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Progress in the mathematical modelling of leaching reactors

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Abstract

Leaching reactors have been described using three different approaches. These models are the overall mass balance, the population-balance model and the segregated-flow model. Each of these models has been used extensively without the relationship between them being either understood or quantified. These models do not only differ in their conceptual basis, but also yield different results for the same reaction conditions. The conceptual relationship between the various approaches to the mathematical modelling of continuous leaching reactors is discussed, and it is suggested that the population-balance model is the most appropriate approach for the modelling of leaching reactors.

The population-balance method of the mathematical modelling of leaching reactors is discussed. The population balance incorporates the kinetic parameters obtained from the analysis of the batch experiments. The model is used to analyse the batch laboratory experiments and to predict the operation of the continuous plant. The model accounts for the particle-size distribution of the feed, the residence-time distribution of the reactor, the leaching kinetics, and the solution mass balance.

The model is used to obtain predictions of the operation of the zinc pressure leaching reactor at Trail, B.C., and the bacterial leaching of a refractory gold ore at Fairview, South Africa. The predictions of the continuous operation are shown to be in excellent agreement with the data from the plant operation.

1. Introduction

Leaching is a central unit operation in the hydrometallurgical treatment of ores and for this reason much attention is focused on the study of the kinetics of leaching reactions. In spite of this, comparatively fewer studies have considered the incorporation of these kinetics into a mathematical model of the reactor or compared the results of the mathematical models with the data obtained from continuous leaching plants. In order to determine the parameters that are important in the efficient design of the hydrometallurgical plant, reliable models of both the reaction kinetics and the leaching reactor are required.

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The leaching of mineral particles by a reagent in solution can be represented by the following reaction:

$$aA(s) + bB(aq) \rightarrow \text{aqueous and solid products} \quad (1)$$

where $A(s)$ represents the solid undergoing leaching, $B(aq)$ represents the reactant in solution, and a and b are stoichiometric coefficients.

The kinetics of leaching reactions are often described by the shrinking-core and shrinking-particle models [1]. This model considers the reaction of the reactant at the surface of the solid particle, which results in both aqueous and solid products which may form on the surface of the particle. As reaction proceeds, the unreacted core of the mineral is reduced in size, while more solid and aqueous products are formed.

The rate of leaching is governed by physical and chemical phenomena. The governing phenomena are the rate of transport of reactants to and products from the particle surface, the diffusion of reactants and products through the porous product layer that forms on the unreacted core, and the rate of the reaction at the surface of unreacted core. Each of these phenomena represents a resistance to the rate of the overall reaction. One or more of these resistances may control the rate of reaction. If the resistances are all linear in concentration, then the rate of shrinkage, $R(l, L)$, of the unreacted core of size l of a particle of initial size L, is given by [2]:

$$R(l, L) = \frac{dl}{dt} = \frac{-2(a/b)[B]}{\rho\left[\frac{1}{k_s} + \frac{1}{2D_B}(l - l^2/L) + \frac{1}{k_f}(l/L)^2\right]} \quad (2)$$

where ρ_A is the molar density of the mineral, k_s is the reaction rate constant at the surface, D_B is the effective diffusion coefficient of the reactant in the porous product layer, k_f is the film transfer coefficient, $[B]$ is the concentration of the reactant in the bulk solution and L is the initial particle size.

Since the conversion, $X(t, L)$, in a batch reactor in which the particles are initially of size L is given by:

$$X = 1 - (l/L)^3 \quad (3)$$

Eq. (2) may written as:

$$\frac{dX}{dt} = \frac{6(a/b)[B]}{\rho_A\left[\frac{L}{k_s}(1-X)^{-2/3} + \frac{L^2}{2D_B}[(1-X)^{-1/3} - 1] + \frac{L}{k_f}\right]} \quad (4)$$

The rate of the reaction at the unreacted mineral surface is often controlled by charge transfer across the solid-solution boundary. If this is the case, then the rate of the reaction at the surface is governed by the mixed-potential model [3], and these reaction kinetics are incorporated in the shrinking-core and shrinking-particle models in order to describe the overall reaction.

