Bioleaching Model of a Copper-Sulfide Ore Bed in Heap and Dump Configurations

J.M. CASAS, J. MARTINEZ, L. MORENO, and T. VARGAS

A two-dimensional (2-D) model for a heap or dump bioleaching of a copper ore containing mainly chalcocite and pyrite has been developed. The rate of the mineral sulfide dissolution was related to the rate of oxidation by bacteria attached onto the ore surface. The latter was calculated using the model of Michaelis–Menten, where both temperature and dissolved oxygen in the leach solution were taken into account by the kinetic equation. Oxygen transport through the ore bed was associated with natural air convection originating from the decrease in gas density inside the ore bed, which was attributable not only to heating, but also to humidification and decrease in the oxygen concentration. The model was used to estimate air-velocity fields and profiles of temperature and oxygen concentrations as well as mineral conversions during the bioleaching operation for ore beds with different pyrite contents, bacterial populations, widths, heights, and permeabilities. The model provides a useful tool for the design, improvement, and optimization of industrial operating conditions.

I. INTRODUCTION

COPPER ores usually contain a mixture of oxide and sulfide minerals. Oxide minerals are solubilized by acid solutions, whereas sulfide minerals are solubilized only under oxidizing conditions. In the latter case, the acidophilic microorganisms, such as the bacterium *Thiobacillus ferrooxidans*, play a crucial role in the sulfur and ferrous-sulfate oxidation by generating the oxidizing environment for mineral leaching.[19,24,29] Bacterial leaching of an ore bed is a complex process that involves at least the following phenomena:[4,11,13,16,26,29]

(a) reactions of mineral species with sulfuric acid, ferric ions, and dissolved oxygen;
(b) hydrolysis and precipitation of complex compounds in solution, which mainly involves ferric-ion species;
(c) transport, attachment, growth, and catalytic actions of microorganisms;
(d) transport of aqueous species inside the ore particles;
(e) transport of oxygen and water through the bed, with an air supply to the bed by natural convection and diffusion; and
(f) heating and cooling of the bed, associated with exothermic and endothermic reactions and heat transfer to the environment.

In order to assess the importance of these phenomena on the overall performance of the operation, it is necessary to take into account the specific characteristics of the ore to be processed, the environmental conditions, and the geometry of the ore bed. The development of bioleaching operations involves very expensive and extensive testing and scale-up activities.[4,11,16,19,24,29] In this context, the development of computational models can be very useful, as they aid the design and operation of bacterial leaching processes on a scientific basis.

Modeling of the leaching of copper-sulfide ores in heaps and dumps has received considerable attention in recent years. In some models, the kinetics of ore leaching are described using the shrinking-core model.[5,7,8,14,21] In general, these models consider chemical oxidation by oxygen or ferric ions, and mixed kinetics where both pore diffusion through the ore particles and chemical reaction at the mineral surfaces are the controlling leaching phenomena.

Other models introduce a more explicit phenomenological description of the bacterial action and growth phenomena involved.[12,17,26] In the process, bacteria that are either attached to the ore or free in solution catalyze the oxidation of ferrous ions to ferric ions. Most of the leaching of sulfide minerals within ore fragments occurs by oxidation with ferric ions. These models are not directly applicable to bioleaching of an ore bed because they ignore macroscale air transport. In fact, the oxygen supply necessary for bacterial growth and mineral sulfide oxidation can be the rate-controlling factor in the bioleaching of heaps or dumps.

Bioleaching models that consider macroscopic heat and air transport within the ore bed have been developed by Cathles and Schlitt[13] and by Pantellis and Ritchie.[27] The gas transport through the ore bed involves both convection and diffusion. The simulations[13,27] showed that when the ore-bed permeabilities are too low, the oxygen supply occurs mainly through air diffusion inside the bed. Under these circumstances, bacterial leaching of the sulfide minerals is too slow because it is limited by the slow supply of oxygen. When the bed permeability is higher, air convection is the predominant mechanism for oxygen supply inside the bed, and consequently the rate of mineral oxidation by bacteria can be improved. In the case of bioleaching of well-aerated dumps containing reactive species like pyrite, temperatures can even reach the boiling point of water.[27]

Several aspects of two-dimensional (2-D) models describing macroscopic transport phenomena occurring in dump- and heap-bioleaching processes need further consideration. For instance, bacterial catalytic activity has

J.M. CASAS, Académico, and T. VARGAS, Associate Professor, are with the Departamento de Ingerniería Química, Unversidad de Chile, Beauchef 861, Santiago, Chile. J. MARTINEZ, Assistant Professor, and L. MORENO, Associate Professor, are with the Department of Chemical Engineering and Technology, Royal Institute of Technology, S-10044 Stockholm, Sweden.

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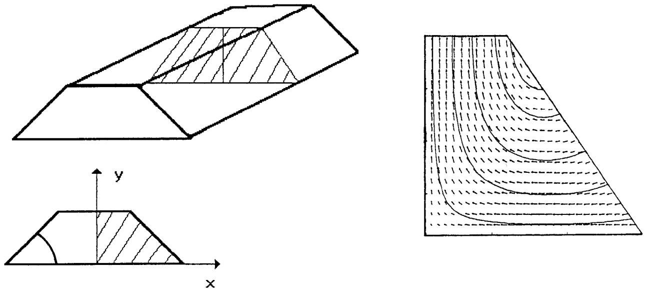

Fig. 1—Cross section of an ore bed used as domain for the calculations. The semi-trapezium picture shows the calculated streamlines for gas transport and the gas velocity field developed through the ore bed.

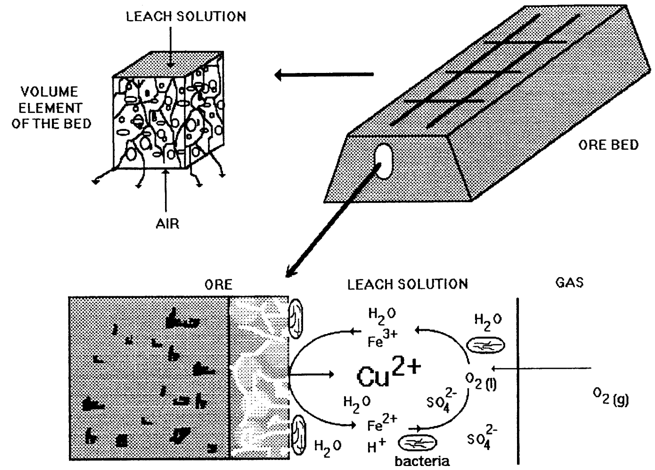

Fig. 2—Bioleaching model of the ore bed. The main steps are both transport phenomena and chemical reactions.

been simply described as a switch that triggers ferrous oxidation when the bed is within a certain temperature range. It is well known that under specific conditions, the bioleaching in heaps or dumps can be determined by the bacterial population in the ore bed, particularly in the initial stages of the operation. In order to detect and to evaluate these situations, a more explicit description of the bacterial activity and its relation to the operating conditions should be included.

In this work, a 2-D model for bioleaching in ore beds is presented. In the model, the activity of the microorganisms is described in an explicit form using the model of Michaelis–Menten.[29] The model also incorporates a more detailed description of the effective bed permeability of the gas phase by introducing a relative gas permeability as a function of the liquid content in the ore bed, which depends on the irrigation rate of the leach solution.

The model was applied in order to analyze the effect of bacterial activity and geometry on the global performance of bioleaching beds and the dependence of the irrigation flow on bed aeration efficiency.

