



Swansea University  
Prifysgol Abertawe



## Cronfa - Swansea University Open Access Repository

---

This is an author produced version of a paper published in :  
*Minerals Engineering*

Cronfa URL for this paper:

<http://cronfa.swan.ac.uk/Record/cronfa18573>

---

### **Paper:**

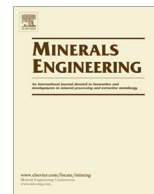
McBride, D., Croft, T., Cross, M., Bennett, C. & Gebhardt, J. (2013). Optimization of a CFD – Heap leach model and sensitivity analysis of process operation. *Minerals Engineering*, 63, 57-64.

<http://dx.doi.org/10.1016/j.mineng.2013.11.010>

---

This article is brought to you by Swansea University. Any person downloading material is agreeing to abide by the terms of the repository licence. Authors are personally responsible for adhering to publisher restrictions or conditions. When uploading content they are required to comply with their publisher agreement and the SHERPA RoMEO database to judge whether or not it is copyright safe to add this version of the paper to this repository.

<http://www.swansea.ac.uk/iss/researchsupport/cronfa-support/>



## Optimization of a CFD – Heap leach model and sensitivity analysis of process operation



D. McBride<sup>a,\*</sup>, T.N. Croft<sup>a</sup>, M. Cross<sup>a</sup>, C. Bennett<sup>a</sup>, J.E. Gebhardt<sup>b</sup>

<sup>a</sup> School of Engineering, Swansea University, Singleton Park, Swansea SA2 8PP, Wales, UK

<sup>b</sup> FLSmidth Salt Lake City, Inc., 7158 S. FLSmidth Drive, Salt Lake City, UT 84047, USA

### ARTICLE INFO

#### Article history:

Available online 2 December 2013

#### Keywords:

Heap leach modeling  
Computational fluid dynamics (CFD)  
Optimization

### ABSTRACT

A comprehensive heap leach model, developed within a computational fluid dynamics software framework, provides a modeling tool to capture reactive dissolution in low grade ores of oxide and sulfide minerals. These systems involve suites of very complex reactions, which are closely coupled with thermal conditions and key microbial populations. One of the key challenges when modeling heap leach scenarios is characterization of the ores and parameterization of the model in order to utilize the model as an investigative tool. The calibration of the model can be a lengthy process requiring many simulation runs. An optimization tool has been incorporated into the model to allow automated searching for multiple 'best fit' parameter values and to determine sensitivity. Once the model has been parameterized, large-scale forecasts can be simulated or a sensitivity analysis can be performed to investigate a range of process variables, such as irrigation rate, lift, air injection, acidity, head grade and dripper emitter spacing, amongst others. One such example is explored here for the Zaldivar ore body.

© 2013 Elsevier Ltd. All rights reserved.

## 1. Introduction

Stockpile or heap leaching for metal recovery from low-grade ore deposits, such as copper, nickel, zinc, uranium, gold and silver ores, increases in importance at a time when demand for metals is continuing to rise. As available metal head values degrade, efficient leaching of large quantities of low-grade metal deposits becomes increasingly essential. In today's operations, expanding heap leach practices see the size of heaps grow larger, increasing lift heights to reduce the amount of land impacted by mining, leaching of run-of-mine ore and crushed ore and leach solution rates designed to optimize metal recovery and chemical consumption. Recovery of the target metal can range from approximately 30% for some difficult to leach sulfide copper ores to over 90% for easier oxide gold ores. Thus, a computational tool to support operational analysis by the engineer to reduce operational costs and maximize recovery is increasingly appealing.

Building a computational model that incorporates the physics and chemistry involved in the heap leach process, with stockpiles of width and depth of hundreds of meters and timescales that may be months and years, offers a considerable challenge. The basic process, applying a reactive solution to a stockpile of low-grade ore and collecting the dissolved metal in the recovered

leach solution, is simple in concept. However, leach systems are very complex physically and chemically, and the variability between different ores and between samples (i.e., mineral concentrations, local blockages, and impurities) makes it difficult to accurately predict the behavior of a particular system unless the model is calibrated against each specific ore. Once the model is calibrated for a specific ore type, then it is possible to determine trends and indicators towards improving leaching at the industrial scale. Computational models have the advantage of being repeatable and fast – simulations of hundreds of days of column tests can take place in a few minutes, whilst years of whole heap leach can be delivered within hours. A helpful general description of leach modeling requirements has recently been given by Petersen (2010).

Developing computational tools that allow different leach strategies to be explored and optimized is a challenging task. There has been an enduring interest for over 30 years in the development of mathematical models of heap leach processes to provide effective engineering management tools (Bartlett, 1998). In the past few years, several models based on computational fluid dynamic (CFD) platforms have been reported in the literature, including Leahy et al. (2005, 2006 and 2007) and Leahy and Schwarz (2009). Flow models have been developed by Cariaga et al. (2005, 2007) and an analytical model developed by Mellado and Cisternas (2008) and Mellado et al. (2011a,b). Heap bioleaching has been considered by Bouffard (2008), Bouffard and Dixon (2009) and

\* Corresponding author.

E-mail address: [d.mcbride@swansea.ac.uk](mailto:d.mcbride@swansea.ac.uk) (D. McBride).

Petersen and Dixon (2007) amongst others. This paper builds upon a CFD based model that combines true heap geometry with all aspects of the various physical, chemical and biological processes present in a heap as a series of sub models to provide a comprehensive solution (Bennett et al., 2006, 2008a,b, 2012b; Cross et al., 2006; McBride et al., 2006, 2012a, b).

Over the past years there has been much interest in developing models of all or part of a heap leaching system to enable the design and optimization of the leaching process. Due to the highly non-linear and complex suite of reactions occurring during the leach process, the influence of small changes in operating parameters can lead to high uncertainty in the effect on recovery. Many modeling approaches have been applied to the heap leaching process and process sensitivity analysis performed to investigate the effect of changing operation variables. Dixon and Hendrix (1993), developed a mathematical model for use in the design and scale up of heap leaching processes. Mellado et al. (2011a,b, 2012) presented analytical models to investigate optimal flow rates and investigates sensitivity of input parameters to the response of the process in applications where scale-up is necessary.

