

Estimation of Hydraulic Parameters under Unsaturated Flow Conditions in Heap Leaching

Emilio Cariaga*

*Departamento de Ciencias Matemáticas y Físicas, Universidad Católica de Temuco,
Casilla 15-D, Temuco, Chile.*

Rubén Martínez

*Instituto de Matemática e Estatística, Universidade de São Paulo, Caixa Postal 66.281,
CEP 05315-970, São Paulo, SP, Brasil.*

Mauricio Sepúlveda

*CPMA and Departamento de Ingeniería Matemática, Universidad de Concepción,
Casilla 160-C, Concepción, Chile.*

Abstract

The mathematical modeling of the unsaturated flow problem requires the simultaneous resolution of two problems: the Richards equation and the estimation of the hydraulic parameters involved in hydraulic conductivity and in the retention curve. Various techniques have been applied to both problems in a wide range of situations. In this article, a novel implementation of the processing techniques involved in copper heap leaching is presented. Specifically, the impact of the used numerical method and the selection of the parametric family are evaluated. From a methodological point of view,

*Corresponding author

Email addresses: ecariaga@uct.cl (Emilio Cariaga), rmart@ime.usp.br (Rubén Martínez), mauricio@ing-mat.udec.cl (Mauricio Sepúlveda)

URL: <http://www.uct.cl/> (Emilio Cariaga), <http://www.ime.usp.br> (Rubén Martínez), <http://www.ing-mat.udec.cl/> (Mauricio Sepúlveda)

a global algorithm is proposed that integrates the solutions of both problems. Finally, our computational experiments are compared with previous experimental results from the Chilean copper mining industry and related works.

Keywords: parameter estimation, heap leaching, Richards equation.

1. Introduction

Leaching is a method of extraction in which a solvent is passed through a mixture to remove some desired substance from it. There are several types of leaching: heap leaching, vat leaching, dump leaching and in-situ leaching. In this work the focus is on heap leaching process of copper ores, where the construction of the heap is preceded by a crushing and agglomeration process that determines the hydrodynamic properties of the stack: mechanical stability, particle size, porosity, and permeability. Two distinct phenomena are of interest in the study of heap leaching: fluid flow and the physicochemical reactions. In this paper the estimation of the hydraulic parameters under unsaturated flow conditions is considered [7].

From a macroscopic point of view, the mathematical modeling of flow and transport in porous media requires the resolution of two main problems: the Differential Equation (DP), and the Parameters Estimation (PE). For both problems, there are several techniques that have been applied in a wide range of situations.

The HeapSim code [6, 14] is a part of the bioleaching model, in which the estimation of different types of parameters is performed by varying one parameter at a time and adjusting regression curves by the least squares

method. The process of estimation in this program is primarily empirical and relies heavily on the expertise of the user. For completeness, we mention [13] where a parameter estimation under saturated flow conditions was performed, and [3, 2, 4] for a brief discussion of the hydraulic parameters for two phase flow in copper heap leaching.

In [10], the fluid flow problem was modeled under unsaturated conditions in copper column leaching, the Richards equation was solved with a finite difference scheme, and the parameters were estimated with the Simplex Search method. Additionally, in [10] the van Genuchten family was applied, with a constant irrigation rate. In [16] the fluid flow problem was also modeled under unsaturated conditions in a copper heap and in column leaching, the Richards equation was solved with a finite difference scheme, and the parameters were estimated by means of fitting regression curves. In [16], a combination of the van Genuchten model along with the Brooks-Corey model was considered, but no adequate justification for this choice was presented. Moreover, in [16] the experimental data outflow from a semi-industrial heap leaching was considered. The simulation was based on a one dimensional mathematical model. Unfortunately, the observed outflow was compared only with the average simulated flow and did not consider daily fluctuations in outflow or the variable irrigation rates. In [12], the fluid flow problem was also modeled under unsaturated conditions in a copper leach pad. The Richards equation and the parameters estimation problems were solved with Hydrus 2D software (cf. [15]). The simulated outflow in [12] considers the variable irrigation rate and daily fluctuations of the outflow, achieving a proper fit to the experimental data. To the best of our knowledge,

[10, 12] and [16] are the only works that have been conducted in this area. This paper provides a novel application of DP and PE problems to copper heap leaching under unsaturated flow conditions. In the DP problem, the Richards equation is solved with the same numerical scheme applied in [10]. The PE problem is solved with the Levenberg-Marquardt algorithm (cf. [9]) from the MATLAB optimization toolbox, [17].

The main objective of this work is to provide a global algorithm that considers the solution of both problems in a way that is easy to implement by the mining industry. This article describes an advantageous method for the estimation of hydraulic parameters. We present a global algorithm that integrates the numerical solution of the Richards equation with the optimization method and provides a numerical error estimation.

We have organized this article into six sections. Section 2 presents the model problem. In Section 3, the numerical solution of the Richards equation is presented. In Section 4, the Global Algorithm of estimation is developed, which combines the optimization and differential problems. Section 5 reports five computational experiments, and Section 6 presents the main conclusions.

2. Model Problem

Figure 1 represents a leaching column of length $H > 0$ that is wet with a liquid irrigation rate $R(t) \geq 0$. At the base of the column, the experimental outflow q_{o_l} is measured at specific time intervals t_l , $l \in \{1, \dots, N\}$.

