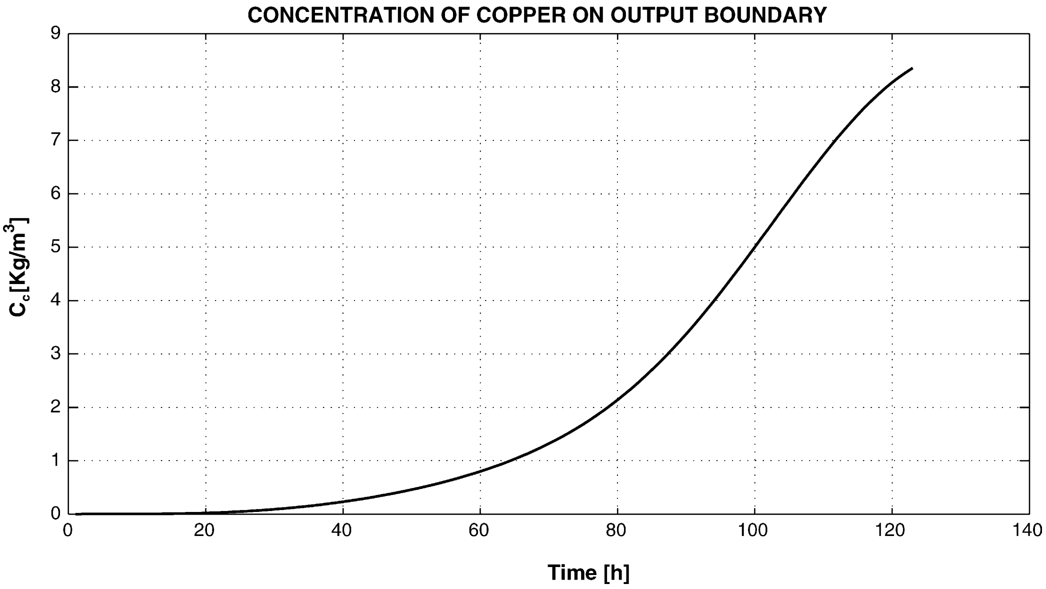

Fig. 13. Plot of concentration of copper in liquid phase vs. time on the drainage boundary.

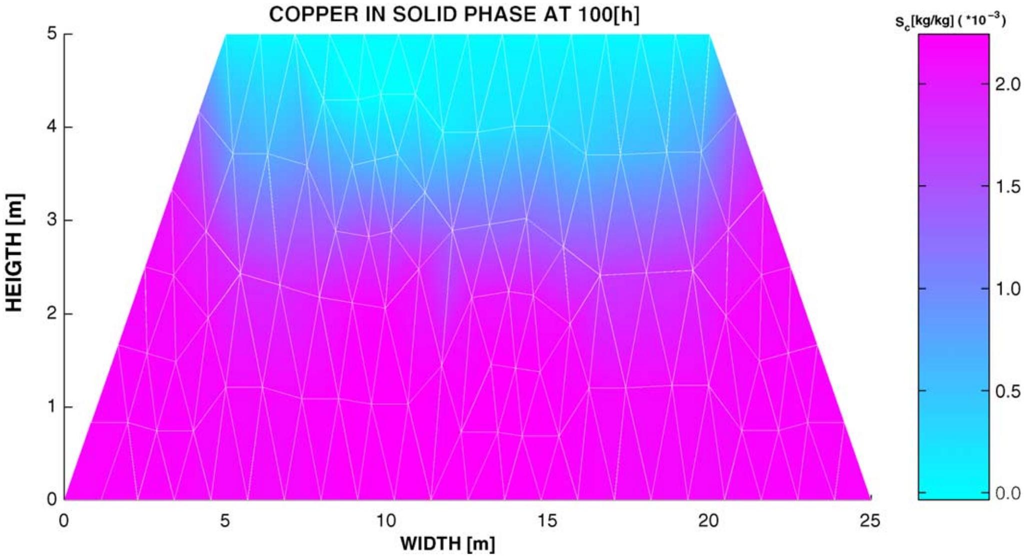

Fig. 14. Plot of concentration of copper in solid phase at 100 h.