One of the key challenges when modeling heap leach scenarios is characterization of the ores and parameterization of the model in order to utilize the model as an investigative tool. Although a computational model can simulate days, months of leaching in minutes, the calibration of the model can be a lengthy process requiring many simulation runs. The focus of this paper is to show how the model can be employed, with characterized and calibrated ore data, to understand which process parameters affect the recovery and to what extent. The paper also details an optimization tool that has been incorporated into the CFD model to allow automated searching for multiple 'best fit' parameter values, thus reducing the calibration times and optimizing the 'fit' of the model. The optimizer tool is a simple automated 'best fit' search, which makes small changes to each parameter and determines if the change improves or worsens the quality of fit of the variables under investigation. The advantage of this type of optimizer is that it is extremely robust for a highly non-linear system but the disadvantage is that it requires many automated simulation runs.

Examples of model calibrated and predicted results are shown for sulfide ore and for a multi-material oxide ore. In any practical investigation, there are really two essential components – one concerns the calibration of the ore complex (for which the above mentioned tools are devised) and the sensitivity analysis of the target commercial heap – what influences the effectiveness of its operation. In the final part of this paper, sensitivity analysis on process operational parameters on a commercial copper sulfide leach heap, for which adequate data is in the public domain, is presented to show how the calibrated simulation tools might be employed.

## 2. Heap leach model

The general heap leach model is implemented within a computational fluid dynamics (CFD) multi-physics software framework. A detailed description of the mathematical models and algorithms is given by (Bennett et al., 2012b) for copper sulfide ores and for oxide ore (McBride et al., 2012b). The host code, PHYSICA, provides a three-dimensional finite volume unstructured mesh modular framework for multi-physics modeling (Croft et al., 1995). The framework supplies generic routines to discretise a general transport equation over a solution domain using cell-centred approximations over an arbitrarily complex three dimensional mesh comprised of a mix of tetrahedral, wedge and hexahedral elements.

### 2.1. Liquid–gas–thermal transport

Flow through variably saturated porous media is typically characterized by the Richards' equation. Saturated and unsaturated liquid flow have individually been well described but modeling systems containing both saturated and unsaturated regions offers considerable challenges. A computational procedure for handling both saturated and unsaturated conditions in the same environment has been developed (McBride et al., 2006). The procedure is based on a transformation method and is fully integrated into the unstructured context within the PHYSICA code. In addition to the liquid solution flow, air may be circulated through the heap. The model solves the gas phase transport and makes the assumption that the liquid flow influences the gas flow but the gas flow does not directly influence the fluid flow. Gas flow is primarily driven by boundary conditions such as gas injection through air lines and wind pressure against the sides of heaps. Temperature gradients can also be very important in driving gas flow and buoyancy forces are also accounted for in the model. In addition oxygen liquid–gas mass transfer can occur due to a number of factors, typically temperature, liquid and gas composition and liquid–gas interfacial area. In the model, oxygen is transported between the liquid and gas phases according to Henry's law. The details of the CFD flow module that is used to calculate the fluxes of chemical species, gas and liquid flows, and heat balance are given by Bennett et al. (2012b).

### 2.2. Mineral reaction chemistry

The reactions module solves the solid–liquid mineral reactions by explicitly solving a shrinking core algorithm, tracking the residual grades and the production and consumption of species from solid to liquid state. The solid fraction of ore is defined by a size distribution of representative particle sizes, each with their own mineral properties, replicating measured data for the properties of a specific ore type. The overall chemistry balance is determined by summing the reaction products for each particle size fraction and scaling according to availability of reactants. Typically in mineral leaching, the chemical reactions occur between raffinate species (commonly, ferric ions and/or acid for copper sulfides, cyanide for gold oxides) and reactive minerals in the solid phase.

The general equation employed to calculate the rate of dissolution of a given mineral is:

$$\frac{dr_m}{dt} = -\frac{3r_m}{4\pi r_o^2} \frac{M_i}{\rho_{ore} x_i} \frac{D_{eff} C_o A_m}{[3D_{eff} r_o C_o + 2(r_o - r_m) r_m^2 (1 - \varepsilon_p) A_m]} \quad (1)$$

where  $r_o$  is the initial particle radius,  $r_m$  is the current mineral radius,  $A_m$  comes from the kinetic rate equation for the current mineral.  $D_{eff}$  is the effective rock diffusion coefficient,  $C_o$  is the concentration of reactant at the ore particle surface,  $\varepsilon_p$  is the rock voidage,  $\rho_{ore}$  is the ore density,  $M_i$  is the molecular weight of the mineral,  $x_i$  is the mass fraction of the mineral.

The value of  $A_m$  comes from the general expression for the kinetic rate equations, which takes the general form;

$$A_m = \frac{d\beta}{dt} = Ae^{\left(\frac{B}{RT}\right)} \quad (2)$$

where  $\beta$  is the fraction of mineral reacted,  $A$  and  $B$  are functions of the individual kinetic rate equation.  $R$  is the gas constant,  $T$  is the temperature in degrees Kelvin

This approach allows minerals to react at different rates in an individual particle size, and although it requires the assumption that the minerals can be treated relatively independently, this is not unreasonable given the low concentration of reactive minerals present. Each mineral in each particle size fraction can be modeled using a single characteristic radius, which indicates how much of

the mineral has reacted. This allows the model to deal with multiple particle sizes and multiple minerals over large meshes without excessive memory usage in the overall CFD model framework.

The advantage of this approach is that it can easily be related to experimental analysis of ore, which is commonly given as mineral content by size classification, making validation easier. It also easily allows for different minerals to dominate the reactions at different stages of the leach cycle. The general kinetic rate Eq. (2) can be modified to incorporate a rate constant,  $R_A$ , thus:

$$A_m = \frac{d\beta}{dt} = R_A A e^{\left(\frac{-\beta}{\tau}\right)} \quad (3)$$

This allows the model to be tuned to a given ore using experimental column data. The rate constants in effect combine to cover factors in the reactions that are not otherwise specified for in any particular ore complex. These can include particular distributions of mineral grains and interactions between different minerals that can be difficult to quantify but may be characteristic of a particular ore body. The rate constants are unrelated to particle size and therefore allow the model to scale from small to large particle size distributions (e.g., from experimental column to heap).

As well as the standard dissolution reactions for minerals, as described previously for copper sulfides (Bennett et al., 2012b) and oxide minerals (McBride et al., 2012b), tracking of gangue minerals has been added to the model and reported in Gebhardt et al. (2012). The dissolution of these gangue species was implemented using simple first order reaction within the shrinking core model for individual particle reactions.

### 2.3. Solution reaction chemistry

In addition to the solid–liquid mineral reactions, other liquid–liquid or liquid–solid reactions may take place, such as the oxidation of ferrous ions to ferric and the precipitation of salts and other compounds.