II. MODEL FORMULATION

A. *General Aspects*

The model proposed describes the bioleaching of an ore bed containing the reactive mineral species chalcocite and pyrite, plus inert gangue. The bacterium *Thiobacillus ferrooxidans* is the only microorganism considered. These bacteria live in mining environments at temperatures between 10 °C and 40 °C and at pH values between 1.5 and 3.5.[24,29]

The configuration analyzed consists of an ore heap or dump that is irrigated on the top and on the slope with a dilute solution of sulfuric acid. The solution percolates through the ore particles and dissolves the minerals. The interparticle space in the bed is filled by both liquid and gas phases. In this system, air flows by both diffusion and natural convection promoted by oxygen concentration and air-density gradients, respectively. Two-dimensional geometry is considered (Figure 1).

The model considers the processes occurring in an ore bed when the oxidation of the copper sulfide is controlled by the activity of the bacteria. This means that the transport of the ferric ions in the particles is sufficiently fast. This assumption is valid, of course, at the initial period when the gangue layer depleted of copper is small. However, it is also valid in other situations; for example, if the particle size is small, if the gangue is sufficiently porous, and if the copper minerals are located in veins that may be reached by the ferric ions directly from the surface. This will be discussed in more detail in the following Section B. If this assumption is satisfied, the leaching rate does not change with time, as long as these conditions are maintained. Therefore, the mathematical model can be formulated for the steady state.

In most of the practical situations, the permeability of the bed varies at the different locations. Dumping procedures result in a segregation of fine material at the top and coarse material at the bottom. However, the model is solved for a permeability that is the same over the whole ore bed because of the lack of detailed data about how the permeability varies inside of the bed. To include the variation of permeability, the equation of flow would be modified in a manner indicated by Stanek and Szekely.[31]

The model considers a constant number of bacteria homogeneously distributed through the bed. Actually, the population of bacteria is dependent on the access of oxygen, nutrients, and temperature, and even on competition between different microorganisms. A constant number of bacteria is assumed anywhere in the ore bed, since the dependence of the number of bacteria on these parameters is not well known. If a function that links the number of bacteria with temperature and oxygen concentration could be obtained the inclusion in the model would be straightforward.

Variations of permeability of the bed and the number of bacteria with time are not considered in the model, since the model is formulated for the steady state.

B. *Ore Balance and Reaction Rate*

The main steps involved in the leaching of a sulfide mineral particle under bacterial action are represented in Figure 2. Mineral sulfides are oxidized and dissolved by ferric ions present in the leaching solution according to the following:

$$MS + 2Fe^{3+} \longrightarrow M^{2+} + 2Fe^{2+} + S \quad \text{(chemical)}$$

where M represents the metal of interest, either copper or iron.

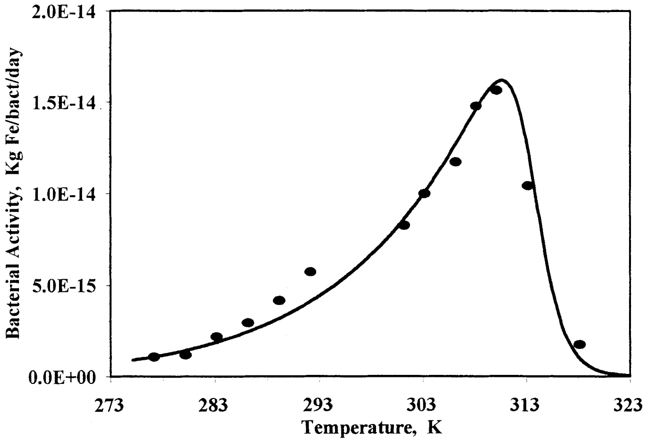

Fig. 3—Temperature effect on the *T. ferrooxidans* activity at pH = 2, K_m = 1 ppm, and O_{2L} = 6.5 ppm.[1,2,10,20]

This reaction produces ferrous ions, which are continuously reoxidized to ferric ions under the catalytic action of the bacteria present either in the solution or attached to the ore, according to the following:

$$2Fe^{2+} + 0.5O_2 + 2H^+ \longrightarrow 2Fe^{3+} + H_2O \quad \text{(bacterial)}$$

This coupled reaction system is sustained if there is an adequate oxygen transfer to the leach solution from the air surrounding the particles.

Models for bioleaching in heaps and dumps have usually described the leaching rate assuming that the global kinetics are controlled by the rate of particle dissolution, which is commonly described in terms of the unreacted core model.[5,7,8,14,21] However, in the bioleaching of sulfide ores by the irrigation of packed ore beds, there are situations in which the leaching rate is controlled by bacterial activity. In fact, bioleaching starts with a low initial bacterial population corresponding to the microflora naturally present in the ore. As the process continues, some bacterial progeny are released into the solution and continuously removed from the bed. The bacteria present in the ore bed are then either attached to the ore or present in the static retained liquid.[15,18,22]

In order to determine under which conditions the process will be controlled by the number of bacteria present, the transport of ferric ions through the reacted part of the ore particle for different thicknesses was calculated. These values, expressed as the oxygen consumption rate, were compared with the oxygen consumption rate of different bacterial populations attached to the ore surface. The results showed that for a maximum population of 10^{11} bacteria/m^2, the dissolution of the mineral is controlled by the bacterial activity for a particle less than 2 cm in diameter. In this estimation, an effective diffusion coefficient for the ferric ions of 5×10^{-11} m^2/s and a Michaelis–Menten behavior for bacterial activity[29] were assumed. A bacterial population of 10^{11} bacteria/m^2 of ore (about 10^{10} bacteria/kg of ore) is a high value, which is observed in oxygenated surface layers of the ore beds.[6,18,19] Therefore, we can expect that the model is valid for particle sizes of several centimeters. For beds with large particles, the model is valid at the initial period. When the reaction has reached several centimeters into the particle, the process is controlled by diffusion and the model is not valid.

When the bacterial activity is the controlling factor, the rate of copper-sulfide dissolution is determined at the particle level by the rate of bacterial generation of ferric ions, and can be expressed in terms of the Michaelis–Menten equation.[29] However, since in this situation ferrous ions are always present in excess, it is better to express the oxidation rate in terms of a modified equation that considers oxygen to be the limiting substrate. This approach also allows one to associate the microphenomena related to the copper dissolution rate at the particle level with the oxygen transport through large beds. Accordingly, the rate of copper-sulfide dissolution is expressed in this model as follows:

$$\frac{d\alpha}{dt} = \frac{\sigma_1}{\rho_B\, G^o} X V_m \left(\frac{C_L}{K_m + C_L}\right) \qquad [1]$$

where σ_1 is the stoichiometric factor, estimated according to the following dissolution stoichiometries:

Chalcocite: $Cu_2S + 2.5O_2 + H_2SO_4 \rightarrow 2CuSO_4 + H_2O$
Pyrite: $FeS_2 + 3.5O_2 + H_2O \rightarrow FeSO_4 + H_2SO_4$

These stoichiometries describe the global reactions resulting from the chemical leaching of chalcocite and pyrite with ferric ions and the bacterial oxidation of residual sulfur and ferrous ions.