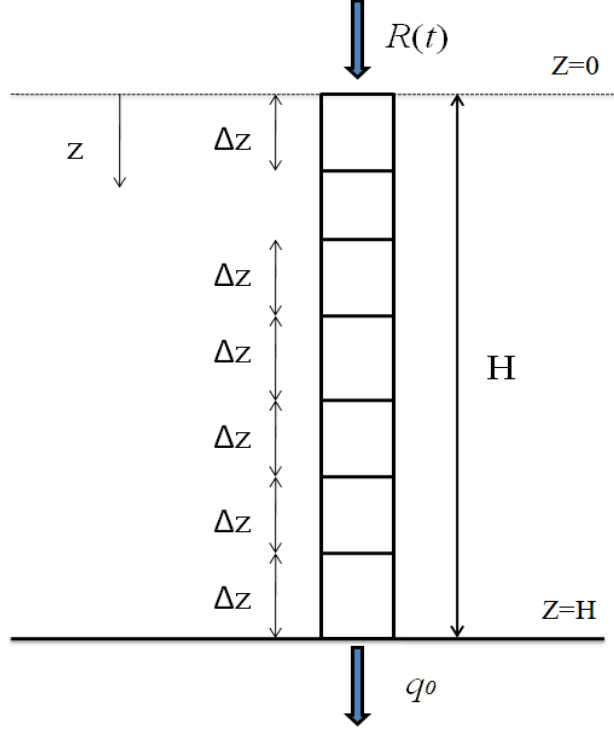


Figure 1. Mathematical Domain.

If $\theta = \theta(z, t)$ is the moisture content (that is, the fraction of the soil's bulk volume occupied by water [1]) in the column at the height $z \in [0, H]$ (the spatial coordinate z is positive in the downward direction) at time $t \in [0, T]$, then according to the mass conservation law, and Darcy's law, the Richards equation (cf. [1] for detailed derivation of this equation) becomes,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(D(\theta) \frac{\partial \theta}{\partial z} \right) - \frac{\partial}{\partial z} K(\theta) \quad (1)$$

with the initial and boundary conditions,

$$\theta = \theta_{initial} \text{ in } t = 0, z > 0 \quad (2)$$

$$-D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) = R(t) \text{ in } z = 0, t > 0 \quad (3)$$

$$\frac{\partial\theta}{\partial z} = 0 \text{ in } z = H, t > 0 \quad (4)$$

where the hydraulic conductivity $K(\theta)$, the diffusivity $D(\theta) = K(\theta)/\frac{d\theta}{dh}$, and the retention curve $h(\theta)$ are all non-linear functions, $\theta_{initial}$ is the initial volumetric water content, and h is the soil water potential.

The differential problem (DP) consists of obtaining an approximation of θ on the rectangle $[0, H] \times [0, T]$, from equation (1), under conditions (2), (3) and (4).

Remark 1. With respect to the functions $K(\theta)$ and $h(\theta)$, in this work the following two parametric families will be considered:

1. **Family VG.** This parametric family corresponds to van Genuchten which is defined as [8]:

$$K(\theta) := K_s \sqrt{S(\theta)} \left(1 - \left(1 - S^{\frac{1}{m}}(\theta) \right)^m \right)^2 \quad (5)$$

$$S(\theta) := \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + (\alpha|h|)^n)^m}, \quad (6)$$

where K_s is the saturated hydraulic conductivity of porous media, θ_r is the residual volumetric content of liquid, θ_s is the volumetric content of liquid saturation, and $m = 1 - \frac{1}{n}$, $n > 1$ and $\alpha > 0$ are the van Genuchten parameters.

2. **Family VGM.** This parametric family corresponds to a modification

of van Genuchten [8], which was applied in [4, 16]. Specifically,

$$K(\theta) = K_s S^\delta(\theta) \quad (7)$$

$$S(\theta) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + (\alpha|h|)^n)^m}, \quad (8)$$

where $m = 1 - \frac{2}{n}$, and $\delta = 3 + \frac{2}{nm}$.

Note that the family VGM is a combination of van Genuchten and Brooks-Corey models [1].

3. Numerical Solution of the Richards Equation

The numerical solution of equation (1) is based on the finite difference method, specifically, the Crank-Nicolson modified method (cf. [5]). The election of this method follows [10] to enable a better comparison with our computational experiments.

Let $[0, H]$ be the spatial domain and $[0, T]$ the temporal domain. Let Nz and Nt be the number of subintervals for $[0, H]$ and $[0, T]$, respectively. We define $\Delta z := H/Nz$, $\Delta t := T/Nt$, and θ_i^j is an approximation of $\theta(i\Delta z, j\Delta t)$, with $i \in \{0, \dots, Nz\}$ and $j \in \{0, \dots, Nt\}$. Therefore, the discretization of (1), for $i \in \{0, \dots, Nz\}$ and $j \in \{0, \dots, Nt - 1\}$, is given by:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} = \frac{1}{2} \cdot (E_i^{j+1} + E_i^j) - \frac{1}{2} \cdot (F_i^{j+1} + F_i^j), \quad (9)$$

where,

$$\begin{aligned} E_i^{j+1} &:= \frac{D_{ff} \cdot (\theta_{i+1}^{j+1} - \theta_i^{j+1}) - D_{bf} \cdot (\theta_i^{j+1} - \theta_{i-1}^{j+1})}{(\Delta z)^2} \\ E_i^j &:= \frac{D_f \cdot (\theta_{i+1}^j - \theta_i^j) - D_b \cdot (\theta_i^j - \theta_{i-1}^j)}{(\Delta z)^2} \\ F_i^m &:= \frac{K_{i+1}^m - K_{i-1}^m}{2\Delta z}; m = j, j+1, \end{aligned}$$

with $D_{ff} := \frac{D_{i+1}^{j+1} + D_i^{j+1}}{2}$, $D_{bf} := \frac{D_i^{j+1} + D_{i-1}^{j+1}}{2}$, $D_f := \frac{D_{i+1}^j + D_i^j}{2}$, $D_b := \frac{D_i^j + D_{i-1}^j}{2}$, $D_i^j := D(\theta_i^j)$ and $K_i^j := K(\theta_i^j)$. With respect to the boundary conditions, the discrete version of (3), that is, for $i = 0$, is given by

$$-D_0^j \frac{(\theta_0^j - \theta_{-1}^j)}{\Delta z} + K_0^j = R^j, \quad \forall j = 0, \dots, Nt. \quad (10)$$