In the case of copper sulfide heap leaching, ferrous ion oxidation is modeled using an algorithm based on a population of ferrous-oxidizing bacteria. An equilibrium relationship is used to determine the ferric ion concentration,  $[\text{Fe}^{3+}]$ , based on the concentrations of ferrous ions,  $[\text{Fe}^{2+}]$ , dissolved oxygen,  $[\text{O}_2]$ , and free acid,  $[\text{H}^+]$ , and an equilibrium constant,  $K$ . Concentrations here are in moles/litre.

The ratio of ferric ions to ferrous is therefore given by:

$$\frac{[\text{Fe}^{3+}]}{[\text{Fe}^{2+}]} = K^{1/4} [\text{O}_2]^{1/4} [\text{H}^+] \quad (4)$$

Once in the solution phase, the solubility and precipitation of several species can be affected by the local chemical environment. For a copper sulfide material, some important precipitates are hydronium and potassium jarosite, ferric hydroxide, alunite, and gypsum. An equilibrium algorithm is included in the model based on the solubility of several species where the solubility and equilibrium constant can be adjusted. The precipitation equations accounted for in the model, default solubilities and relationships are detailed in Gebhardt et al. (2012).

## 3. Parameter optimization

The parameterisation of the reaction kinetics for a given set of minerals for a particular ore type is achieved by calibration of the reaction rate,  $R_A$  in Eq. (3), for each species. The reaction rates are essentially tuned to enable the best fit possible for the data on small column tests. These reaction rates are material specific so will require tuning for each ore type. These reaction parameters can then be used to predict the bulk behavior, from large column

leach tests to multi-material large scale heaps. So the data from the small scale column can be used to parameterize the model for a specific ore and then the model used to predict the behavior of a large-scale column leach thus providing a validation test for the parameterized model. It is worth noting that it is not too difficult to ‘tune’ model parameters so that a reliable match can be obtained for the overall extraction of a metal. It is, however, much more challenging to enable the model to match the behavior of both the species concentrations and pH within the pregnant leach solution, and the dissolution in the column by particle size fraction. This requires that the formation of the model capture all the key details of the extraction process.

The calibration and parameterization of the model can be a lengthy process. Each mineral has its own characteristic reaction rate for each material and there are inevitably other unknown ore properties, such as particle effective diffusivity, that will require ‘fitting’ to experimental data. The calibration and parameterization of the model is often the most time consuming part of the modeling process, requiring study results from multiple sets of simulations, many simulation runs and an experienced operational modeler.

An optimization and sensitivity analysis tool has been incorporated into the model to allow automated searching for multiple ‘best fit’ parameter values and to determine sensitivity. The optimizer determines how the parameters should change by using an error function that compares data sets from simulation and experiment. The error function determines the variance between matched pairs of values. The optimizer tool finds the best values for selected control parameters to fit the model to a set of experimental results. Typically, it will be used to calibrate the model to new column test data. A sensitivity analysis tool enables data to be easily generated to show model behavior against variations in selected parameter values.

### 3.1. Parameter optimization

Applying the heap leach model to a new mineral or ore body requires control parameters, such as mineral reaction rates and particle diffusion, to be optimized. The optimization algorithm, incorporated into the model, automates this process of generating model control parameters (e.g., reaction rate parameters, particle diffusion coefficients, bacteria growth parameters and others).

The optimization algorithm is designed for the case where there are multiple dependant control parameters and it is difficult to generate values from physical data. When the set of input data is simple, it may be possible to do a more direct optimization to determine the best values, but this becomes increasingly hard with a large number of input parameters. The algorithm optimizes the parameters to give a ‘best fit’ to experimental data by running the same data set repeatedly and minimizing an error function. The ‘best fit’ is determined by comparing model output data to a given data set or sets that may contain multiple records. The user can set the error function to a weighted combination of fits to multiple data, such as copper recovery, and PLS concentrations of acid and ferric. The user can select and weight the most important data. The data sets can be modified by time to allow features that are difficult to model precisely in the PLS recovery, such as start up and rest periods, to be discounted. The algorithm also allows a fit to individual point values and utilizes multiple experimental and simulation data files to build the error function.

### 3.2. Error estimation

The error function is a weighted combination of fits of different data sets and fixed points. A data set consists of a set of experimental and simulated values between a set of defined time ranges.

Defining a set of time ranges allows features, such as start up and rest periods, to be ignored for the purposes of fitting. Linear interpolation is applied to experimental data to achieve experimental values that correspond in time.

For data set  $j$  the measure of fit is calculated according to the formula

$$\varepsilon_j = \frac{\left[ \sum_{t=1}^n (X_{tj}^{sim} - \bar{X}_j^{sim})(X_{tj}^{exp} - \bar{X}_j^{exp}) \right]^2}{\sum_{t=1}^n (X_{tj}^{sim} - \bar{X}_j^{sim})^2 \sum_{t=1}^n (X_{tj}^{exp} - \bar{X}_j^{exp})^2} \left( 1 - \left| \frac{\bar{X}_j^{sim} - \bar{X}_j^{exp}}{\bar{X}_j^{sim} + \bar{X}_j^{exp}} \right| \right) \quad (5)$$

In (5) the summation is over the defined time range,  $X_{tj}^{sim}$  and  $X_{tj}^{exp}$  are the simulated and experimental values at a given time  $t$  within data set  $j$  respectively and  $\bar{X}_j^{sim}$  and  $\bar{X}_j^{exp}$  are the mean of the simulated and experimental of the data sets respectively. Experience has shown that the individual data points contain a level of experimental noise that is damped when calculating the mean values. In the measure of fit equation small errors in the estimation of the individual data reduce the value of the measure by a very small amount due to the squaring of the deviation. For the mean values a linear function is used due to improved confidence in the experimental value and therefore a greater need to penalize even small variations between the simulated and experimental values.