According to these reactions, the stoichiometric factor σ_1 can be expressed as follows:

$$\sigma_1 = \frac{M_{\text{Ch}} M_{\text{Py}}}{5/2\, M_{\text{Ox}}\, M_{\text{Py}} + 7/2\, (\text{FPY})\, M_{\text{Ox}}\, M_{\text{Ch}}} \qquad [2]$$

where M is the molecular weight and FPY is the ratio of the mass of pyrite leached to the mass of chalcocite leached. The dissolved oxygen concentration is assumed to be in local equilibrium with the oxygen concentration in the gas phase and was calculated using Henry's law.[28] The relationship between the maximum specific respiration rate of the bacteria, (V_m), and the temperature was obtained by fitting a model equation[3] to experimental data[1,2,10,20] for ferrous oxidation by *T. ferrooxidans* as follows:

$$V_m = \frac{6.8 \times 10^{-13}\, T \exp\left(-\dfrac{7000}{T}\right)}{1 + \exp\left(236 - \dfrac{74000}{T}\right)} \qquad [3]$$

In fact, the general temperature dependence of the specific respiration rate is unknown, because in real ore beds there are frequently a number of different microorganisms that are active depending on the temperature.[29] In Figure 3, experimental and calculated values of *T. ferrooxidans* activity at different temperatures are shown. These data will be used in the simulations.

C. *Gas Flow*

The velocity of gas through the bed is described by Darcy's law:

$$\varepsilon_g \mathbf{v_g} = \mathbf{q_g} = -\frac{K\, k_{rg}}{\mu_g} \left(\nabla P - \rho_g \mathbf{g}\right) \qquad [4]$$

The gas movement inside the bed is driven by natural convection originating in the decrease in the gas density, which was attributable to heating, humidification, and oxygen consumption. The gas-flow distribution within the bed may be described by the stream function (Ψ), which is defined as follows:

$$q_x = -\frac{\partial \Psi}{\partial y}, \quad q_y = \frac{\partial \Psi}{\partial x} \qquad [5]$$

Combining Eqs. [4] and [5] (refer to the Appendix for details) allows one to obtain the following equation for determining the streamlines as a function of the gas density variations inside the bed:

$$g K k_{rg} \frac{\partial \rho_g}{\partial x} = -\mu_g \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} \right) \qquad [6]$$

D. *Mass Balance of Gaseous Oxygen*

The oxygen balance includes the transport by molecular diffusion, bulk transport due to natural convection of air, and the rate of oxygen consumption, as follows:

$$\varepsilon_g D_g \left(\frac{\partial^2 C_g}{\partial x^2} + \frac{\partial^2 C_g}{\partial y^2} \right) - \varepsilon_g \left(\frac{\partial (v_g C_g)}{\partial x} + \frac{\partial (v_g C_g)}{\partial y} \right) = \frac{\rho_B G^o}{\sigma_1} \frac{d\alpha}{dt} \qquad [7]$$

E. *Energy Balance*

There are several mechanisms by which heat may be transferred in the bed. The most important are the transport by the downward liquid flow, the gas flow through the bed, including the effect of water evaporation, and the heat generated by the leaching reactions. Local thermal equilibrium between solid, liquid, and gas phases is assumed. Furthermore, only vertical liquid movement is taken into account in the system. Considering these assumptions, the equation for the energy balance of the bed may be written as follows:

$$k_B \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) - \frac{\partial h_L}{\partial y} - \left(\frac{\partial h_g}{\partial x} + \frac{\partial h_g}{\partial y} \right) = (-\Delta H_R) \frac{\rho_B G^o}{\sigma_1} \frac{d\alpha}{dt} \qquad [8]$$

where h represents the enthalpy flow per unit area ($h_g = G[-\lambda H_{\text{air}} + \{Cp_g + Cp_v H_{\text{air}}\} \{T - T_{\text{ref}}\}]$; $h_L = -q_L \rho_L Cp_L [T - T_{\text{ref}}]$) and ΔH_R represents the mean reaction enthalpy ($\Delta H_R = \Delta H_{\text{Ch}} + FPY \cdot \Delta H_{\text{Py}}$). The terms on the left-hand side of Eq. [8] are the conductive and convective heat transports and the term on the right-hand side is the heat generated by the reactions.

F. *Boundary Conditions*

It is assumed that the ore bed rests on an insulating and impermeable ground surface. Along the central axis of bed, no transverse flows of air, heat, and liquid are assumed because of symmetry conditions. At the top and on the slopes, air flows freely into or out of the bed with a given temperature and oxygen concentration.

At the bottom, where $y = 0$, the following holds:

$$\Psi = 1 \text{ (constant value of the stream function)} \qquad [9]$$

$$\frac{\partial C_g}{\partial y} = \frac{\partial T}{\partial y} = 0 \text{ (no flux of oxygen or heat across the bottom boundary)} \qquad [10]$$

At the center, where $x = 0$, the following holds:

$$\Psi = 1 \text{ (constant value of the stream function)} \qquad [11]$$

$$\frac{\partial C_g}{\partial x} = \frac{\partial T}{\partial x} = 0 \text{ (no flux of oxygen or heat across the center boundary)} \qquad [12]$$

At the top, where $y = H$, and on the sloped surface, the following holds:

$$\frac{\partial \Psi}{\partial n} = 0 \text{ (gas velocity perpendicular to the surface)} \qquad [13]$$

$$T = T_L,\ C_g = C_{\text{air}} \text{ (constant temperature and oxygen concentration)} \qquad [14]$$

G. *Transport and Thermodynamics Properties*

The porosity occupied by the gas and the relative gas permeability were calculated as a function of water content in the ore bed. A constant permeability and a steady liquid irrigation flow were assumed and the following equations were used:[32]

$$q_L = \frac{K g \rho_L}{\mu_L} \left(S_{ef} \right)^4 \qquad [15]$$

$$\varepsilon_g = 1 - \varepsilon_s - \phi S_w \qquad [16]$$

$$k_{rg} = \left(1 - S_{ef}^2 \right) \left(1 - S_{ef} \right)^2 \qquad [17]$$

where S_{ef} is the effective liquid saturation ($S_{ef} = [S_w - S_{wr}]/[1 - S_{wr}]$) and S_w is the liquid content ($S_w = \varepsilon_w / \phi$).

The rate of pyrite dissolution is related to the rate of chalcocite dissolution through the FPY parameter, defined here as the ratio of the mass of pyrite leached to the mass of chalcocite leached. Thus, if FPY increases, the total heat generated by chemical reactions (ΔH_R) increases and the stoichiometric factor (σ_1) decreases, indicating that a smaller fraction of oxygen is consumed in the chalcocite reaction.

Figure 4 shows the chalcocite conversion vs time for different pyrite contents in the ore. The calculations were made using Eq. [1] and the bacterial population that reproduces the mineral-leaching kinetics under ideal conditions. These values were taken from literature.[6,9] The chalcocite conversion decreases when the pyrite content increases, indicating that a smaller fraction of oxygen is consumed by the chalcocite oxidation in competition with the pyrite oxidation.