3. The approximations P_K^{n+1} and $\boldsymbol{v}^{n+1}(\boldsymbol{x}, \cdot)$ are replaced in (12) to obtain the approximation $\boldsymbol{v}_{\mathrm{w}}^{n+1}(\boldsymbol{x}, \cdot)$.
4. The approximations $s_{\mathrm{w},j}^{n+1}$ and $\boldsymbol{v}_{\mathrm{w}}^{n+1}(\boldsymbol{x}, \cdot)$ are replaced in (30) to obtain the approximation $c_{\mathrm{a},j}^{n+1}$.
5. The approximations $s_{\mathrm{w},j}^{n+1}$, $\boldsymbol{v}_{\mathrm{w}}^{n+1}(\boldsymbol{x}, \cdot)$ and $c_{\mathrm{a},j}^{n+1}$, are replaced in (31) to obtain the approximation $c_{\mathrm{c},j}^{n+1}$.

Eq. (29) gives origin to a system of nonlinear equations which was solved using the inexact Newton method [1]. For the convective fluxes we use the Lax–Friedrich flux [8]. Our subroutines allows to modify all relevant parameters, such that, height and width of the heap, porosity, absolute permeability, residual saturation, ratio of irrigation, acid concentration on the input boundary of the heap, extraction coefficient, adsorption coefficient and the consumption coefficient.

6. Application to the heap leaching of a copper ore

6.1. Global parameters

We will use the following numerical values of the global parameters: $k = 6.23 \times 10^{-11}\,\mathrm{m}^2$, $g = 9.8\,\mathrm{m/s}^2$, $\mu_{\mathrm{w}} = 9 \times 10^{-4}\,\mathrm{kg/m\,s}$, $\mu_{\mathrm{n}} = 1.85 \times 10^{-5}\,\mathrm{kg/m\,s}$, $\alpha_{\mathrm{L}} = 1.704 \times 10^{-2}\,\mathrm{m}$, $\alpha_{\mathrm{T}} = 0.637 \times 10^{-2}\,\mathrm{m}$, $\phi = 0.459$, $\rho_{\mathrm{w}} = 1011\,\mathrm{kg/m}^3$, $\rho_{\mathrm{n}} = 1.165\,\mathrm{kg/m}^3$, $\lambda_{\mathrm{BC}} = 1$, $p_{\mathrm{d}} = 101{,}325\,\mathrm{Pa}$.

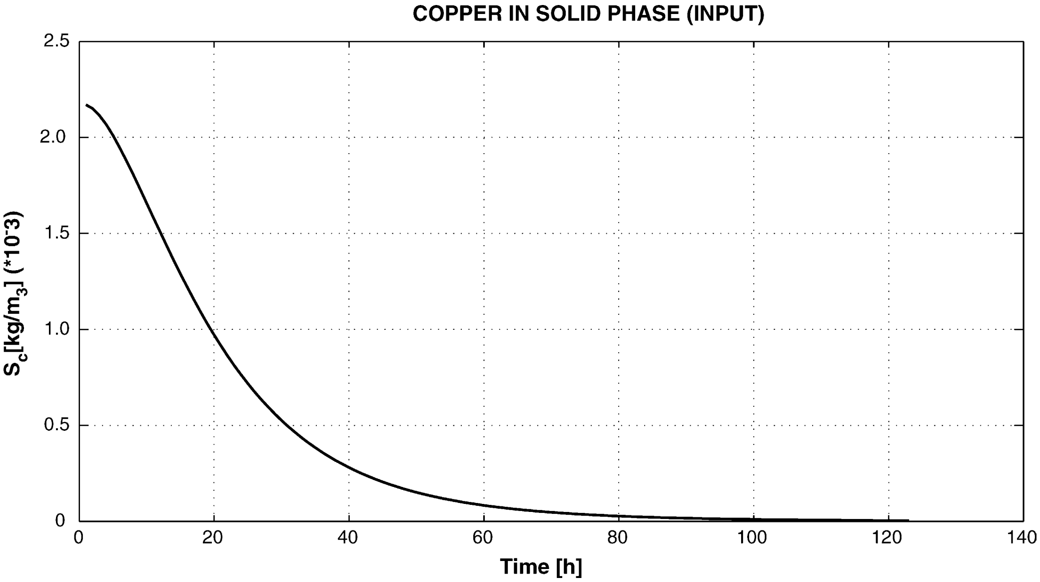

Fig. 15. Plot of concentration of copper in solid phase vs. time on the irrigation boundary.