Fixed points are taken at a set time from an available data set. An example of a fixed point that might be used is copper recovery at the end of the simulation, or another example might be residual particle grade. The quality of fit  $R_i$  for the named point  $i$  is calculated using the formula

$$R_i = 1 - \left| \frac{X_i^{sim} - X_i^{exp}}{(X_i^{sim} + X_i^{exp})} \right| \quad (6)$$

The total fit is calculated using the equation

$$\varepsilon_i = \frac{\left( \sum_{j=1}^{n_1} w_j \varepsilon_j + \sum_{j=n_1+1}^{n_2} w_j R_j \right)}{\sum_{j=1}^{n_2} w_j} \quad (7)$$

### 3.3. Optimizer algorithm

The algorithm minimizes the error function for all parameters on a stepwise basis. The step size for each increase or decrease in a parameter is defined initially as a fixed value or as a multiplier of the starting value. This reflects the fact that some parameters may vary by orders of magnitude. At the start, the optimizer determines the 'best strategy' and starting search direction for each parameter by measuring the quality of fit and ranking all parameters by the degree of sensitivity of the quality of fit. When the optimizer is required to change the search direction, it assumes that it has gone past a local minima and the size of the step is reduced.

The parameters are evaluated during the optimization phase in order of the largest effect on fit, positive or negative. The ordering of parameters is redone at the end of each sweep, allowing parameters that become insensitive to be ignored in subsequent sweeps. Sensitivity analysis can be performed with selected parameters varying over a defined range to determine sensitivity to key parameters without having to set up and run large numbers of separate simulations thus reducing the user input required and managing the simulation data. A schematic of the algorithm is shown in Fig. 1.

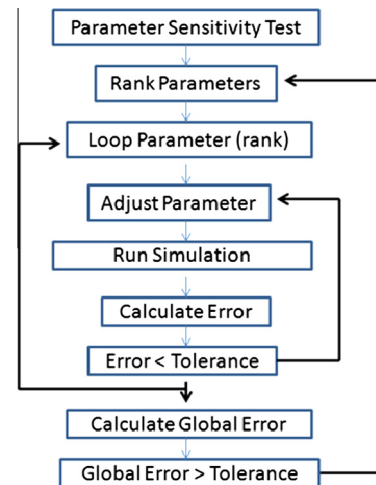


Fig. 1. Schematic for optimization algorithm.

The optimizer algorithm makes small changes to each parameter and determines if the change improves or worsens the quality of fit of the variables under investigation. Initially, the optimizer ranks the parameters in order of sensitivity. An initial learning stage determines the degree of sensitivity of the quality of fit to a small change in the parameter value. The algorithm then loops through all the parameters in order of rank. Each parameter is adjusted by its present step size and a new simulation is run. A new error is calculated for each variable under investigation. The parameter error function is a weighted combination of the error in each variable, where weights have been defined by the user, else equal weighting is applied. If the error function of the parameter under investigation is below  $10^{-4}$  or a user defined tolerance, the algorithm loops to the next parameter. When all the parameters have been investigated, the global error is calculated to determine the quality of fit for the new set of parameter values. If the global error is more than  $10^{-4}$  or a user defined tolerance, the algorithm loops through all the parameters again.

## 4. Calibration and forecast results

The optimizer tool has been employed to calibrate the model to a varying range of ore types. The leach tests reported here utilize the optimization tool to obtain reactivity parameters for both oxide and sulfide minerals.

### 4.1. Calibration result

An example of a weighted combination of fits of different data sets and fixed point calibration is the optimization of reaction parameters, which are mineral dependent, and diffusivities, which are particle dependent, to fit PLS concentration over time and particle residual grades at the simulation end. Fig. 2, shows the calibrated fits for a chalcocite-type ore, 0.32% copper mass fraction and 2.8% pyrite mass fraction, for copper recovery and residual particle grades.

Large-scale leach forecasts illustrate the model's ability to predict large-scale leaching scenarios once the model has been calibrated to a particular ore type and parameters have been optimized. In the following column leach test, the model is calibrated against a small column leach test and the parameters are used to predict a large column leach test of the same copper sulfide material. In the multiple-material case, the model is calibrated

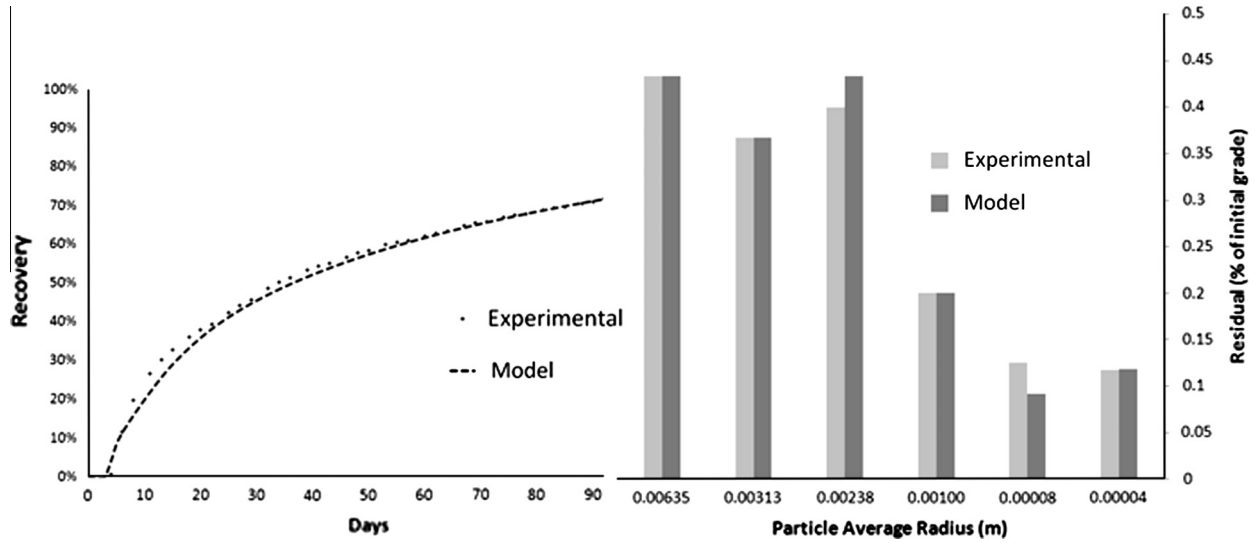


Fig. 2. Calibrated results of copper recovery and copper residual in particle distribution.

against multiple column oxide leach tests to obtain a range of optimum parameters for different ore types, and the model is used to predict the gold recovery in a full-scale heap leach comprised of these different materials.

4.2. Column leach tests

The model was calibrated against a chalcocite-type ore, 0.59% copper mass fraction and 2.15% pyrite mass fraction, small scale, 1.8-m tall, 1/2-inch crush, column leach test. The reaction rates,  $R_A$ , for the chalcocite and pyrite reactions were optimized together with particle diffusivities and the ferrous to ferric equilibrium ratio in the ferrous oxidation reaction. The column was leached with a raffinate solution containing 4.08 gpl ferric at an application rate of  $3.6 \times 10^{-7}$  m/s. The column temperature was approximately 25 °C and air was injected into the column at  $8.64 \times 10^{-5}$  m/s.