On the other hand, the discrete version of (4), that is, for $i = Nz$, is given by

$$\frac{\theta_{Nz+1}^j - \theta_{Nz}^j}{\Delta z} = 0, \quad \forall j = 0, \dots, Nt, \quad (11)$$

where the unknowns θ_{-1}^j and θ_{Nz+1}^j are auxiliary unknowns.

The Crank-Nicolson method is a second order method on time [5]. By another hand, the discretization in space is at most first order as the diffusion coefficients are not constant. For this reason the first-order discretization (10) and (11) is sufficient.

The matrix form of the nonlinear system (9), for $j \in \{0, \dots, Nt - 1\}$ and $i \in \{0, \dots, Nz\}$, is given by

$$A(\theta^{j+1})\theta^{j+1} = b(\theta^j) + c(\theta^{j+1}), \quad (12)$$

where $\theta^{j+1} = (\theta_i^{j+1})_{(Nz+1) \times 1}$ and the entries of $A(\theta^{j+1})$, $b(\theta^j)$ and $c(\theta^{j+1})$ are defined as follows. The matrix $A = A(\theta^{j+1})_{(Nz+1) \times (Nz+1)}$ is given by

$$A = \begin{bmatrix} 1 + w_1(D_{ff} + D_{bf}) & -w_1 D_{ff} & 0 & \cdots & \cdots \\ -w_1 D_{bf} & 1 + w_1(D_{ff} + D_{bf}) & -w_1 D_{ff} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & 0 & -w_1 D_{bf} & 1 + w_1(D_{ff} + D_{bf}) & -w_1 D_{ff} \\ \cdots & \cdots & 0 & -w_1 D_{bf} & 1 + w_1(D_{ff} + D_{bf}) \end{bmatrix}$$

where $w_1 := \frac{\Delta t}{2(\Delta z)^2}$. The entries of $b = b(\theta^j)_{(Nz+1) \times 1}$, for $i \in \{0, \dots, Nz\}$, are given by

$$b_{i+1} = \theta_i^j + w_1[D_f(\theta_{i+1}^j - \theta_i^j) - D_b(\theta_i^j - \theta_{i-1}^j)] - w_2(K_{i+1}^j - K_{i-1}^j),$$

where $w_2 := \frac{\Delta t}{4\Delta z}$, and the entries of $c = c(\theta^{j+1})_{(Nz+1) \times 1}$, for $i \in \{0, \dots, Nz\}$ are

$$c_{i+1} = -w_2(K_{i+1}^{j+1} - K_{i-1}^{j+1}).$$

In particular, note that for $i = 0$

$$c_1 = -w_2(K_1^{j+1} - K_{-1}^{j+1}) + w_1 D_{bf} \theta_{-1}^{j+1},$$

where θ_{-1}^{j+1} is computed from the boundary condition (10), and for $i = Nz$

$$c_{Nz+1} = -w_2(K_{Nz+1}^{j+1} - K_{Nz-1}^{j+1}) + w_1 D_{ff} \theta_{Nz+1}^{j+1},$$

where θ_{Nz+1}^{j+1} is computed from the boundary condition (11).

Remark 2. The system in (12) is implicit in time and will be solved by a corrector-predictor method. Specifically, in this work we consider two versions for this method:

1. **Version CP1.** This version corresponds to the method applied in [10].

For $j \in \{0, \dots, Nt - 1\}$, the system solved is

$$A(\theta^j)\theta_{aux} = b(\theta^j) + c(\theta^j), \quad (13)$$

for θ_{aux} and then θ^{j+1} is computed from

$$A(\theta_{aux})\theta^{j+1} = b(\theta^j) + c(\theta_{aux}). \quad (14)$$

2. **Version CP2.** This version corresponds to the method applied in [5].

For $j \in \{0, \dots, Nt - 1\}$, the vector θ_p is computed from

$$A(\theta^j)\theta_p = b(\theta^j) + c(\theta^j) \quad (15)$$

where θ_p is a prediction of θ^{j+1} . Next, θ_c which is a correction of θ_p , is calculated from

$$A(\theta_p)\theta_c = b(\theta^j) + c(\theta_p), \quad (16)$$

which is a correction that is acceptable as an estimation of θ^{j+1} when

$$\|A(\theta_c)\theta_c - (b(\theta^j) + c(\theta_c))\|_2 < \epsilon, \quad (17)$$

where ϵ is a user's value; otherwise, $\theta_p = \theta_c$, where θ_c is computed again from (16) until (17) is satisfied. In this case,

$$\theta^{j+1} = \theta_c.$$

Note that the application of CP1 and CP2 is based in the resolution of a linear tridiagonal system (12) which is diagonal dominant. This system was solved with the Thomas algorithm [5], which is based on a LU factorization when is applied to a tridiagonal matrix.