In general, and in industrial practise, the particulate feed to a continuous leaching reactor has a distribution of sizes, and this distribution of sizes changes with reaction and time spent in the reactor. In this communication, we review the three different models that have been

proposed as descriptions of continuous leaching reactors, and we discuss the relationship between these models. We also review the results of the comparison between the model predictions of the performance of the continuous plant and the data from the plant. These comparisons have been performed for a pressure leaching reactor, and for a bacterial leaching reactor.

2. Review of the mathematical models of leaching reactors

Three different, but related, approaches have been used to describe leaching in a continuous-stirred-tank reactor (CSTR). These models all incorporate the unreacted shrinking-core model, represented by Eq. (2) or Eq. (4), to describe the reduction in particle size on reaction. However, they differ in their description of the distribution of particle sizes in the material in the feed to the reactor, and in their assumptions concerning the state of micromixing in the continuous reactor.

2.1. Monosized-particle model of leaching reactors

Henein and Biegler [4] and Pritzker [5] presented a model of continuous leaching. They assumed that the particles in the feed are monosized and that the particles in the exit are monosized. However, both Sepulveda and Herbst [2] and Crundwell and Bryson [6] showed that changes in the variance of the size distribution of the feed can result in large differences in the model predictions. Even if the distribution in the feed to the first tank in a cascade of CSTR is monosized, the distribution leaving that first tank will have an exponential distribution, reflecting the residence-time distribution of the first tank. The size distribution of the feed to the second and subsequent tanks would then be required. Henein and Biegler [4] and Pritzker [5] have assumed that these complexities of the changing size distributions in modelling a cascade of leaching tanks have little effect on the conversion.

2.2. Segregated-flow model of leaching reactors

The segregated-flow model [7,8] has been used by a number of different authors [9–14] to describe the conversion achieved in a reactor. The segregated-flow model is a general model describing the performance of a continuous reactor. The model supposes that the fluid entering the reactor is dispersed into small elements of fluid that remain intact for the duration of their residence in the reactor, and that each element behaves as a batch reactor [7]. For particulate reactors, the particles themselves have been considered to represent individual batch reactors [8]. For a particulate reactor with a residence-time density $f(t)$, the segregated-flow model is given as [8]:

$$1-X=\int_0^\infty\int_0^\infty \{1-X(t, L, [B]_t)\}m_f(L)f(t)\mathrm{d}L\,\mathrm{d}t \tag{5}$$

where $X(t, L, [B]_t)$ is the batch conversion of a particle initially of size L in contact with solution of concentration $[B]_t$ after time t. $m_f(L)$ is the particle-size density of the feed on

a mass basis. $X(t, L, [B]_t)$ is obtained from the integration of Eq. (4), which must be expressed in the mathematically correct manner so that the conversion does not exceed one.

The segregated-flow model is solved in conjunction with the solution mass balance, which is given by:

$$[B]_t = [B]_f - F_f \eta X(t, L, [B]_t) \tag{6}$$

where $[B]_t$ represents the concentration of B at the corresponding residence time t, $[B]_f$ represents the concentration of B in the feed, F_f represents the molar concentration of mineral into the reactor and η represents the stoichiometric factor. When the reactant is in stoichiometric proportion to the mineral, $F_f\eta/[B]_f$ is equal to one, and the concentration of B tends to zero as the conversion tends to one.

In the application of the segregated-flow model to leaching reactors, researchers have assumed that the concentration of reactant, $[B]_t$, is constant with residence time and is equal to the exit concentration [8–14]. This is equivalent to assuming that the particles themselves are batch reactors, and represents a different model to the segregated-flow model formulated by Danckwerts [7] for homogeneous reactors. A limiting case is that in which the concentration of reactant is in vast excess; in this situation both the assumption that $[B]_t$ is constant and Eq. (6) are obviously redundant.

It is clear from Eq. (6) that if the reactant is consumed in sufficient quantity on reaction, the concentration $[B]_t$ will decrease with residence time. The interaction between the particles and the reactant is the key to the understanding of the difference between the segregated-flow model and the population-balance model. This is discussed later in this paper.