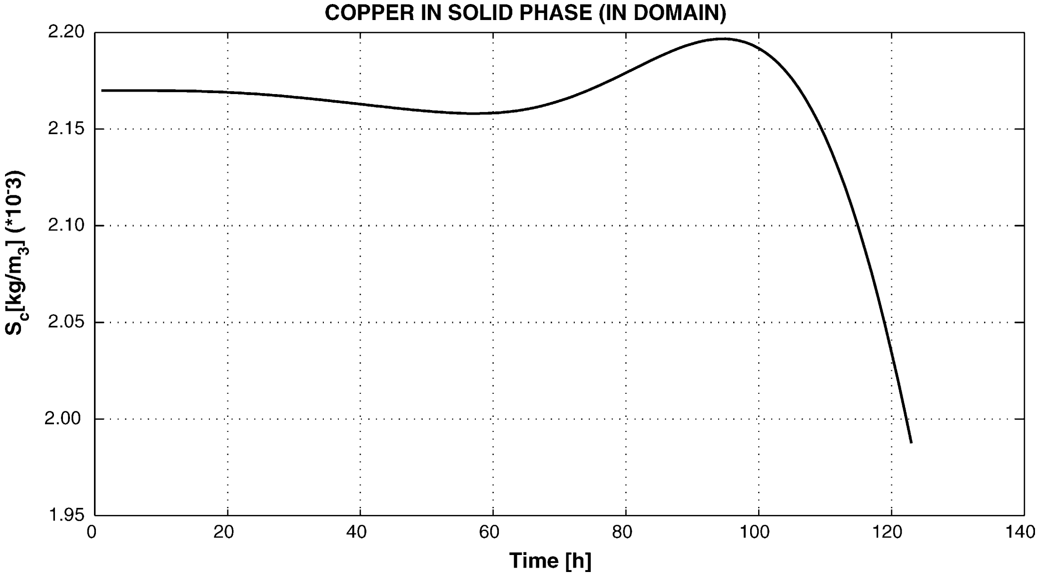

Fig. 16. Plot of concentration of copper in solid phase vs. time in the domain.

6.2. *Saturation of the leach solution*

Assume the residual saturation in the heap to be: $s_{\mathrm{wr}} = 0.28322$, the initial condition for the saturation $s_{\mathrm{w}}(x, t = 0) = 0.34858$, and the rate of irrigation: $R = 1.6 \times 10^{-5}$ m/s. Fig. 2 shows the saturation of leaching solution in 2D. Additionally, we present results in three plots: Fig. 3 shows the evolution of the saturation s_{w} on the input boundary Γ^{i} where the irrigation process occurs, Fig. 4 shows s_{w} in an arbitrary point $x \in \Omega$, and Fig. 5 shows s_{w} on the output boundary where the drainage process occurs. The total time of simulation is $T = 12$ h, with $\Delta t = 350$ s. As you can see, the numerical solution is in agreement with the physical expected behavior.

6.3. *Concentration of sulfuric acid*

Assume the concentration of sulfuric acid in the irrigation solution to be: $C_{\mathrm{a}}^{\mathrm{i}} = 6\,\mathrm{kg/m^3}$, for each $t \geq 0$, and the first-order reaction constant $\mu = 2 \times 10^{-5}\,\mathrm{s^{-1}}$. Fig. 6 shows the concentration of acid in 2D. Additionally, we present three plots: Fig. 7 shows the evolution of the acid concentration c_{a} on the input boundary Γ^{i} where the irrigation process occurs, Fig. 8 shows c_{a} in an arbitrary point $x \in \Omega$, and Fig. 9 shows c_{a} on the output boundary where the drainage process occurs. The total time of simulation is $T = 123$ h, with $\Delta t = 1$ h. As you can see, the numerical solution is in agreement with the physical expected behavior.