The air humidity was calculated considering that the air in the bed is saturated with water. The water pressure was obtained using the Antoine equation[28] ($H_{\text{air}} = [M_w / M_{\text{air}}] \cdot P^{\text{sat}} / [P - P^{\text{sat}}]$; $\log [P^{\text{sat}}] = 8.07 - 1730/[T - 39.75]$; P^{sat} is given in mm Hg). Henry's constant was obtained as a function of the temperature using the oxygen solubility in the

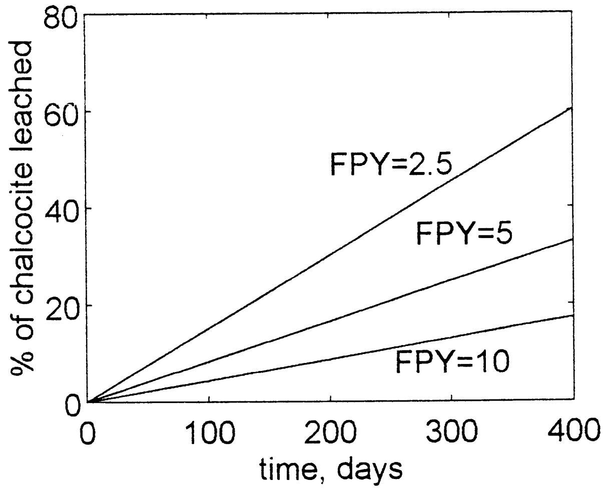

Fig. 4—Chalcocite conversion *vs* time for different pyrite contents in the ore. These kinetic predictions were made using the simulation parameters indicated in Table I.

leach solution at different temperatures[18,28] ($C_L = C_g{\cdot}He$; $He = 21.312 + 0.784 \times T - 0.00383 \times T^2$; T is given in °C).

H. *Numerical Solution*

The mathematical model represented by the aforementioned equations was transformed into a set of dimensionless equations and then discretized using the integrated finite-difference methodology.[25] The resulting algebraic equation system is nonlinear and was solved with the successive over-relaxation iterative method,[30] using a personal computer.

A computational code was developed to solve the model equations by an iterative algorithm. At the first step, a distribution of gas densities was assumed and Eqs. [5] and [6] were solved to obtain an estimation of the stream function and the air velocities through the ore bed.

Then, Eqs. [7] and [8] were solved to obtain the oxygen concentration and the temperature profiles, respectively. Finally, the gas density was recalculated using the calculated values of temperature and oxygen concentration, and Eqs. [5] and [6] were solved again to obtain new values of the stream function and the air velocities. The process was repeated to reach the desired convergence.

III. RESULTS AND DISCUSSION

The model was used to describe the bioleaching of an ore bed containing chalcocite (0.63 wt pct) and pyrite (3 wt pct) as the main mineral species. The model was solved assuming that bacterial population, irrigation flow rate, and both environmental temperature and pressure were constant throughout the bioleaching process. The specific parameters used in the simulations were estimated from literature sources and are listed in Table I.

As a first stage, simulations were made for different bed sizes, using the values of bacterial population, ore-bed permeability, and irrigation flow (Table II). For each case, air-velocity distribution, oxygen concentration, temperature, and chalcocite conversion profiles inside the bed were obtained.

Table I. Model Parameters Used for the Simulation of the Bioleaching Operation in an Ore Bed

Parameter	Unit	Value
Average density[21]	kg/m^3	$\rho_{air} = 1.16$
		$\rho_L = 1050$
		$\rho_s = 2700$
		$\rho_B = 1800$
Average specific heat[21]	kJ/kg/K	$Cp_g = 1.0$
		$Cp_L = 4.0$
		$Cp_s = 1.172$
		$Cp_v = 1.864$
Average viscosity[21]	kg/m/s	$\mu_g = 1.85 \times 10^{-5}$
		$\mu_L = 9 \times 10^{-4}$
Bed density[4]	kg/m^3	$\rho_B = 1800$
Bed porosity[4]	m^3/m^3	$\phi = 0.3$
Chalcocite reaction enthalpy[6]	kJ/kg	$\Delta H_{Ch} = -6000$
Diffusion coefficient for the oxygen in gas phase[20]	m^2/s	$D_g = 1.5 \times 10^{-5}$
Heat of water vaporization[21]	kJ/kg	$\lambda = 583$
Irreducible liquid content[4]	m^3/m^3	$S_{wr} = 0.27$
Michaelis constant[15]	kg/m^3	$K_m = 10^{-3}$
Pyrite reaction enthalpy[6]	kJ/kg	$\Delta H_{Py} = -12{,}600$
Thermal conductivity of the bed[6]	kJ/m/K/s	$k_B = 2.1 \times 10^{-3}$
Volumetric liquid fraction[4]	m^3/m^3	$\varepsilon_L = 0.12$

In the second stage, the influence of bacterial population, bed permeability, and irrigation flow rate on the profiles obtained in the first stage was studied for the specific case of an ore bed with a height of 10 m and a base width of 30 m.

A. *Air Flow Inside the Ore Bed*

Air-velocity distributions for the case of a 10-m-high ore bed are shown in Figure 5, which includes both a contour plot for the stream function and the gas-velocity field represented as vectors. Gas convects along the streamlines, and the closer the streamlines in the diagram, the faster the gas flows. According to Figure 5, the air gets into the bed through the slope of the bed and exits on the flat top. The lowest air-flow rates occur in the central part of the bed, where air flows mainly in the vertical direction. The highest air-flow rates are reached under the bed slope and closer to the bottom. Air-flow rates in the center of the bed range from 3×10^{-5} m^3/m^2/s at the top to 3×10^{-6} m^3/m^2/s at the bottom. The air-flow rate in the slope region reaches up to 4×10^{-5} m^3/m^2/s.

Significant changes in the air distribution pattern result from an increase in the size of the bed. Simulations performed with large ore beds indicate that not all the air sucked through the slope leaves it through the flat top. In fact, an important fraction of the inflow air leaves on the upper region of the slope. The central zone, in which air flows vertically and at a slow rate, is consequently much larger.

B. *Profiles Inside the Ore Bed*

The calculated distributions of stream function, relative oxygen concentration, temperature, and chalcocite conver-

Table II. Model Variables Used for the Simulation of the Bioleaching Operation in an Ore Bed

Variable	Unit	Value
Atmospheric temperature	K	$T = 298$
Atmospheric pressure	kPa	$P = 101$
Bacterial population	number of bacteria/m^3	$X = 5 \times 10^{13}$
Bed permeability[20]	m^2	$K = 5 \times 10^{-10}$
Copper grade	wt pct	$G_{Cu} = 0.5$
Pyrite factor	kg pyrite leached/kg chalcocite leached	FPY = 5
Liquid temperature	K	$T_L = 298$
Liquid flow density rate[4]	m^3/m^2/s	$q_L = 1.4 \times 10^{-6}$
Oxygen concentration (at 298 K and 101 kPa)	kg/m^3	$O_{2_g} = 0.26$

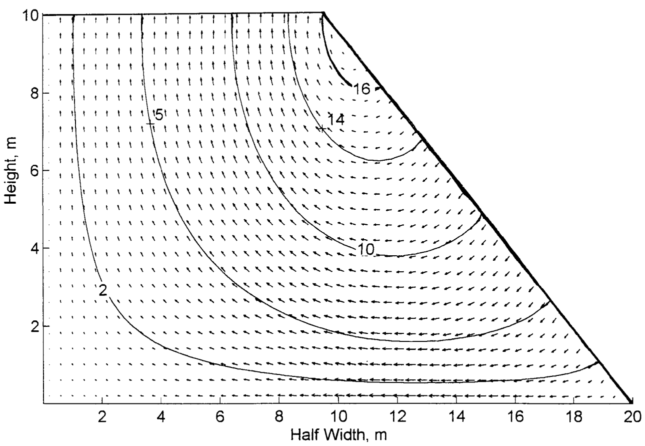

Fig. 5—Contour plot for the stream function and air velocity field calculated in an ore bed with a height of 10 m and a base half-width of 20 m. The simulation parameters are indicated in Table I.