2.3. *Population-balance model of leaching reactors*

Sepulveda and Herbst [2] and Crundwell and Bryson [6] applied the population balance [15,16] to the modelling of leaching reactors. The population balance is a general method for the description of the disperse phase in a particulate process, and it is premised on the conservation of number. Particulate processes differ from homogeneous processes in that the particles undergoing reaction are not all the same. In a homogeneous reaction, all the reactants are identical, whereas in a particulate process, the particles differ in size, composition, reactivity, etc. For leaching reactions, the most important property that is distributed is the size of the particles. Thus, we define $n(l, L)\,\mathrm{d}l\,\mathrm{d}L$ as the number of particles per unit volume in the size range l to $l+\mathrm{d}l$ which had an initial size in the range L to $L+\mathrm{d}L$. The population balance for a well-mixed leaching reactor is given by [2,6,15,16]:

$$\frac{\mathrm{d}[R(l, L)n(l, L)]}{\mathrm{d}l} = \frac{1}{\tau}[n_f(l, L) - n(l, L)] \tag{7}$$

with the boundary condition that $R(l, L)n(l, L) \to 0$ as $l \to \infty$. τ is the mean residence time of the tank reactor, and $R(l, L)$ is obtained from the unreacted shrinking-core model, given by Eq. (2).

The size density of the unreacted cores of the particles is given by:

$$n(l) = \int_{l}^{\infty} n(l, L)\mathrm{d}L \tag{8}$$

The third moment of the size density of the unreacted cores of the particles gives the total volume of unreacted mineral. The third moment is defined as:

$$\mu_3 = \int_{0}^{\infty} l^3 n(l)\mathrm{d}l \tag{9}$$

The conversion for the tank is given by:

$$X = 1 - \mu_3/\mu_{3,\mathrm{f}} \tag{10}$$

The concentration in the tank is given by:

$$[B] = [B]_{\mathrm{f}} - F_{\mathrm{f}}\eta X \tag{11}$$

where η is the stoichiometric factor describing change in the concentration of the reactant on reaction. If the reactant is in large excess, then $F_{\mathrm{f}}\eta/[B]_{\mathrm{f}}$ is approximately zero and the concentration of B remains constant. If the reactant is in stoichiometric proportion to the mineral, then $F_{\mathrm{f}}\eta/[B]_{\mathrm{f}}$ is equal to one, and the concentration of B tends to zero as the conversion of mineral tends to one.

The predictions of the performance of the continuous plant from the population-balance model were shown to be in good agreement with the plant data for the pressure-leaching reactor at Trail, B.C. [6] and for the bacterial leaching plant at Fairview, South Africa [17,18]. These results are reviewed later in this paper.

3. Comparison between the segregated-flow model and the population-balance model

Although the segregated-flow and the population-balance models have been known since the 1960's [1,7,15,16,20], direct comparison between the numerical results for these two models for particulate reactors has only been performed recently [19]. In order to illustrate this comparison, consider the following example, which represents amongst the most straightforward of the leaching operations [19]. Mineral particles and the solution containing the reactant are fed to a single well-mixed reactor. The amount of reactant that is present in the feed is in stoichiometric proportion to the amount of mineral added, so that the concentration of the reactant, B, tends to zero as the conversion tends one. The concentration of the reactant in the tank is described by Eq. (11), which, in this case, can be expressed as:

$$[B] = [B]_{\mathrm{f}}(1 - X) \tag{12}$$

The kinetics of leaching are independent of the particle size, and are described by:

$$R(l) = -k_{\mathrm{s}}[B] \tag{13}$$

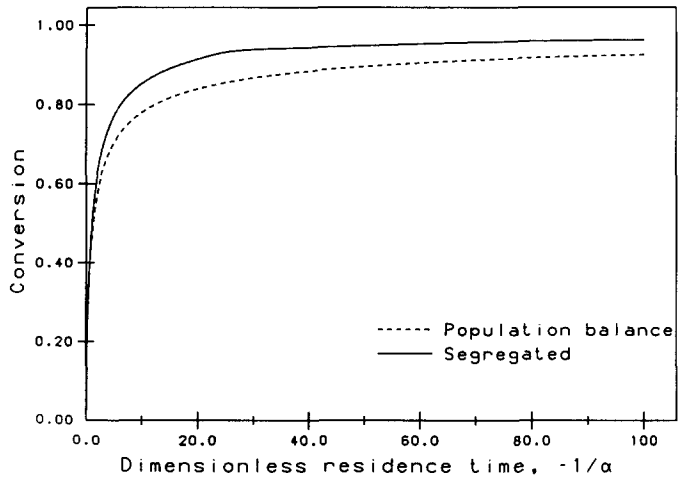

Fig. 1. The conversion calculated from the segregated-flow model (Eq. 5 and 6) and the population-balance model (Eqs. 7–11) for a single ideally-mixed tank. The amount of leaching reactant, B, is in stoichiometric proportion to the amount of mineral in the feed. The reaction kinetics are described by Eq. (13).