The optimized model was employed to predict species concentration and pH in the recovered pregnant solution on a large scale, 6.1-m tall, 1 1/2-inch crush, column leach test of the same material. The raffinate solution contained 3.5 gpl ferric at an application rate of  $1.58 \times 10^{-6}$  m/s. All other properties were the same. The graphs in Figs. 3 and 4 show the calibrated model results on the small column leach and the model predicted results, employing the optimized parameters obtained from the small column, against measured data on the large scale column leach test. Fig. 3 shows

the copper recovered during the leach period, and as can be seen, the model calibrated and predicted results are in good agreement with measured data. Fig. 4 shows the pH of the recovered solution during the leach period, the model predicted pH is slightly lower than measured but the general pH trend is captured.

4.3. Multiple-material heap leach

The same parameter optimization strategy can be applied within the context of a multi-material ore body as well, such as that characterized by a gold oxide system, where the ore body consists of a gold-copper-silver oxide complex. Here the model was calibrated against several 2-m high column leach tests to obtain reaction and diffusivity parameters for three base ore types. The oxide ores contained a mixture of gold, silver, copper and a gangue-type mineral, which acted as a cyanide consumer. Fig. 5 shows the particle size distribution and gold grade for each ore type. A leach solution of 50 ppm cyanide was applied to the ore at a rate of 10 l/h/m<sup>2</sup>. The gold recovered over the leach period is shown for the different ore types in Fig. 6. The calibrated model predicted results give a good match with measured data.

The different ore types were stockpiled and leached with a 50 ppm cyanide leach solution. The heap was built up over a year with new ore being added on a monthly basis. The composition of material added each month is shown in Fig. 7. The reaction param-

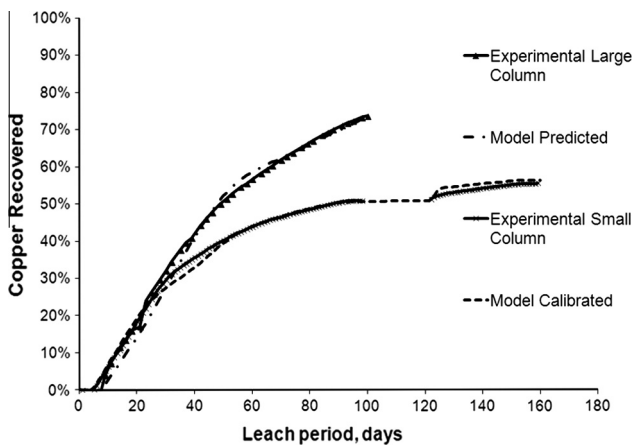


Fig. 3. Copper recovered in pregnant leach solution.

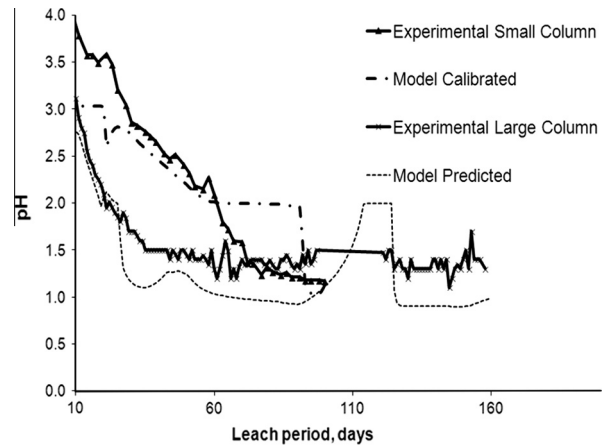


Fig. 4. pH of pregnant leach solution.

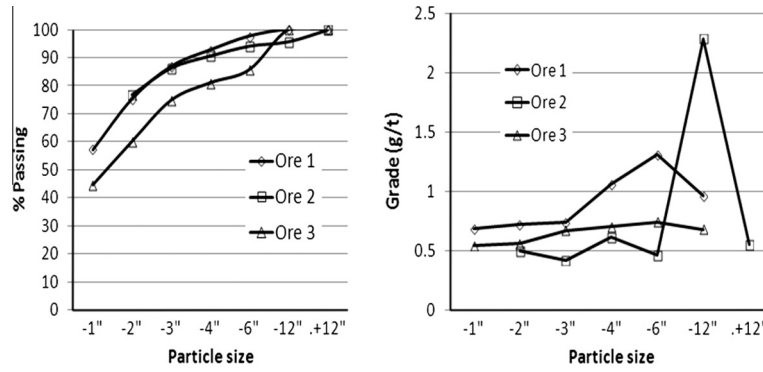


Fig. 5. Particle size distribution and gold grade.

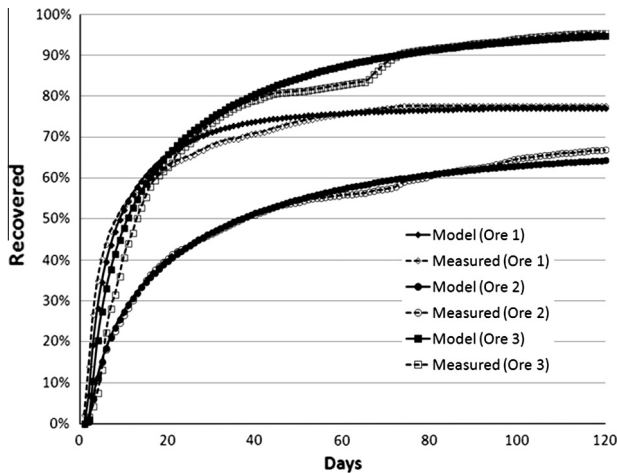


Fig. 6. Percent gold recovered over leach period.