4. Global Algorithm of Parameter Estimation

In this work the parameter vector considered is (α, n) (cf. Remark 1). Comparing the experimental outflow q_{ol} , $l = 1, \dots, N$ with the numerical solutions of the DP: $q(\theta; (\alpha, n)) = -D(\theta; (\alpha, n)) \frac{\partial \theta}{\partial z} + K(\theta; (\alpha, n))$ (maintaining the same notation for discrete and continuous solutions), the objective function is defined as

$$\Omega(\alpha, n) = \sum_{l=1}^N \left(q_{ol} - \hat{q}(\hat{\theta}_l(\alpha, n)) \right)^2, \quad (18)$$

where $\hat{q}(\hat{\theta}_l((\alpha, n)))$ is the numerical outflow estimated in t_l , with $l = 1, \dots, N$. Note that the outflow is measured at the bottom of the domain, $z = H$, where the boundary condition (4) applies. Thus, the expression for $q(\theta; (\alpha, n))$ is $q(\theta; (\alpha, n)) = K(\theta; (\alpha, n))$ on $z = H$.

The minimization of the function (18) is based on the Levenberg-Marquardt algorithm, which will be applied using the MATLAB function *lsqnonlin* (cf. [17]), which is based on [11]. A complete analysis of the convergence and a detailed discussion of the computational implementation of the algorithm is presented in [9] and was also discussed in [11]. Here, the primary application of the Levenberg-Marquardt algorithm is curve fitting using the least squares method.

The input for the optimization algorithm of (18) are: q_o (vector of experimental flow), (α_0, n_0) (vector of initial values), T (length of temporal interval of simulation for DP), H (height of leaching column), and Nt and Nz (the size of partitions in time and space, respectively). This data is applied to *lsqnonlin* and the output is the vector (α_{opt}, n_{opt}) , where $\Omega(\alpha, n)$ is minimum.

Figure 2 describes the computational structure of the routine and its

subroutines by showing the order in which the calculations are made and the order in which the functions are used, where the *qfunction* is a MATLAB function that computes the vector r and its components

$$r(\theta_l(\alpha, n)) = q_{o_l} - \hat{q}(\hat{\theta}_l(\alpha, n)), \quad l = 1, \dots, N.$$

After the incorporation of the specified data by the user in Section 5, the *lsqnonlin* function is invoked, which in turn invokes the *qfunction* (m-function created by the user), which in turn invokes the subroutine Solve **DP**. This process is repeated as many times as seems necessary by the function *lsqnonlin*.

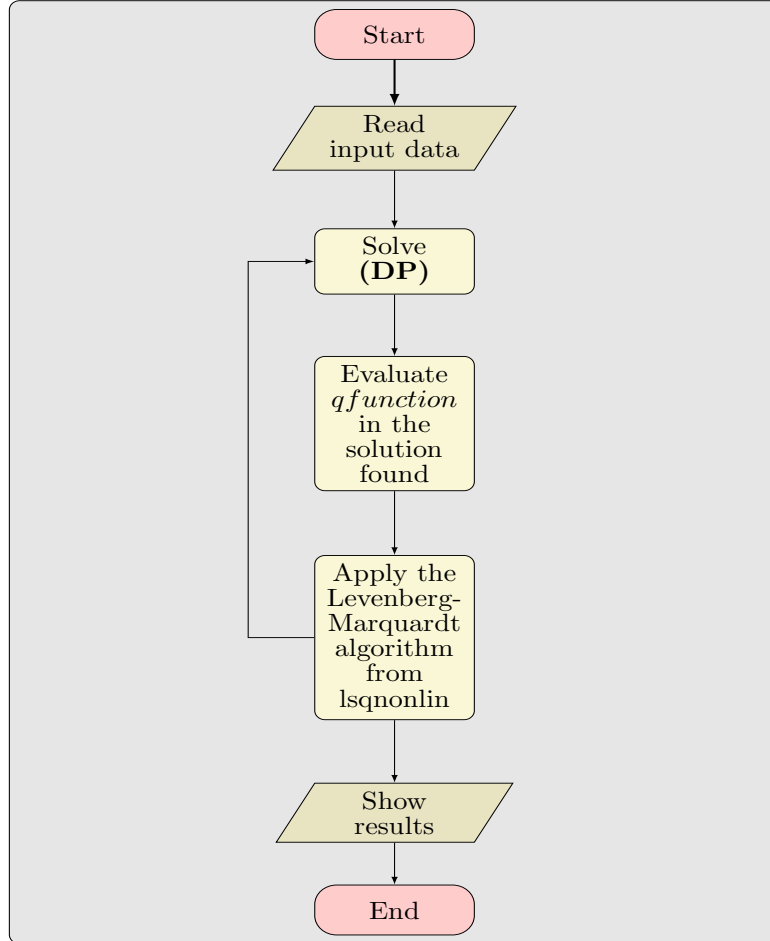


Figure 2. Flowchart of the Global Estimation Algorithm.

The subroutine **Solve (DP)**, which is detailed in Figure 3, takes the data from the *qfunction* and solves the Richards equation. Specifically, applies de Predictor-Corrector method and the Thomas's algorithm (cf. Section 3 and Remark 2).