Leaching kinetics such as those given by Eq. (13) arise when chemical reaction is the controlling mechanism in the shrinking-core model, or when the kinetics are described by the shrinking-particle model (cf. Eq. 2).

The size distribution on a number basis for the mineral particles in the feed is described by the gamma distribution:

$$n_f(l) = \frac{1}{\Gamma(p)} l^{p-1} \exp(-pl) \tag{14}$$

The value of p used in this example is 2.

Crundwell [19] presented solutions to the segregated-flow model and population-balance model for this example.

The segregated-flow model is described by Eq. (5). Expressions for $X(t, L, [B]_t)$, $m_f(l)$ and $f(t)$, which are required for the calculation of the conversion using Eq. (5), are obtained from the kinetics of the reaction Eq. (13), the feed-size density Eq. (14) and the residence-time density, respectively. (Note that the feed-size density given in Eq. (14) is in terms of the number basis, while Eq. (5) requires the feed-size density on a mass basis.) The segregated-flow model describing the conversion for a reactor with exit concentration $[B]$ is solved simultaneously with the solution mass balance, given by Eq. (6). In this example, Eq. (6) is expressed in a form analogous to Eq. (12).

The population-balance model is described by Eq. (7) in which the feed-size density is given by Eq. (14). This differential equation is expressed in integral form using the method of integrating factors, and the integral is evaluated numerically. The conversion is calculated using Eq. (10). This calculation is performed simultaneously with Eq. (12) describing the concentration of reactant in the tank.

The results for these two calculations are given in Fig. 1. Full details of these calculations for this example and for similar examples can be found in Ref. [19]. The results are given in terms of the dimensionless residence time, $-1/\alpha$, where α is given by:

$$\alpha = \frac{\bar{l}_f}{k_s[B]_f \tau} \tag{15}$$

where $\bar{l}_f$ represents the mean size of the feed distribution.

The results shown in Fig. 1 indicate that there is a large difference in the results obtained from these two models. Fig. 1 indicates that the segregated-flow model gives a higher conversion than does the population-balance model.

The largest difference in the conversion for this example is 0.0767, representing a difference in conversion of approximately 10%. Examination of Fig. 1 indicates that for a conversion of 0.9 there is factor of approximately four between the values for the dimensionless residence time. This means that if the required design conversion was 0.9, the tank size calculated by the two methods would differ by approximately four times. Similarly, if experimental data was analysed on this basis, there would be a factor of approximately four between the rate constants calculated by the two methods. This difference is likely to increase in other cases, such as the case of non-linear kinetics or the case of bacterial leaching, in which the kinetics of reaction resemble those of auto-catalytic reactions.

The reason for the difference in the conversions obtained from these two models is not obvious. This difference is not the result of numerical approximation in the calculation procedure.

It is worth noting that if the concentration of reactant, B, is assumed to be constant with residence time and equal to the exit concentration (that is, described by Eqs. 11 or 12) [8–14], then the segregated-flow and the population-balance models are equivalent for a single ideally-mixed tank reactor. However, ambiguities arise when the process consists of more than one tank in series and this assumption is made. For example, consider a leaching plant comprised of a number of tanks in series. The concentration of reactant in the inlet, in the first tank and in the second tank will all be different, so that the concentration down the train of reactors can be represented by a series of step changes. This leaching process is easily described by the population-balance model, which describes only one tank at a time. The segregated-flow model describes the whole series of reactors with a single residence-time density in one equation. If the concentration is considered to be constant, an assumption that is common [8–14], then the concentration profile will be different for the two models. With this assumption, the segregated-flow model will yield a different result to that of the population-balance model. Obviously, the segregated-flow model can be applied one tank at a time down the train of reactors, but this method seems to defeat the point of being able to describe the whole train of reactors with one residence-time density.