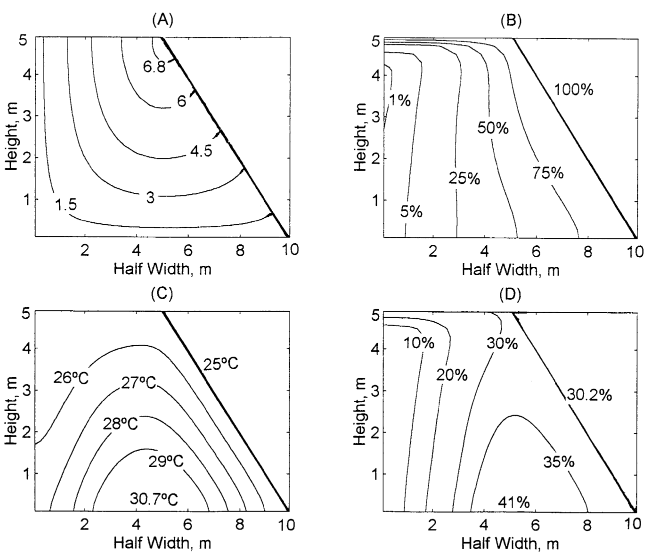

Fig. 6—Contour plot for (*a*) stream function, (*b*) relative concentration of gaseous oxygen ($C \times 100/C_{AIR}$), (*c*) temperature, and (*d*) chalcocite conversion at 1 year in an ore bed with a height of 5 m and base half-width of 10 m. The simulation parameters are indicated in Table I.

sion for bioleaching of a bed with a height of 5 m are presented in Figure 6. The oxygen concentration is expressed as a percentage with respect to the atmospheric oxygen concentration. The mineral conversion is presented at 1 year of operation.

The resulting oxygen-concentration profile is linked to the air convection patterns combined with oxygen diffusion at the top. A minimum in the oxygen concentration is found at an intermediate height in the central zone of the bed (Figure 6(b)). At this point, the oxygen is practically depleted from the convective air flow. The oxygen concentration increases above this zone, due mainly to direct oxygen diffusion from the atmosphere. It is observed that in this small bed, there is no anoxic zone and mineral sulfide oxidation proceeds throughout the whole bed, although at different oxidation rates.

In general, the temperature inside the bed increases with increasing depth, because the leaching solution accumulates the thermal energy liberated by oxidation reactions as it flows downward. The highest temperature zone is located at the bottom, approximately 5 m from the center, where a large liquid flow path with an adequate oxygen supply is found. The reduction in temperature of the ore located under the bed slope with increasing horizontal distance from the hot zone is attributed to the shorter liquid flow paths under the slope zone. However, the reduction in temperature in the central zone with decreasing horizontal distance from the center is associated with the decrease in oxygen availability, which leads to a reduction in the heat generated. In this case, the maximum temperature increase in the bed was 5.7 °C above the temperature of the bed surface. This relatively small temperature increment is attributable to a heat-generation rate, which is small compared with the heat removed by the percolating solution.

The degree of chalcocite conversion in the bed is determined by a combination of the availability of oxygen and the temperature distribution. The position of the zone with the highest conversion is determined mainly by the temperature profiles established in the bed and is displaced only slightly to the right of the highest temperature spot (Figure 6(c)). Under the flat irrigation zone, close to the bed center, the conversion is small and is mainly determined by the reduction in oxygen availability. Under the slope, the conversion is slightly smaller than the maximum value, mainly because of the lower temperature (Figure 6(c)).

C. *Influence of the Ore-Bed Geometry*

The influence of the bed size on the bioleaching behavior in beds can be observed by comparing the results in Figure 6 of oxygen, temperature, and conversion profiles with the profiles obtained in Figures 7 and 8 for 10- and 20-m-high beds, respectively.

It is observed that in the 10-m-high bed, there is an inner central part of the bed where there is no oxygen and there-

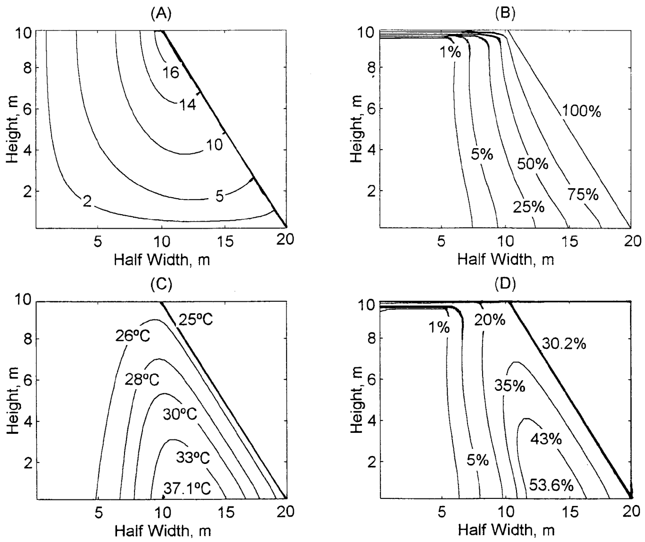

Fig. 7—Contour plot for (*a*) stream function, (*b*) relative concentration of gaseous oxygen ($C \times 100/C_{AIR}$), (*c*) temperature, and (*d*) chalcocite conversion at 1 year in an ore bed with a height of 10 m and a base half-width of 20 m. The other parameters are as in Fig. 5.

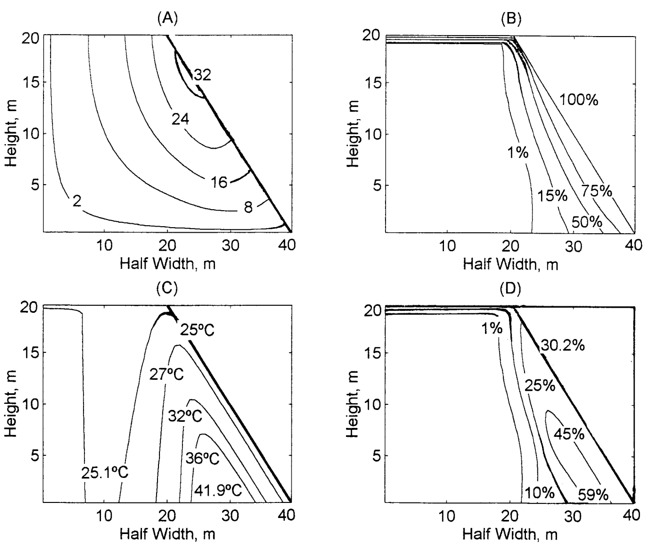

Fig. 8—Contour plot for (*a*) stream function, (*b*) relative concentration of gaseous oxygen ($C \times 100/C_{AIR}$), (*c*) temperature, and (*d*) chalcocite conversion at 1 year in an ore bed with a height of 20 m and a base half-width of 40 m. The other parameters are as in Fig. 5.

fore no reaction. The size of this zone increases with increasing height of the bed, and in the case of the 20-m-high bed, this zone corresponds to more than 50 pct of the bed volume. In fact, in these large beds, bioleaching occurs mainly in the ore that is located under the slope. This indicates that even though the air flow reaches the inner zones, oxygen is depleted by bacterial action before it reaches the inner zones of the bed.