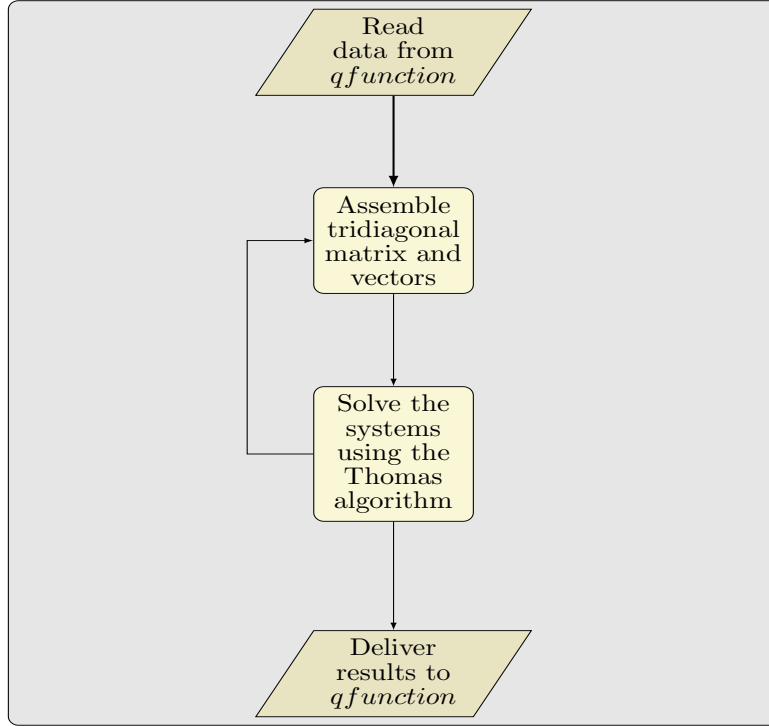


Figure 3. Flowchart for subroutine Solve (**DP**)

5. Computational Experiments

The copper heap in Tranque Barahona, Chile that was researched in articles [12, 16] was also investigated for this article. The heap is 550 *cm* high, 220 *cm* wide, and has a base of length 500 *cm*, with lateral slopes 1:1. Drip irrigation was conducted on a surface of 308 m^2 . Additionally, a programmed variable irrigation was applied to the heap for 44 days. For more details see Table 1 (where vG is used as acronym for van Genuchten).

In experiments 1, 2, 3 and 4, (see sections 5.1, 5.2, 5.3, and 5.4, respectively) the parametric family VGM defined by (7) and (8) was considered. In experiment 5 (see section 5.5), the parametric family VG defined by (5)

Parameter	Symbol	Value
Total Time	T	44 [day]
Height	H	550 [cm]
Initial Moisture	$\theta_{initial}$	0.14 [cm^3/cm^3]
Saturated Moisture	θ_s	0.33 [cm^3/cm^3]
Residual Moisture	θ_r	0 [cm^3/cm^3]
Saturated Hydraulic Conductivity	K_s	170 [cm/day]
vG Parameter	α	0.035 [1/cm]
vG Parameter	n	2.267
Size of Time Step	Δt	1/24 [day]
Size of Space Step	Δz	2.5 [cm]

Table 1: Simulation Parameters

and (6) was considered (cf. Remark 1).

5.1. Experiment 1

In this experiment only the DP problem was solved, that is, the Richards equation, following the parameters outlined in Table 1. The values of the van Genuchten parameters were $(\alpha_1, n_1) = (0.035, 2.267)$. The parametric family utilized was VGM: (7)-(8), and the corrector-predictor method was CP1: (13)-(14). In Experiment 1, the numerical value of the relative residual norm is

$$100 \cdot \|q_o - \hat{q}(\hat{\theta}(\alpha_1, n_1))\|_2 / \|q_o\|_2 = 47.39\%,$$

where $\|q_o\|_2 = 133.4280[m^3/day]$.

Figure 4 contains the evolution of influent, effluent and modeled flows.

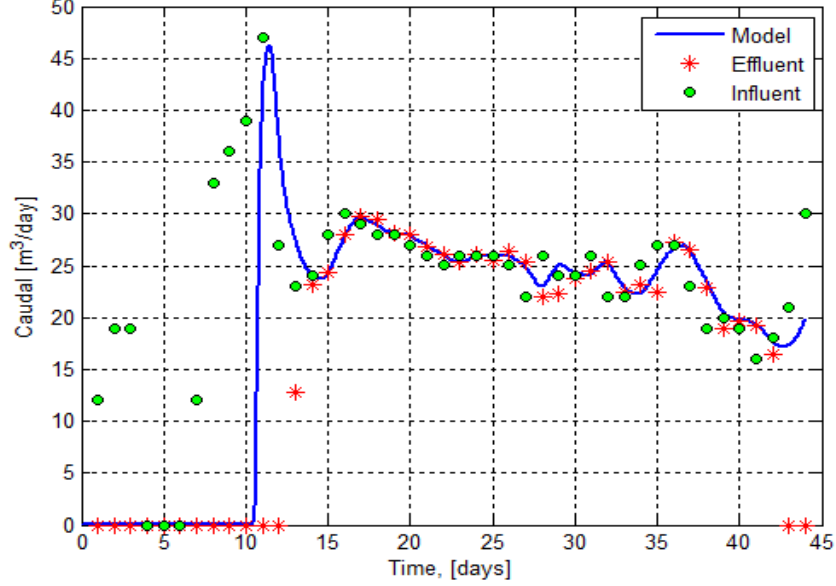


Figure 4. Measured and Modeled Outflow in Experiment 1

In Figure 4, we can see that the model is better adjusted to the observed outflow from the 14 day simulation, and this situation is maintained until day 42.