Crundwell [19] showed that the relationship between the segregated-flow model and the population-balance model is to be understood in terms of the concept of micro-mixing in continuous reactors (Danckwerts [7] and Zwietering [20]).

4. The relationship between the segregated-flow model and the population-balance model

4.1. Micro-mixing in continuous homogeneous reactors

Danckwerts [7] proposed that the state of micro-mixing in a reactor with a given residence-time distribution $F(t)$ falls between two limits. The limit represented by segregated

flow is that in which the material in the feed to the reactor is dispersed on entering the reactor into discrete packets, or elements of fluid. These elements of fluid are small compared to the volume of the reactor, and remain intact while in the reactor, so that each element of fluid behaves as a batch reactor.

The other limit is that in which the material in the feed to the reactor is completely dispersed on entering the reactor on a molecular scale. In other words, volume elements of fluid do not contain molecules that have entered the reactor at the same time, and that there is significant exchange of material between elements of fluid in the reactor, so that no element of fluid has a single history. This limit is called the maximum-mixedness model [20].

Zwietering [20] showed that these two models of the micro-mixing in a reactor gave different results for the conversion in a reactor, except in one case.

The case in which there is no difference between the maximum-mixedness model and the segregated-flow model for a homogeneous reactor is that in which the reaction is an elementary first-order reaction. This is explained as follows. For a first-order reaction, the molecules undergoing reaction do not interact with their environment; the probability of whether the molecule reacts or not depends only on the time the molecule has spent in the reactor. Thus the rate of reaction in an element of fluid is not dependent on the composition of the element. For all other orders of reaction, the rate of reaction in the element of fluid is dependent on its composition, and the composition of elements of fluid in the segregated-flow model and the maximum-mixedness model are completely different.

Zwietering [20] also showed that the maximum-mixed model with a residence-time distribution of a well-mixed tank reduced to the usual form of the mass balance for a CSTR for all reaction kinetics.

4.2. Micro-mixing in continuous particulate reactors

In particulate reactors, such as leaching, each particle is an aggregate of molecules that remains intact for the duration of its residence in the reactor. Because of this physical difference between the particles and the fluid, the particles have previously been regarded as the volume elements of fluid referred to by Danckwerts [7] and Zwietering [20]. Each particle is regarded as a batch reactor in which the concentration of the fluid remains constant, and the segregated-flow model is used to describe the performance of the continuous reactor [8]. In contrast to this model, Crundwell [19] proposed that the different physical state of the particles has little to do with the concept of micro-mixing. Rather, he proposed the following segregated-flow model for particulate reactors [19]. The material in the feed on entering the reactor is dispersed into volume elements composed of both particles and fluid. These elements remain intact, and react as batch reactors. The reaction of the mineral particles with the solution results in the lowering of the concentration of reactant within each volume element. The particles in each element are subject to the concentration of reactant in that element only. This is the model represented by Eqs. (5) and (6).

In addition, the number balance for the maximum-mixed reactor for particulate reactions was derived [19]. This reactor requires that elements of fluid and particles that leave the reactor at the same time are completely mixed.

The segregated-flow and the maximum-mixedness models for particulate reactors give different results for the performance of the reactor for all residence-time distributions and all reaction kinetics, except for one case. This case is that in which the reaction is zero order with respect to the concentration of the reactant. This is expected from Zwietering's results for homogeneous reactors. For a zero order leaching reaction, the rate of leaching is independent of the concentration of reactant in solution. This means that for a zero-order reaction the rate of leaching does not depend on the environment of the mineral particle; in other words, for a zero-order reaction the rate of leaching does not depend on the state of micro-mixing in the reactor. (Note that a reaction may be pseudo-zero order if the concentration of the reactant does not change during the course of the reaction.)

The maximum-mixedness model for a particulate reactor with a residence-time distribution of a single well-mixed tank reduced to the usual form of the population balance, given by Eq. (7) [19] for all reaction kinetics. This means that the population-balance model of continuous particulate reactors, as represented by Eq. (7), is analogous to the mass balance for continuous homogeneous reactors.