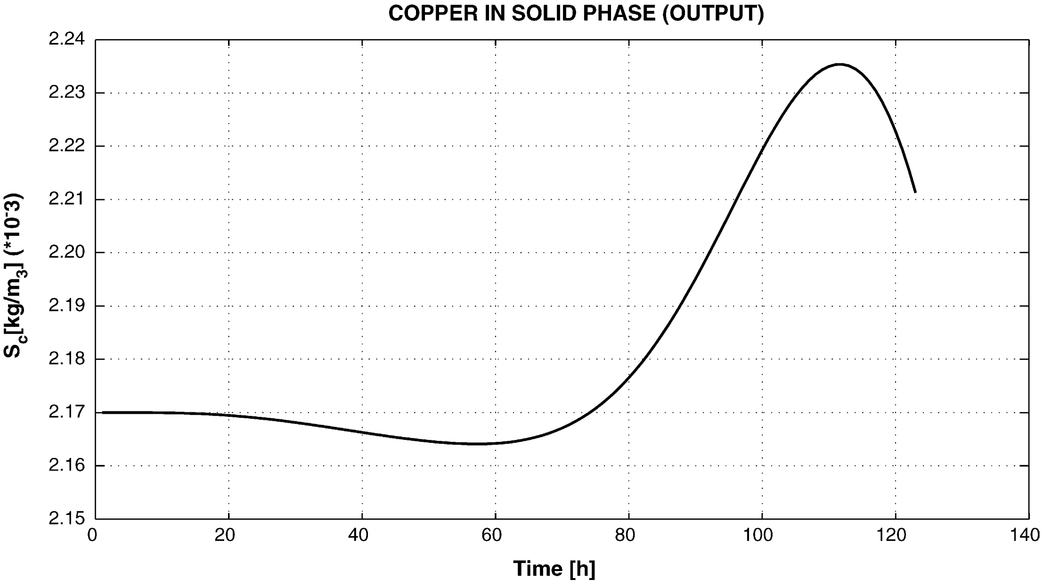

Fig. 17. Plot of concentration of copper in solid phase vs. time on the drainage boundary.

6.4. Concentration of copper in leaching solution

Assume the adsorption coefficient to be $k_d = 8.67 \times 10^{-5}\,m^3/kg$ and the extraction coefficient $k_e = 8.3 \times 10^{-7}\,m^3/kg\,s$. Fig. 10 shows the concentration of copper in leaching solution in 2D. Additionally, we present three plots: Fig. 11 shows the evolution of the copper concentration in the leach solution c_c on the input boundary Γ^i where the irrigation process occurs, Fig. 12 shows c_c in an arbitrary point $x \in \Omega$, and Fig. 13 shows c_c on the output boundary where the drainage process occurs. The total time of simulation is $T = 123\,h$, with $\Delta t = 1\,h$. As you can see, the numerical solution is in agreement with the physical expected behavior.

6.5. Concentration of copper in solid phase

The initial condition is $S_c(x, t = 0) = \lambda_S G_S$, where λ_S is the leachable fraction of the total copper contained in the heap, and G_S is the grade of the ore. In our simulations $\lambda_S = 0.62$, $G_S = 0.0035\,kg/kg$, i.e., $S_c(x, t = 0) = 2.17 \times 10^{-3}$. Fig. 14 shows the concentration of copper in solid phase in 2D. Additionally, we present three plots: Fig. 15 shows the evolution of the copper concentration in the solid phase S_c on the input boundary Γ^i where the irrigation process occurs, Fig. 16 shows S_c in an arbitrary point $x \in \Omega$, and Fig. 17 shows S_c on the output boundary where the drainage process occurs. The total time of simulation is $T = 123\,h$, with $\Delta t = 1\,h$. As you can see, the numerical solution is in agreement with the physical expected behavior.

7. Conclusions

A mathematical model in $\Omega \subset \Re^2$ was developed for the heap leaching process of copper ores which considers simultaneously a two phase flow (leach solution and gas) and transport of two components by the fluid phase (leach solution), i.e., sulfuric acid and copper, for the production of copper. Our model generalizes previous models, for example [3,9], which considers only one phase flow. The model is solved approximately by using a mixed-hybrid finite element method (MHFE) combined with the finite volume (FV) method. Our application of the MHFE method generalizes, to the nonlinear case, the procedure developed by [4]. This generalization is very useful for engineering applications. The FV method is useful for the transport equations (s_w, c_a, and c_c) because the convective fluxes dominate the diffusive fluxes. The numerical solution is in agreement with the behavior reported in leaching process literature, for example [9], and allows to simulate the leaching process under different conditions, for example, height and width of the heap, porosity, absolute permeability, residual saturation, ratio of irrigation, acid concentration on the input boundary of the heap, extraction coefficient, adsorption coefficient and the consumption coefficient.

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