5.2. Experiment 2

In this experiment, we performed the Global Estimation Algorithm, as described in Figure 2. The data in Table 1 was used except for the vG parameters vector, which was changed by the initial parameter vector $(\alpha_0, n_0) = (0.035, 2.315)$. The parametric family utilized was VGM: (7)-(8), and the corrector-predictor method was CP1: (13)-(14). The results are summarized in Table 2, where α_{opt2} and n_{opt2} are the optimal values obtained with the Levenberg-Marquardt algorithm. The observed influent and effluent versus the estimated outflow with the optimal parameters is similar to Experiment 1 (to see Figure 4). In Table 2, one iteration includes the evaluation of the

Parameter	Value
α_0	0.035 [1/cm]
n_0	2.315
α_{opt2}	0.049 [1/cm]
n_{opt2}	2.230
$\ q_o - \hat{q}(\hat{\theta}(\alpha_{opt2}, n_{opt2}))\ _2$	55.3768 [m ³ /day]
N iterations	15
Mean time by iteration	890 [s]

Table 2: Optimal Values for α and n in Experiment 2

q function by *lsqnonlin* and the solution of the DP. This process takes approximately 890 [s] . In Experiment 2, the numerical value of the relative residual norm is

$$100 \cdot \|q_o - \hat{q}(\hat{\theta}(\alpha_{opt2}, n_{opt2}))\|_2 / \|q_o\|_2 = 41.50\%.$$

5.3. Experiment 3

This experiment is a continuation of Experiment 2. In Experiment 3, the impact of changing the size of the steps in space and time is evaluated. Four tests were performed with the same data in Table 1, with α , n , Δt and Δz reported in Table 3. The data concerning the residual norms, the number of iterations, and the mean time elapsed are located in Table 4. In these four tests, the initial vector parameters were $(\alpha_0, n_0) = (0.035, 2.315)$.

The results of Experiment 3 show that the initial values $\Delta z = 2.5[cm]$ and $\Delta t = 1/24[day]$ are suitable, this is, are sufficiently small. The only impact observed after reducing the values of Δz and Δt was an increase in the mean

time of calculation. The decrease of the relative residual norm was only marginal. In tests 1 to 4 the parameters estimated were $\alpha_{opt3} = 0.04999999$ and $n_{opt3} = 2.2300000$, where only the first four decimal places are physically significant. Finally, note that the differences observed between 9 and 14 decimal places can be explained by the internal computer arithmetic.

Test	Δt	Δz	$(\alpha_{opt3}, n_{opt3})$
1	$\frac{1}{24}$ [day]	2.5 [cm]	(0.04999999823866, 2.23000002251736)
2	$\frac{1}{29}$ [day]	2.0 [cm]	(0.04999999999996, 2.23000000000012)
3	$\frac{1}{36}$ [day]	1.5 [cm]	(0.04999999780221, 2.23000004077647)
4	$\frac{1}{48}$ [day]	1.0 [cm]	(0.04999999738890, 2.23000004007278)

Table 3: Optimal Values in Experiment 3

Test	Relative Residual Norm	Iterations	Mean Time
1	41.50%	15	890 [s]
2	40.59%	18	2326 [s]
3	40.27%	15	3590 [s]
4	40.02%	15	5229 [s]

Table 4: Residual Norm, Iterations, and Mean Time in Experiment 3

The observed influent and effluent versus the estimated outflow in test 1,2,3 and 4, is similar to Experiment 1 (to see Figure 4).

5.4. Experiment 4

In this experiment the impact of corrector-predictor method (cf. Remark 2) is evaluated. The parametric family utilized was VGM: (7)-(8), and

the corrector-predictor method was CP2: (15)-(16). In Figure 5, the same comparison between the influent and effluent experimental flows, and the simulated outflow is made, but with the under improved corrector-predictor method (cf. Remark 2 and compare the Figures 4 and 5).

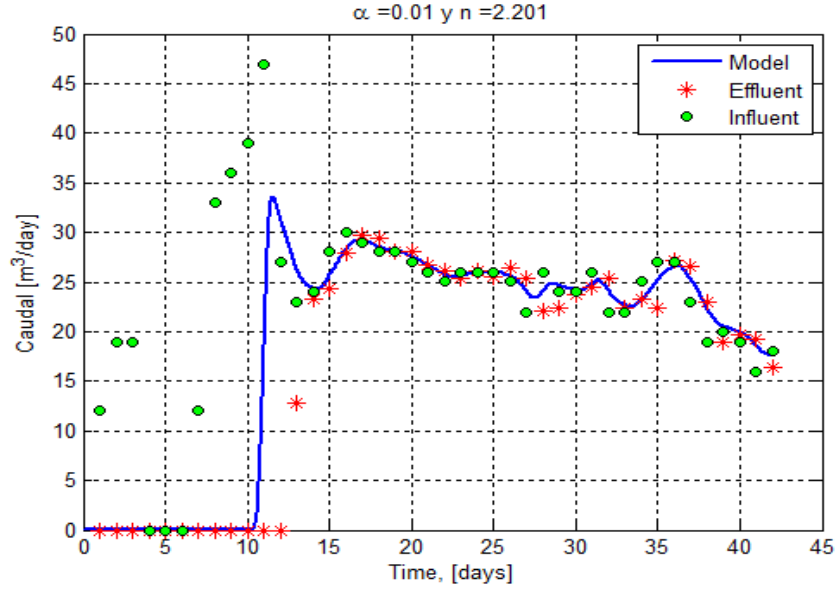


Figure 5. Measured and Modeled Outflow in Experiment 4

The new optimal parameters vector is $(\alpha_{opt4}, n_{opt4}) = (0.01, 2.201)$.