Therefore, the relationship between the segregated-flow model and the population-balance model centres on the assumptions made in these models concerning the conditions of micro-mixing in the reactor. These models are not identical (even for a single CSTR), except in the limited case where the concentration of reactant is in such excess that its concentration does not change between the feed and outlet of the reactor (i.e., pseudo-zero-order reaction).

4.3. Choice of mathematical model for continuous leaching reactors

The differences in the effects of micro-mixing between complete segregation and maximum-mixedness tend to be small for homogeneous reactors, except if the reaction kinetics are highly non-linear, and the physical nature of the flow in the reactor allows segregation as a possibility [30]. Most gas and liquid phase reactors operate close to the limit of maximum-mixedness. Segregated flow usually results from a combination of high viscosity and low diffusivity, which is not typical of most industrial reactions.

No research has investigated the effects of micro-mixing in particulate systems. However, the experience with liquid homogeneous reactors has been that most operate close to the limit of maximum-mixedness. Therefore, we suggest that most leaching reactors operate close to the limit of maximum-mixedness. Most leaching reactions are not highly non-linear, so the effects of micro-mixing are not very pronounced [19]. We suggest that the most appropriate mathematical model for leaching reactors is the population balance, given by Eq. (7). This model is the maximum-mixedness reactor for a residence-time distribution of a single tank, and is analogous to the ordinary mass balance for homogeneous reactors.

5. Modelling continuous reactors using the population balance

The results of the mathematical modelling of leaching reactors using the population-balance model have been compared to the plant data for two different operations, those of the pressure leaching of a zinc concentrate and the bacterial leaching of a pyrite concentrate.

Both these models of the continuous operation are predictions of the plant performance using parameters obtained from the batch data. This is a stringent test of the model of the continuous plant. The results of these models are reviewed below.

5.1. Model of the zinc pressure leaching reactor at Trail, British Columbia [6]

The zinc pressure leaching reactor at Trail, B.C., has a working volume of 100 m^3 and a mean residence-time of 100 min [21]. The sphalerite concentrate is obtained from the Sullivan Mine, and has an iron content of 11.6%. The main reactions that occur in the autoclave are the following:

$$ZnS + 2Fe^{3+} \rightarrow Zn^{2+} + 2Fe^{2+} + S$$

$$Fe^{3+} + 1/6PbSO_4 + 1/2SO_4^{2-} + 2H_2O \rightarrow 1/3Pb_{0.5}Fe_3(OH)_6(SO_4)_2 + 2H^+$$

$$Fe^{2+} + H^+ + 1/4O_2(aq) \rightarrow Fe^{3+} + 1/2H_2O$$

$$FeS + 2Fe^{3+} \rightarrow 3Fe^{2+} + S$$

$$O_2(g) \rightarrow O_2(aq)$$

The kinetics of the dissolution of sphalerite in both ferric sulphate and ferric chloride solutions has received a large amount of attention [22–25]. Since no information was available on the kinetics of leaching of the sphalerite concentrate from the Sullivan Mine, it was assumed that the mechanism of reaction of this concentrate is similar to that of other sphalerite concentrates, and the rate of reaction is similar if the impurity content of iron is similar [6]. Sphalerite from the Gamsberg deposit has an iron content of 9.08%, which is similar to the value of 11.6% from the Sullivan deposit. The kinetics of dissolution of the Gamsberg sample were described by Eq. (2) with $k_s = 542.3 \exp(-5533/T)$ m/min and $D_B = 5.46 \times 10^{-7} \exp(-2887/T)$ m^2/min [6]. The value of k_f in Eq. (2) was found to be small.

The concentration quotient for the precipitation of jarosite was obtained from the exit conditions of the reactor, and at 150°C is given by [6]:

$$K = 10^{-3.608} = \frac{[Fe^{3+}]}{[H^+]^2} \text{ m}^3/\text{mol} \tag{16}$$

The rate of the oxidation of ferrous sulphate has been thoroughly studied [25,26], and is given by [6]:

$$r_{Fe^{2+}} = k_3[Fe^{2+}]^2[O_2] \text{ mol/m}^3 \text{ min} \tag{17}$$

where $k_3 = 7.4 \times 10^5 \exp(-8251/T)$ $m^6/(mol^2\ min)$.

The iron in the sphalerite concentrate is assumed to leach at the same rate as the sphalerite.