The temperature of the hot zone increases with an increasing bed height: 30.7 °C for 5 m, 37.1 °C for 10 m, and 41.9 °C for 20 m. This is because in the larger beds, the leach solution follows a longer path, experiences a greater temperature increase, and transfers some heat to the ore below. The distance from the hot zone to the slope surface increases with increasing bed height, from 5 m in

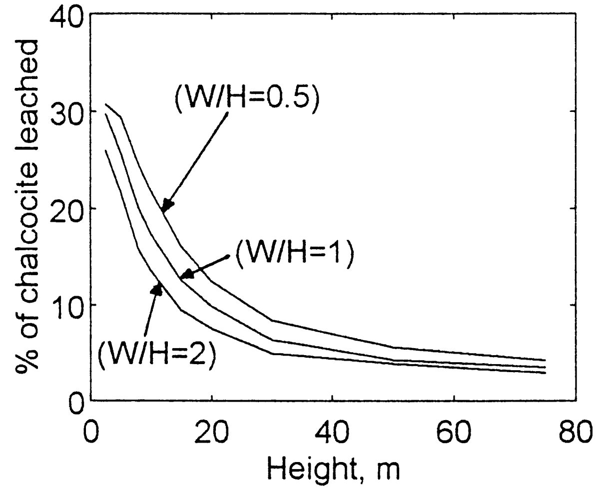

Fig. 9—Chalcocite conversion reached in 1 year averaged over the whole volume of the ore bed *vs* height, for different width/height ratios (W/H). The other parameters are as in Fig. 5.

the 5-m-high dump to 8 m in the 10-m-high dump and 12 m in the 20-m-high dump. This displacement is also related to the increase in the leaching solution path flow. However, this distance will not necessarily continuously increase in higher beds because the depletion of oxygen in the incoming air will eventually play a limiting role in the generation of heat from exothermic reactions.

In the three bed sizes, the conversion profiles are closely related to the temperature profiles established. Accordingly, the conversion reached in the hot zone after 1 year of bioleaching increases with increasing bed height, from 41 pct in the 5-m-high ore bed, to 53.6 pct in the 10-m-high ore bed, and to 59 pct in the 20-m-high ore bed. However, as the increase in the bed height also results in an increase in the size of the oxygen-depleted zone, the average conversion decreases with increasing bed size. Figure 9 shows the influence of bed height on the conversion reached in 1 year, averaged over the whole bed volume.

For a given bed height, the size of the oxygen-depleted zone also increases with increasing width and this leads to a reduction in the average conversion. Figure 9 shows the influence of an increasing bed width on the conversion reached in 1 year, averaged over the whole volume of the ore bed.

D. *Influence of Bacterial Population*

Figure 10 shows the extent of chalcocite conversion reached in 1 year, averaged over the whole bed volume, in a bed with a height of 10 m and a base width of 30 m, for different populations of bacteria. There is a zone with less than 2×10^{13} bacteria/m^3, in which the conversion is directly proportional to the bacterial population. This behavior indicates that in this range, the bioleaching rate is controlled by the oxidative activity of the bacteria. For populations over 2×10^{13} bacteria/m^3, the conversion increases are smaller and continuously decay with increasing bacterial population.

The reasons behind this behavior can be explained by examining Figure 11. Curve (a) in Figure 11 shows the oxygen consumption as a function of the bacterial population, calculated from Eq. [1]. This curve represents the ox-

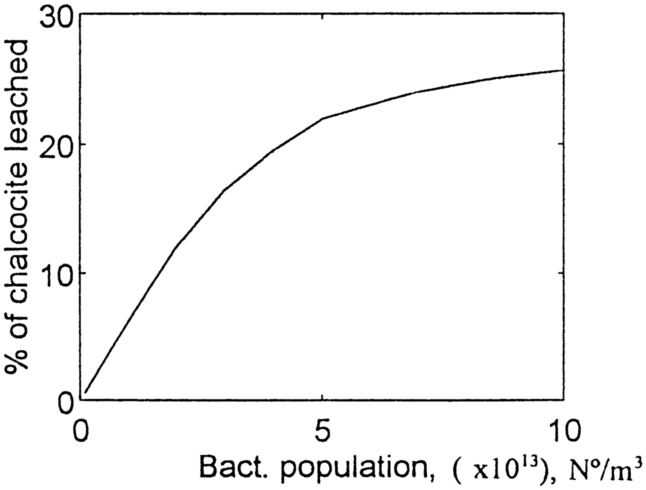

Fig. 10—Chalcocite conversion reached in 1 year averaged over the whole volume of the bed *vs* bacterial population. Parameters: height = 10 m, base half-width 15 m, and the other parameters are as in Fig. 5.

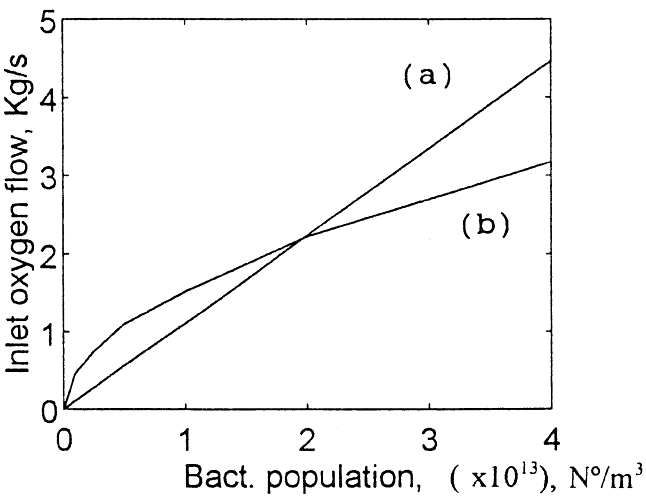

Fig. 11—Inlet oxygen flow *vs* bacterial population in the ore bed. Curve (*a*) represents the oxygen consumption in the ore bed for the case of full availability of oxygen in the system, and curve (*b*) represents the convective flow of oxygen into the ore bed. The other parameters are as in Fig. 10.

ygen consumption when there is full availability of oxygen in the bed (21 pct of oxygen). Curve (b) represents the flow of oxygen that convects, as part of the air, into the bed as a function of the bacterial population. In fact, in this system, the chimney effect, which moves air into the ore bed, increases with increasing bacterial population, because the bioleaching reactions induce density changes inside the bed by both oxygen consumption and heating.

The chimney effect associated with a certain bacterial population, in the range of 0 to 2 × 10^{13} bacteria/m^3, pulls into the bed a flow of oxygen greater than the amount these microorganisms require for oxidation. This is why the conversion is directly linked to the amount of bacteria present in the ore. However, when the population is greater than 2 × 10^{13} bacteria/m^3, the maximum oxidative bacterial oxygen demand is larger than the oxygen flow driven into the bed. Therefore, once a limiting bacterial population is reached, the conversion does not increase directly with further increases in the population; instead, the conversion follows the convective air flow (curve (b) in Figure 11).

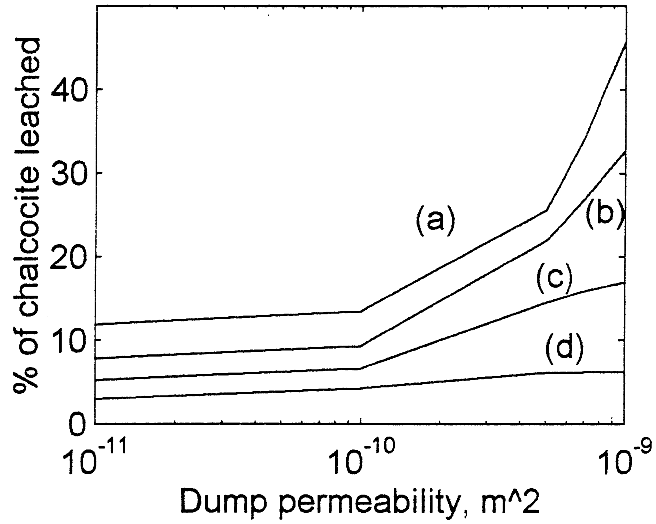

Fig. 12—Chalcocite conversion reached in 1 year averaged over the whole volume of the ore bed *vs* the ore bed permeability, for different bacterial populations: (*a*) =10^{14}, (*b*) =5 × 10^{13}, (*c*) =2.5 × 10^{13}, and (*d*) =10^{13}, number bacteria/m^3. The other parameters are as in Fig. 10.