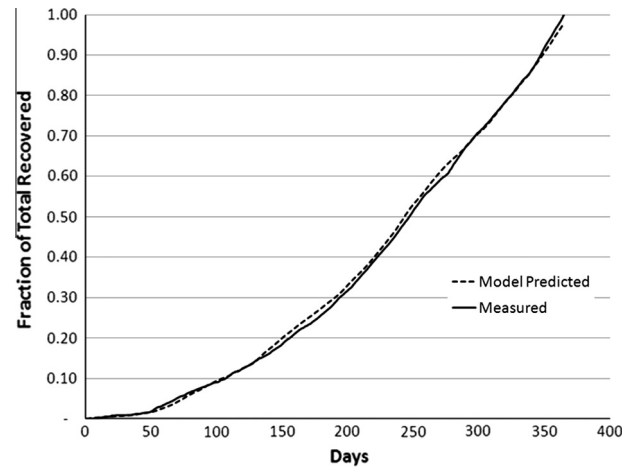


Fig. 8. Comparison of model predicted and measured gold recovery.

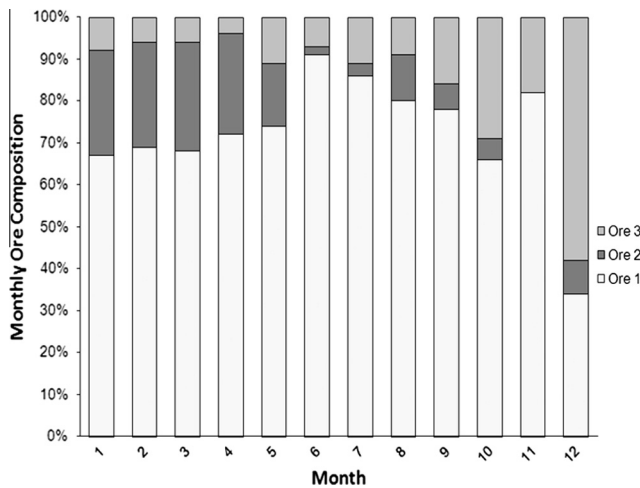


Fig. 7. Composition of material added to heap each month.

eters for each ore type were obtained from the column test model calibration study, shown in Fig. 6. The ore specific rate parameters were applied to the stockpile material, but it is also worth noting that the mineral recovery from the ore is also influenced by the solution flow path and available cyanide. As the leaching solution travels through the heap, the available reactant is consumed hence limiting the mineral reactions. Fig. 8 compares the fraction of actual total gold recovered against the model predicted recovery.

The model predicted 98% of the total gold recovered over a period of a year.

### 5. Process sensitivity analysis

Once the model has been parameterized for an ore body, the next natural stage in any simulation based investigation is to set up a model of the commercial heap operation and then to perform a process sensitivity analysis to enable a detailed understanding of which and to what extent operating parameters can affect the rate of as well as the ultimate recovery from a heap. A process sensitivity analysis was performed on a copper sulfide ore from published operating data (Bouffard and Flores Godoy, 2007) in order to explore the possible impact of operational changes at the Zaldivar mine in Chile. Bouffard's paper details a number of strategies that have been used to optimize leaching from copper sulfide ores on a dynamic leach pad. There is sufficient information in the paper combined with existing knowledge of similar ores to build a computational model that should respond to the different strategies appropriately and to investigate the extent to which the model supports the analysis and its conclusions. The model utilized in this paper has been calibrated to published data on the ore body and a detailed analysis of the effect of changing a wide range of process parameters and model assumptions is given in the paper by Bennett et al. (2012a).

The basic material investigated is a mixture of chalcocite, 1% copper, pyrite content of 2% and no acid consuming gangue. The ore is a p80 0.5-inch crush, agglomerated and treated to reduce

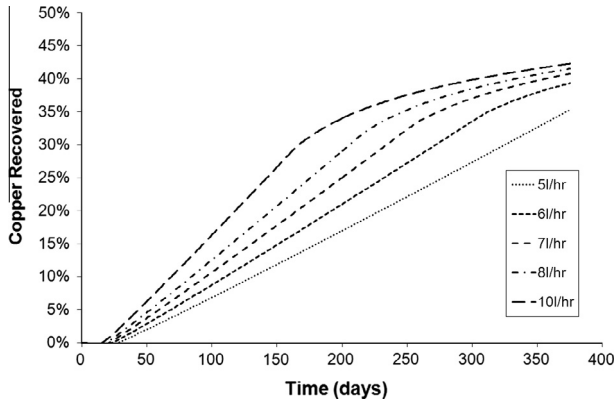


Fig. 9. Copper recovery for various application rates.

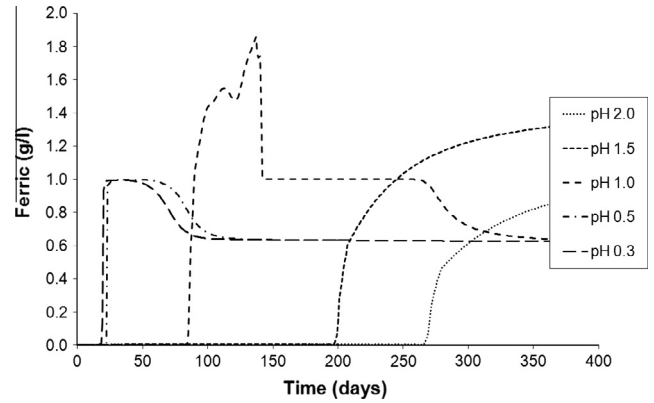


Fig. 12. Ferric in PLS for different acidity of raffinate.

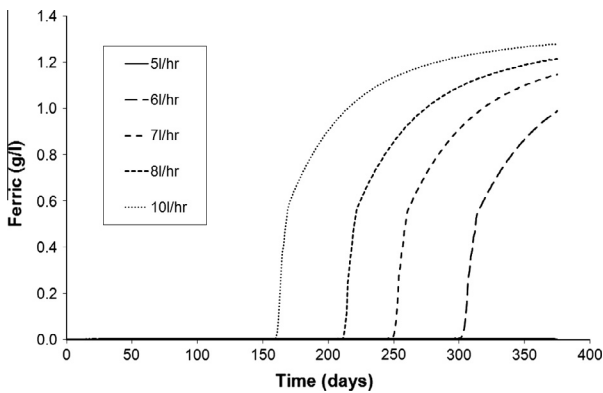


Fig. 10. Ferric in PLS for various application rates.

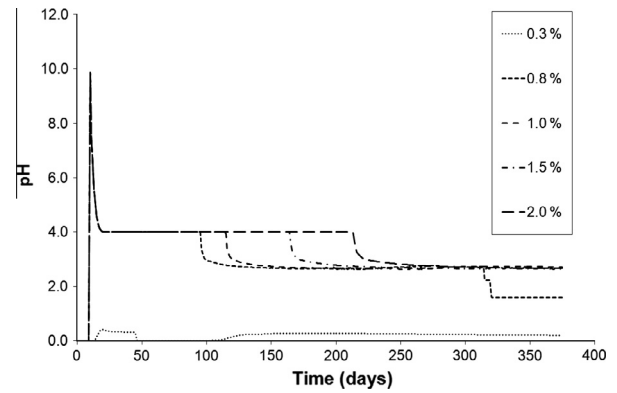


Fig. 13. Acidity of PLS for a range of ore grades.