In Experiment 4, the numerical value of the relative residual norm is

$$100 \cdot \|q_o - \hat{q}(\hat{\theta}(\alpha_{opt4}, n_{opt4}))\|_2 / \|q_o\|_2 = 29.01\%.$$

5.5. Experiment 5

Experiment 5 reports the results of two main modifications made to the previous results. The parametric family utilized was VG: (5)-(6), and the corrector-predictor method was CP2: (15)-(16). Under these new conditions, the optimal parameter vector was $(\alpha_{opt5}, n_{opt5}) = (0.013, 1.306)$. In

Experiment 5, the numerical value of the relative residual norm is

$$100 \cdot \|q_o - \hat{q}(\hat{\theta}(\alpha_{opt5}, n_{opt5}))\|_2 / \|q_o\|_2 = 3.49\%.$$

Figure 6 shows the experimental data and the estimated data. The improved conditions were compared with the works [10, 12, 16].

The purpose of experiment 4 was to evaluate the impact of replace the method CP1 by CP2. The results of experiment 4 were compared with of experiment 2, showing a decrease of 12.49 ($= 41.5-29.01$) percentage points of relative error. On the other hand, the purpose of experiment 5 was to evaluate the impact of replace simultaneously the parametric family VGM by VG, and the method CP1 by CP2. The results of experiment 5 were compared with the experiment 2, showing a reduction of 38.01 ($= 41.50-3.49$) percentage points of relative error. This significant reduction of 38.01 percentage points of relative error, can be partially explained by the impact of changing simultaneously the method CP1 by CP2, and family VGM by VG. The simulations obtained show the importance of evaluating different parametric families (VG, VGM, or other) for a better fit of the model. Indeed, given different functional expressions is expected that adjustment levels between simulations and experimental data are not the same.

In [12], the heap was divided into three layers (top, middle and bottom), and the estimation of the van Genuchten parameters, α and n , were made for each of these layers. For the parameter α , the values obtained were 0.03023[1/cm], 0.01368[1/cm], and 0.07060[1/cm], respectively. For the parameter n , the values obtained were 1.265[-], 1.411[-] and 1.200[-], respectively. Therefore, our estimates of $(\alpha_{opt5}, n_{opt5}) = (0.013, 1.306)$ correlate well with those obtained with the Hydrus Software 2D. However, the error

of our fit is lower.

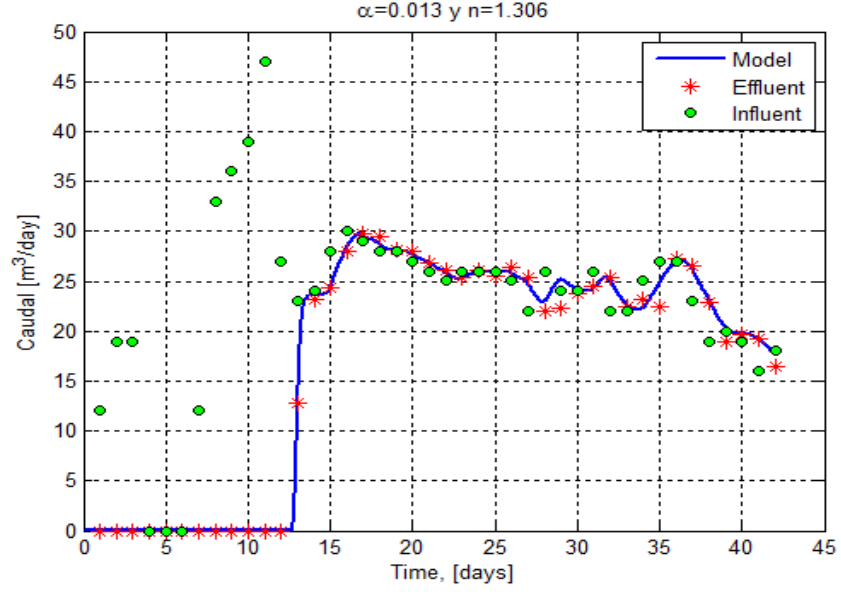


Figure 6. Measured and Modeled Outflow in Experiment 5

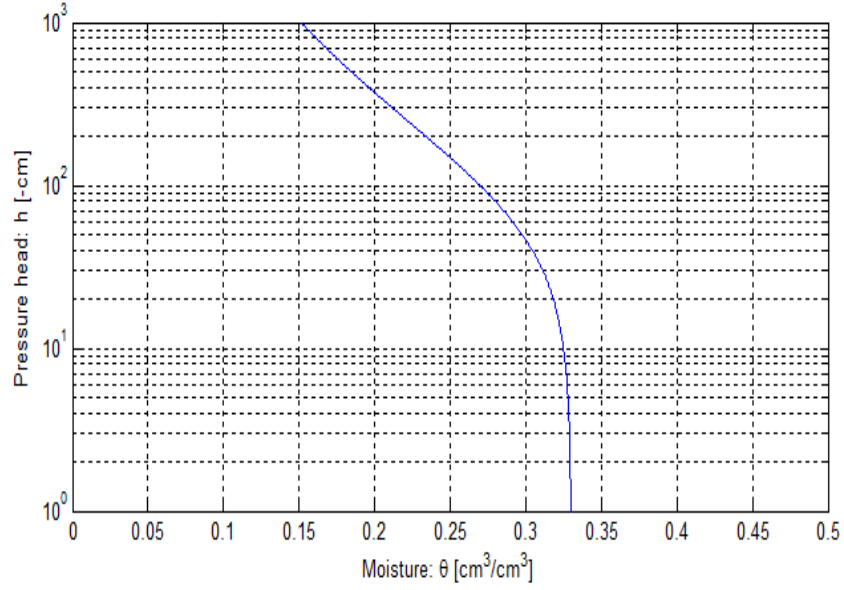


Figure 7. Retention Curve $h(\theta)$ in Experiment 5

Finally, Figure 7 shows the Retention Curve (6) with the same data and

under the same conditions as in Figure 6.