The influence of the bacterial population on the degree of dissolution of the ore is closely linked to the permeability of the bed that is being bioleached. This interdependence is clearly shown in Figure 12, which shows the extent of the chalcocite conversion reached in 1 year averaged over the whole volume of the ore bed, as a function of the bed permeability for different bacterial populations. An increase in the bacterial population from 10^{13} to 10^{14} bacteria/m^3 in ore beds for permeabilities ranging between 10^{-11} and 10^{-10} m^2 produces an increase of only 10 pct in the average conversion. In this permeability range, the weak influence of bacterial population on conversion is attributable to the fact that dissolution of the ore is controlled by the convection of air, which varies weakly with the number of bacteria (Figure 1).

The influence of the bacterial population on the average degree of conversion is more significant with larger ore permeabilities (Figure 12). For instance, for a bed permeability of 10^{-9} m^2, an increase in the bacterial population between 10^{13} and 10^{14} bacteria/m^3 results in an increasing conversion degree of approximately six times. In this permeability range, the convection of air is large enough and the dissolution of the ore is mainly controlled by the number of bacteria present. As mentioned previously, bacteria activate oxygen consumption in bioleaching reactions and this results in density changes, which are the driving force for air convection into the bed. It is then clear that maximization of bed oxygenation by convection demands an adequate level of bacteria and adequate bed permeability.

E. *Influence of the Irrigation Rate*

Figure 13 shows the degree of chalcocite conversion reached in 1 year averaged over the whole volume of the bed, for different liquid irrigation flow rates, for a bed with a height of 10 m and a base width of 30 m. The conversion decreases with the increasing of the liquid-flow rate. For example, the conversion is 17.74 pct for q_L = 5 L/h/m^2 and

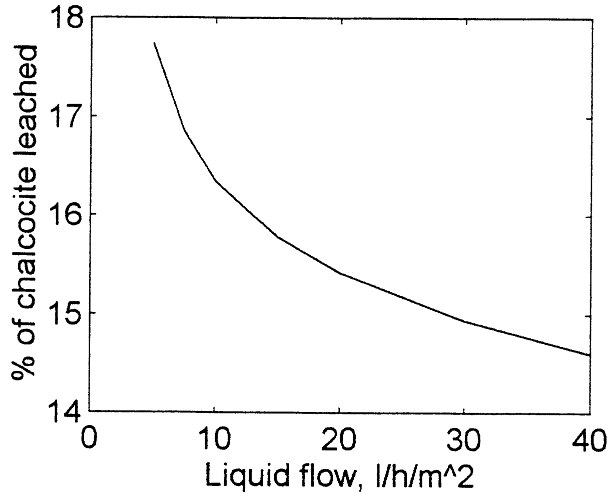

Fig. 13—Average chalcocite conversion over the whole bed volume after 1 bioleaching year *vs* the liquid irrigation rate. Parameters: height = 10 m, base half-width = 15 m, T_L = 20 °C, and the other parameters are as in Fig. 10.

14.6 pct for q_L = 40 L/h/m^2. This is explained by the fact that the liquid removes an important part of the heat generated when it leaves the bed. So, increasing the irrigation-flow rate reduces the temperature of the bed, and consequently the rate of mineral oxidation is decreased. For this simulated case, with a liquid input temperature of 20 °C, the maximum temperatures are 27.9 °C and 20.9 °C for q_L = 5 L/h/m^2 and q_L = 40 L/h/m^2, respectively.

F. *Practical Implications of the Results*

1. *Bacterial population in the ore bed*

Bacterial population measurements in copper-sulfide bioleaching in industrial heaps or dumps show maximum values in the range of 10^9 to 5×10^{10} bacteria/kg[6,9] (about 10^{12} to 10^{14} bacteria/m^3 of ore bed). Considering the specific available surface of mineral particles in these beds, it is possible to show that with these bacterial populations, there is still a low coverage of the particles. Therefore, the availability of active sulfide surface for bacterial attachment can be discarded as the factor that limits further growth of the total population. The measured values of bacterial population are of the same order of magnitude as the values determined for the limiting case, in which oxygen supplied by convection is equal to the oxygen demanded by bacteria, 2×10^{13} bacteria/m^3. This agreement between experimental and calculated values suggests that, in the bioleaching of large beds such as heaps or dumps, the balance between supply of oxygen and bacterial demand for oxygen may well self-regulate the population of bacteria. According to this interpretation, when the bacterial population is below the critical level, say 2×10^{13} bacteria/m^3, an increase in the population is well balanced by the air convection induced by the bacterial activity itself. The bacterial population is not expected to grow much over this level, and any further increase in population will imply, in practice, a decrease in the specific availability of oxygen for the bacteria already present.

Data obtained from copper-bioleaching plants show that bacterial population varies throughout the bed. Bhappu *et al.*[6] measured bacterial activity in the copper ore beds at different distances from the surface. They found that most of the bacterial population is localized in an ore layer close to the surface, at a depth that does not exceed 2.4 m (8 ft). In this zone, the bacterial population (of iron and sulfur oxidizer) in the ore reaches 4.5×10^{10} bacteria/kg dry weight. The presence of this bacterial population is a good demonstration of the localized availability of oxygen in the top of the bed supplied by diffusion. The supply of oxygen by air convection was apparently negligible in the bed analyzed, as evidenced by the low bacterial population, 10^4 bacteria/kg dry weight, that developed along the height of the bed.

2. *Bacterial population control*

According to modeling results, there is a range of bacterial population in which the rate of copper conversion is directly proportional to the number of bacteria present. The present model simulates bioleaching considering the bacterial population to be constant during the process. However, the tendencies observed when simulating the bioleaching for different values of the bacterial population can be applied to analyze the development of a concrete bioleaching operation in which the number of bacteria evolves in time during the process. According to the simulations, when there is a relatively small number of bacteria, the whole process is limited by the bacterial population. Therefore, in this stage, it is critical to promote the rapid increase of bacterial population in the whole bed. In plant practice, for instance, additional bacteria could be incorporated into the fresh ore through the irrigation leach solution, which can be recirculated from the effluent of other heaps that are already fully colonized by bacteria. Mixing a fraction of colonized leached residue into the fresh ore is another possible alternative. Inoculation of bacteria at this stage could reduce leaching times, particularly in heap leaching. However, model simulations showed that, over a critical population of bacteria in the bed, a further increase in the number of bacteria does not necessarily lead to a proportional increase in the rate of ore conversion, because the rate of bioleaching eventually becomes controlled by the supply of oxygen.