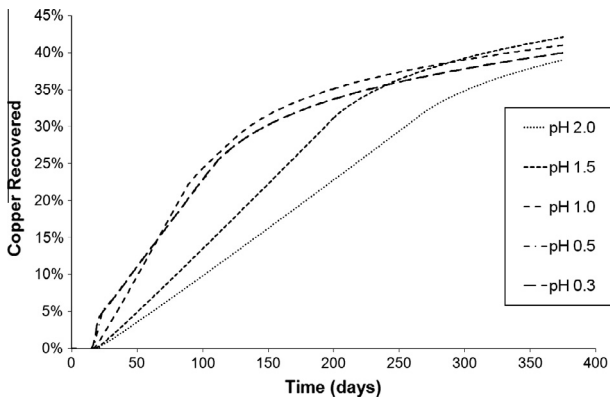


Fig. 11. Copper recovery for different acidity of raffinate.

finer. The dominant reactions are therefore the oxidation of the copper and iron minerals with ferric iron and the subsequent oxidation of ferrous iron with gaseous oxygen to regenerate the ferric. The base heap is modeled as a one dimensional column with a height of 10 m. The leach cycle is 375 days with a constant flow rate of 8 l/h/m<sup>2</sup>. Total iron in the raffinate is 1 g/l, which is almost entirely ferric. The pH is 1.6 and the copper content is 0.24 g/l. A gas flow rate of  $1 \times 10^{-5}$  m/s/m<sup>2</sup> from the base is assumed. Although temperature is allowed to vary, the ambient temperature is set to 25 °C and there is little thermal variation in the PLS. Healthy populations of bacteria are assumed to exist in the heap and therefore do not limit the ferrous oxidation process. Precipitation of iron (III) hydroxide is relatively high. Generally copper recovery to the PLS is about 50%.

The model was used to simulate raffinate flow rate varying from 5 to 8 l/h/m<sup>2</sup>. Overall recovery varies only slightly with the different levels of solution applied. Generally the lower flow rates slow the initial recovery but the long leach period allows for only a slight reduction in the final copper recovery, as shown in Fig. 9. Generally there are low iron levels in all the simulations, any iron in the raffinate is rapidly consumed and ferrous oxidation tends to consume the available acid. Measurable levels of ferric do not appear until after 100 days, see Fig. 10.

The acidity in the raffinate was varied between a pH of 2–0.5, equivalent to varying sulphuric acid content from 0.49 to 15.5 g/l. Generally there is little impact on recovery. The overall pH levels drop with increased raffinate acidity. However, there is a considerable increase in recovery in the early part of the leach period with higher acidity, see Fig. 11. This is due to higher availability of ferric ions, Fig. 12, for reaction due to reduced precipitation. The main acid consumer in this system is the reaction for oxidation of ferrous to ferric ions. Low levels of acidity reduce ferrous oxidation, the most obvious result being the absence of ferric in the PLS until 100 days or later at a pH of 1 or higher.

The head grade can be varied per particle size in the model, but in this simulation was assumed constant over all particle sizes. The copper head grades investigated were 0.3%, 0.8%, 1.0%, 1.5% and 2% chalcocite. The different grades gave considerable variation in recovery rates. This is driven by the availability of the ferric reagent inside the heap, which in turn is driven by regeneration of ferrous that depends on bacteria and acidity. It takes considerably longer for significant acidity to appear in the PLS, see Fig. 13, while leaching higher grades of copper due to its consumption by the oxidation of ferrous. Fig. 14 shows that there is some general improvement in leach behavior with poorer copper grades.



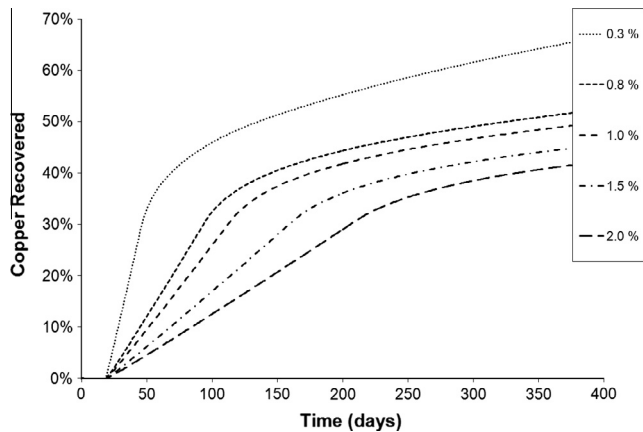


Fig. 14. Copper recovery for a range of ore grades.

The key result of all the simulations is that there is very little overall variation in copper recovery between the different leaching scenarios for the same mineralogy over the time span. What differences there are, tend to occur during the initial leach period. The simulations are all consistent with the analysis of (Bouffard and Flores Godoy, 2007) except that Bouffard and Flores Godoy (2007) recommended that the irrigation rate should be increased to 8 l/m<sup>2</sup>/h whilst the simulation here indicates that overall the recovery is insensitive to the flow rate. However, the available copper will be recovered faster at higher irrigation rates. High flow rates also tend to lead to lower average PLS grades.

## 6. Conclusion

The comprehensive heap leach model has been shown to capture the reactive dissolution kinetics of oxide and sulfide minerals in low grade ores once the model has been parameterized for a particular ore type. The calibration and parameterization of the model is often the most time consuming part of the modeling process, requiring study results from multiple sets of simulations, many simulation runs and an experienced operational modeler. The optimization tool, incorporated into the model, reduces user input enabling automated searching for multiple 'best fit' parameter values. Thus, ore parameter data can be easily generated to allow large scale recovery predictions of multiple materials.

One of the key activities in the simulation based analysis of commercial heaps is a sensitivity analysis to understand which process parameters affect the recovery and to what extent. Such a sensitivity study on characterized and calibrated data can give insight into the effect of operational process changes and, therefore, provide a useful tool for heap operation optimization. The example provided demonstrated a sensitivity analysis investigation performed by the heap leach model and compared the results to a substantial operational analysis by Bouffard and Flores Godoy (2007) for the Zaldivar mine in Chile. The laudable efforts of Bouffard and Flores Godoy demonstrate how challenging such sensitivity analysis is on industrial scale operations. The work reported here may allow ultimately more insightful conclusions to be reached through suitably parameterized and comprehensive simulation studies with heap leach models.