6. Conclusions

In this paper, the problem associated with the parametric estimation from the soil water retention curve and the hydraulic conductivity function, has been solved in the context of mathematical modeling of the fluid flow in copper heap leaching, under unsaturated conditions.

In relation to the numerical solution of the algebraic nonlinear system from the discretization of the Richards equation, we evaluated two cases: first, the corrector-predictor method in [10], and second, a better version of the same method. With respect to the parametric families, we evaluated two cases: a combination of the van Genuchten and Brooks-Corey models following [4, 16], as well as the van Genuchten family following [10, 12]. The optimization problem was solved with the Levenberg-Marquardt algorithm taken from MATLAB. All simulations were compared with experimental data, so that our method would have less error associated with it in comparison with the methods of [2, 4, 10, 12, 16].

This article presents a detailed description of the estimation process and emphasizes the importance of carefully selecting the parametric family and the method employed in the numerical solution of the differential problem. The algorithm developed in this article may be useful in the pre-industrial stages of the design process of leach pads, especially in the experiments conducted in columns where an efficient and exact estimation of the hydrodynamic characteristics assists in the establishment of optimal extraction conditions on an industrial scale. This work is expected to impact the de-

cision making process of metallurgical engineers. Indeed, when the outflow in a leaching pad is simulated, a significant percentage of unexplained variability in the model can be attributed to the methods of approach and/or optimization used.

Our main conclusion for the industrial practice is the need to use software in experimental leaching columns to evaluate: the best solution choice for the differential problem and different parametric families and, to achieve an optimum fit to the experimental data obtained in the pre-industrial stage.

We will continue to examine these methods through the repetition of these tests with different numerical methods, the evaluation of other parametric families, the analysis of changes in critical parameters, and through the evaluation of an the improved version of the optimization algorithm.

ACKNOWLEDGMENTS: EC acknowledges support by Fondecyt project 11100358. MS has been supported by Fondecyt project 11105404; BASAL project CMM, Universidad de Chile and CI2MA, Universidad de Concepción; CONICYT project Anillo ACT1118 (ANANUM); and Red Doctoral RE-DOC.CTA, project UCO1202 at Universidad de Concepción.

References

- [1] J. Bear, Dynamics of fluids in porous media, Dover Publications, Inc. New York, first edition, 1988.
- [2] E. Cariaga, F. Concha, M. Sepúlveda, Flow through porous media with applications to heap leaching of copper ores, Chemical Engineering Journal 196 (2005) 2541–2554.

- [3] E. Cariaga, F. Concha, M. Sepúlveda, Simultaneous modeling of liquid and gaseous phases in heap leaching of copper production, in: J.M. Casas, J.M. Menacho (Eds.), Proceeding of the III International Copper Hydrometallurgy Workshop, pp. 301–315, 2005.
- [4] E. Cariaga, F. Concha, M. Sepúlveda, Convergence of a mfe-fv method for two phase-flow with applications to heap leaching of copper ores, *Computer Methods in Applied Mechanics and Engineering* 196 (2007) 2541–2554.
- [5] M. Davis, Numerical methods and modeling for Chemical Engineers, John Wiley & Son USA, second edition, 1990.
- [6] D. Dixon, J. Petersen, Modeling the dynamics of heap bioleaching for process improvement and innovation, in: T. Vargas (Ed.), Proceeding of the International Colloquium Hydrometallurgical on Processing of Copper Sulfides, pp. 13–45, 2004.
- [7] E. Domíć, Hidrometalurgia: Fundamentos, Procesos y Aplicaciones, first edition, 2001.
- [8] T. van Genuchten, A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.* 44 (1980) 892–898.
- [9] D. Marquardt, An algorithm for least-squares estimation of nonlinear parameters, *Journal of the Society for Industrial and Applied Mathematics* 11 (1963) 431–441.

- [10] S. Mejía, Modelación y simulación de la visualización del transporte de fluido a través de pilas de lixiviación de minerales de cobre, Master's thesis, Universidad de Chile, 2000.
- [11] J. Moré, The levenberg-marquardt algorithm: implementation and theory, *Lecture Notes in Math.* 630 (1978) 105–116.
- [12] J. Munhoz, C. Ortiz, Estudio experimental y modelación numérica de una pila de relave de cobre aglomerado, in: *Actas del XV Congreso Chileno de Ingeniería Hidráulica*, pp. 359–369, 2001.
- [13] J. Munhoz, P. Rengifo, M. Vauclin, Acid leaching of copper in a saturated porous material: parameter identification and experimental validation of a two-dimensional transport model, *Journal of Contaminant Hydrology* 27 (1997) 1–24.
- [14] J. Petersen, H. Watling, D. Dixon, P. Franzmann, J. Plumb, J. Johnson, S. Harrison, G. Hansford, Progress on the development of comprehensive understanding and a model of copper heap bioleaching, in: J.M. Menacho, J.M. Casas (Eds.), *Proceeding of the III International Copper Hydrometallurgy Workshop, The AMIRA P768 Project*, pp. 333–342, 2005.
- [15] J. Simunek, M. Sejna, T. van Genuchten, The Hydrus-2D software package for simulating the two-dimensional movement of water, heat and multiple solutes in variably saturated media, Version 2.0, Technical Report, U.S. Salinity Laboratory, USDA, ARS, Riverside, California, 1999.

- [16] A. Suazo, Lixiviación ácida en pilas de relave aglomerado, Ph.D. thesis, Pontificia Universidad Católica de Chile, 2003.
- [17] P. Venkataraman, Applied optimization with MATLAB programing, Wiley, second edition, 2009.