3. *Oxygen supply in industrial heaps*

Model-simulation results suggest that, in heaps of large dimensions such as those used in industrial practice, oxygen supply by air convection is important only close to the bed slopes. Diffusion, therefore, becomes the predominant mechanism for oxygen supply to the bulk of the bed and efficient aeration is then restricted to the top layer of the ore. Oxygen-profile determinations conducted by Montealegre *et al.*[23] in 6-m-high, 200-m-wide industrial copper-bioleaching heaps also confirmed the model predictions with regard to oxygen distribution. Results showed that oxygen is completely depleted at 2 m from the top of the heap, which is also evidence that oxygen is supplied solely by diffusion from the top surface. In this situation, the bioleaching rate of copper is controlled by the rate of supply of oxygen by diffusion.

According to the results of the simulations, the size of the bed has a strong influence on the efficiency of aeration in the bioleaching of heaps and dumps. Therefore, from an industrial point of view, it should be desirable to operate with heaps with a height not exceeding 10 m and a width not exceeding 20 m. In beds with these dimensions, convection is the predominant mechanism of oxygen supply and most of the bed is well aerated, producing optimum rates of dissolution of copper. In industrial practice, however, it is not convenient to operate with such small heaps because of the larger total operational area required and the ore loading difficulties that would be involved.

An alternative way of improving the efficiency of aeration in large industrial heaps is by avoiding the flooding caused by the accumulation of the leach solution at the base of the bed. In plant practice, the flooded zone forms a continuous barrier that practically prevents the flow of incoming oxygen by air convection into the base of the heap. It has been proved that flooding greatly affects the aeration efficiency. Simulation results obtained with copper-sulfide ores in 6-m-high pilot columns under controlled conditions showed that the rate of copper bioleaching can be increased by about 25 pct (or the leaching time can be reduced by about 50 pct) when flooding is impeded.[23] Manipulation of the flooding level in industrial practice, however, requires a deep understanding of the fluid-mechanical factors that determine the liquid flow and its retention in large ore beds.

IV. CONCLUSIONS

The model presented in this article was developed particularly to describe the bacterial leaching of chalcocite ores, which dissolve relatively more rapidly than other copper sulfides. The simulations permitted an estimation of the maximum ore-bed size in which copper bioleaching can proceed with a sufficient oxygen supply. To satisfy this condition, the ore beds used in the bioleaching process should not be greater than about 10-m high and 20-m wide, with the model parameters used in the simulations.

In this model, the most important parameters are permeability, bacterial population, and liquid irrigation rate. These parameters have a great influence on the results of the ore-bed bioleaching simulations. The reacting system in the ore beds is heterogeneous, *i.e.*, the oxidation rate changes with position and there are different bacterial activities linked to the bacterial population, the specific oxygen concentration, and the temperature at any given location in the bed.

The rate of copper-sulfide bioleaching depends on several factors, and the main ones are bacterial activity, the type of mineral, and the permeability and size of the ore bed. The bioleaching rate is controlled by the slowest of the following four steps: (1) oxygen supply, (2) bacterial oxidation of ferrous sulfate to ferric sulfate, (3) ferric sulfate diffusion through the ore particles, and (4) the intrinsic reaction of the sulfide minerals with the ferric sulfate. These controlling steps may coexist in different zones in the ore bed.

Oxygen supply is the oxidation-rate-limiting mechanism in most interior regions of the large ore beds. In this case; the bioleaching process of the ore bed displays the macroscopic properties rather than the microscopic behavior of the intrinsic kinetics of mineral oxidation. In small beds, the oxygen supply is sufficient for the development of the microorganisms and the rate of the bioleaching process is related to the rate of reaction of the oxidizing agent and minerals at a microscopic level.

Small flow irrigation rates (5 to 10 L/h/m^2) produce higher mineral oxidation rates than high liquid flow rates. In addition, the solution that leaves the bed has a higher copper concentration than at high irrigation rates.

This model can be a tool of great help in the design and operation of bacterial leaching processes. Further development of ore bed bioleaching models is needed, incorporating a monitoring-testing program involving real mining ore beds together with the incorporation of other factors, such as bacterial growth, ferric iron diffusion through the ore particles, and metals precipitation.

ACKNOWLEDGMENTS

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APPENDIX

Deduction of Eq. [6] used to calculate the streamlines of gas transport

At low velocities, the flow of a fluid in a porous medium is governed by Darcy's law:

$$\mathbf{q_g} = -\frac{K_{ef}}{\mu} \cdot (\nabla P - \rho \mathbf{g}) \qquad \text{[A1]}$$

where $\mathbf{g} = -g\hat{j}$ and $K_{ef} = Kk_{rg}$. Multiplying Eq. [A1] by (∇x) and letting $f = \mu/K_{ef}$, the equation becomes

$$\nabla \times (f\mathbf{q_g}) = -\nabla \times \nabla P - \nabla \times (\rho g_{\hat{j}}) \qquad \text{[A2]}$$

Taking $\nabla \times \nabla \mathbf{P} = 0$ (irrotational flow) and assuming f to be constant,

$$f\left(\frac{\partial q_y}{\partial x} - \frac{\partial q_x}{\partial y}\right) = -g\frac{\partial \rho}{\partial x} \qquad \text{[A3]}$$

The fluid flow distribution may be visualized by means of the stream function (Eq. [5]). Introducing Eq. [5] into [A3], the following relationship is obtained:

$$f\left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2}\right) = -g\frac{\partial \rho}{\partial x} \qquad \text{[A4]}$$

Equation [A4] permits the streamlines for fluid transport to be calculated as a function of its density variation.

NOMENCLATURE

C	oxygen concentration, kg/m^3
$C\rho$	average specific heat, kJ/kg/K
D_g	diffusion coefficient for the oxygen in gas phase, m^2/s
FPY	pyrite reaction factor, kg of pyrite leached/kg chalcocite leached
g	gravitational acceleration constant, m/s^2
G	mass flow of dry air per unit area, kg/m^2/s
G^o	chalcocite ore grade, wt pct
h	enthalpy flow per unit area, kJ/m^2/s
H	height of the ore bed, m
H_{air}	air humidity, kg water/kg dry air
He	Henry's constant for oxygen

k_B effective thermal conductivity of the bed, kJ/m/K/s
k_r relative permeability
K permeability of the ore bed, m^2
K_m Michaelis constant, kg/m^3
M molecular weight, kg/kmol
n normal coordinate, m
P pressure, Pa
P^{sat} saturation pressure of the water vapor, Pa
q volume flow per unit area, $m^3/m^2/s$
S_{ef} effective liquid saturation
S_w liquid content, m^3 water/m^3 of voids
S_{wr} irreducible liquid content, m^3 water/m^3 of voids
t time, s
T temperature, K
v velocity, m/s
V_m maximum specific respiration rate by bacteria, kg O_2/number of bacteria/s
X bacterial population, number of bacteria/m^3 of ore bed
x width coordinate, m
y height coordinate, m
z depth coordinate, m

Greek letters

α chalcocite conversion or copper recovery
ε volumetric fraction of a fluid phase within the bed, m^3/m^3 of ore bed
λ heat of vaporization, kJ/kg
ρ average density, kg/m^3
ϕ porosity of the ore bed, m^3 of voids/m^3 of bed
σ_1 stoichiometric factor of reaction, kg chalcocite/kg O_2 consumed
Ψ stream function, m^2/s
μ viscosity, kg/m/s
ΔH_R mean reaction enthalpy, kJ/kg
∇ gradient of a scalar, 1/m

Subscripts

B ore bed or dump
Ch chalcocite
ef effective
g gaseous phase
L liquid phase
i position on the *x*-axis
j position on the *y*-axis
Ox oxygen
Py pyrite
ref reference
s solid phase
v vapor water
w liquid water

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