## References

- Bartlett, R.W., 1998. *Solution Mining*, second ed. Gordon & Breach Science Publishers, Amsterdam, The Netherlands, p. 325.
- Bennett, C.R., McBride, D., Cross, M., Gebhardt, J.E., Taylor, D.A., 2006. Simulation technology to support base metal ore heap leaching. *Miner. Process. Extr. Metall. (Trans. Inst. Min. Metall. C)* 115 (1), 41–48.
- Bennett, C.R., McBride, D., Cross, M., Croft, T.N., Gebhardt, J.E., 2008a. Computational modelling of reactive porous media in hydrometallurgy. In: Topping, B.H.V., Papadarakakis, M. (Eds.), *Trends in Engineering Computational Technology*. Saxe-Coburg Publications, pp. 151–171.
- Bennett, C.R., McBride, D., Cross, M., Gebhardt, J.E., 2008b. Computational modelling of reactive multiphase flows in hydrometallurgical processes. *Conference Proceedings, WCCM8 ECCOMAS*.
- Bennett, C.R., Gebhardt, J., McBride, D., Cross, M., 2012a. Sensitivity analysis of heap optimization techniques using a copper sulfide heap leach CFD model. *SME meeting preprints*, Seattle, USA.
- Bennett, C.R., McBride, D., Cross, M., Gebhardt, J.E., 2012b. A comprehensive model for copper sulphide heap leaching: basic formulation and validation through column test simulation. *Hydrometallurgy* 127–128, 150–161.
- Bouffard, S., 2008. Application of the heapsim model to the heap bioleaching of the Pueblo Viejo ore deposit. *Hydrometallurgy* 93 (3–4), 116–123.
- Bouffard, S., Dixon, D., 2009. Modeling pyrite bioleaching in isothermal test columns with the heapsim model. *Hydrometallurgy* 95 (3–4), 215–226.
- Bouffard, S.C., Flores Godoy, D., 2007. The impact of heap operational changes on the copper production at Zaldivar, Cu2007-volume IV (Book 1), The John E. Durrizac International Symposium on Copper Hydrometallurgy 427–438.
- Cariaga, E., Concha, F., Sepulveda, M., 2005. Flow through porous media with applications to heap leaching of copper ores. *Chem. Eng. J.* 111 (2–3), 151–165.
- Cariaga, E., Concha, F., Sepulveda, M., 2007. Convergence of a MFE-FV method for two phase flow with applications to heap leaching of copper ores. *Comput. Methods Appl. Mech. Eng.* 196 (25–28), 2541–2554.
- Croft, N., Pericleous, K.A., Cross, M., 1995. PHYSICA: a multiphysics environment for complex flow processes. In: Taylor, C., Durbetaki, P. (Eds.), *Numerical Methods in Laminar and Turbulent Flow*, 95, 2, pp. 1269–1280.
- Cross, M., Bennett, C.R., Croft, T.N., McBride, D., Gebhardt, J.E., 2006. Computational modeling of reactive multi-phase flows in porous media: applications to metals extraction and environmental recovery processes. *Miner. Eng.* 19, 1098–1108.
- Dixon, D.G., Hendrix, J.L., 1993. A mathematical model for heap leaching of one or more solid reactants from porous ore pellets. *Metall. Trans. B* 24 (6), 1087–1102.
- Gebhardt, J.E., McBride, D., Bennett, C.R., Cross, M., 2012. Considering Gangue and Precipitation Reactions within a Copper Heap Leach CFD Model. *IMPC*, New Delhi, India.
- Leahy, M.J., Davidson, M.R., Schwarz, M.P., 2005. A model for heap bioleaching of chalcocite with heat balance: Bacterial temperature dependence. *Miner. Eng.* 18, 1239–1252.
- Leahy, M.J., Schwarz, M.P., Davidson, M.R., 2006. An air sparging CFD model of heap bioleaching of chalcocite. *Appl. Math. Modell.* 30, 1428–1444.
- Leahy, M.J., Davidson, M.R., Schwarz, M.P., 2007. A model for heap bioleaching of chalcocite with heat balance: mesophiles and moderate thermophiles. *Hydrometallurgy* 85, 24–41.
- Leahy, M.J., Schwarz, M.P., 2009. Modelling jarosite precipitation in isothermal chalcocite bioleaching columns. *Hydrometallurgy* 98, 181–191.
- McBride, D., Cross, M., Croft, T.N., Bennett, C.R., Gebhardt, J.E., 2006. Computational modelling of variably saturated flow in porous media with complex three-dimensional geometries. *Int. J. Numer. Methods Fluids* 50, 1085–1117.
- McBride, D., Cross, M., Gebhardt, J.E., 2012a. 'Heap leach modelling employing CFD technology: a 'process' heap model. *Miner. Eng.* 33, 72–79.
- McBride, D., Gebhardt, J.E., Cross, M., 2012b. A comprehensive oxide heap-leach model: development and validation. *Hydrometallurgy* 113–114, 98–108.
- Mellado, M.E., Cisternas, L.A., 2008. An analytical-numerical method for solving a heap leaching problem of one or more solid reactants from porous pellets. *Comput. Chem. Eng.* 32, 2395–2402.
- Mellado, M.E., Casanova, M.P., Cisternas, L.A., Gálvez, E.D., 2011a. On scalable analytical models for heap leaching. *Comput. Chem. Eng.* 35, 220–225.
- Mellado, M.E., Gálvez, E.D., Cisternas, L.A., 2011b. On the optimization of flow rates on copper heap leaching operations. *Int. J. Miner. Process.* 101, 75–80.
- Mellado, M.E., Gálvez, E.D., Cisternas, L.A., 2012. Stochastic analysis of heap leaching process via analytical models, stochastic analysis of heap leaching process via analytical models. *Miner. Eng.* 33, 93–98.
- Petersen, J., Dixon, D.G., 2007. Modeling and optimization of heap bioleach processes. In: Rawlings, D.E., Johnson, D.B. (Eds.), *Biomining*. Springer, Berlin, pp. 153–175.
- Petersen, J., 2010. Modelling of bioleach processes: connection between science and engineering. *Hydrometallurgy* 104, 404–409.