The rate of dissolution of the oxygen gas into solution is governed by the rate of mass transfer, described by [6]:

$$r_{O_2} = k_5([O_2]_{sat} - [O_2]) \text{ mol/m}^3 \text{ min} \tag{18}$$

The population balance, Eq. (7), was used to describe the rate of leaching, while the concentrations of the species in solution were described by the usual material balances [6].

Table 1
Cumulative conversions obtained in each compartment in % at 105% of design capacity

Compartment	1	2	3	4
Calculated	88.12	95.76	97.86	98.67
Actual plant Data [21]	88.7	96.5	97.9	98.4

The conversion and concentrations of the reactants and the molar flow rates of the reactants between each compartment were determined from the conditions of the feed to the reactor. The comparison between the data from the plant operation [21] and the model calculation [6] are given in Table 1. These results indicate the model is an excellent description of the plant operation.

5.2. *Model of the bacterial leaching of a refractory gold ore at Fairview, Barberton, South Africa [17,18]*

In the last decade a number of full-scale plants employing bacterial oxidation as a pre-treatment process for refractory gold ores have been commissioned [27]. Miller [28] presented data on the batch and continuous leaching of a pyrite/arsenopyrite concentrate from the Fairview Mine, Barberton, South Africa, using a mixed culture. A model for the batch experiments and continuous plant was developed [17,18] and is discussed here.

In order to apply the population-balance model to leaching reactors, the kinetics of reaction must be in the form of $R(l)$, such as those that are obtained from the unreacted shrinking-core model. The derivation of a model of bacterial leaching in a batch reactor that yields a kinetic expression in this form is discussed, and the parameters from this model are used in the population-balance model to describe the continuous plant.

It is thought that the leaching of the pyrite occurs at the point of the attachment of the bacteria to the surface of the pyrite particles. Two factors affect the rate of leaching: the rate of growth of the population of bacteria that are attached to the surface, and the amount of surface area available for attachment.

The rate of growth of the bacteria on the pyrite surface, r_b, is given by:

$$r_b = k_b M(M_{max} - M) \tag{19}$$

where M is the number of bacteria on the mineral surface per unit volume of slurry and k_b is the rate constant for bacterial growth. The maximum number of bacteria that can be supported, M_{max}, is given by $N_{max}A$, where N_{max} is the maximum number of bacteria that can be supported per unit surface area, and A is the surface area per unit volume of slurry.

The batch number balance gives:

$$\frac{dM}{dt} = k_b M(M_{max} - M) \tag{20}$$

The rate of consumption of pyrite by bacterial leaching is proportional to the rate of growth of the bacteria, given by:

$$F_0\frac{dX}{dt}=k_{dl}M(M_{max}-M) \tag{21}$$

where F_0 is the initial molar concentration of pyrite per unit volume, X is the conversion of pyrite, and k_{dl} is a rate constant for the direct leaching of pyrite.

Assuming that the particles may be approximated as spheres, the surface area is give by:

$$A=A_0(1-X)^{2/3} \tag{22}$$

where X is the conversion, and A_0 is the initial surface area per unit volume.

The solution of Eqs. (20), (21) and (22) gives a model equation for bacterial leaching:

$$\frac{dX}{dt}=\frac{k_D}{L}(1-X)^{2/3}(1+k_BX)\left[1-\frac{k_{MAX}(1+k_BX)}{(1-X)^{2/3}}\right] \tag{23}$$

where:

$$k_D=\frac{k_{dl}\phi N_{max}M_0}{\rho}\quad k_B=\frac{k_bF_0}{k_{dl}M_0}\quad k_{MAX}=\frac{M_0}{N_{max}A_0}$$

Note that $A_0/F_0=\phi/\rho L$, where ϕ is the shape factor, ρ is the molar density of pyrite, and L is the initial particle size.

Eq. (23) was fitted to the data of Miller [28,29]. Fig. 2 shows the data and the fitted model, indicating that the model is a good description of bacterial leaching. The parameters are given in Table 2. The parameters k_D and k_B are independent of size, as expected from the model. The model indicates that the parameter k_{MAX} is dependent on size, but that $k_{MAX}A_0$ is independent of particle size. The values of $k_{MAX}A_0$ obtained from parameter estimation are independent of particle, as expected.

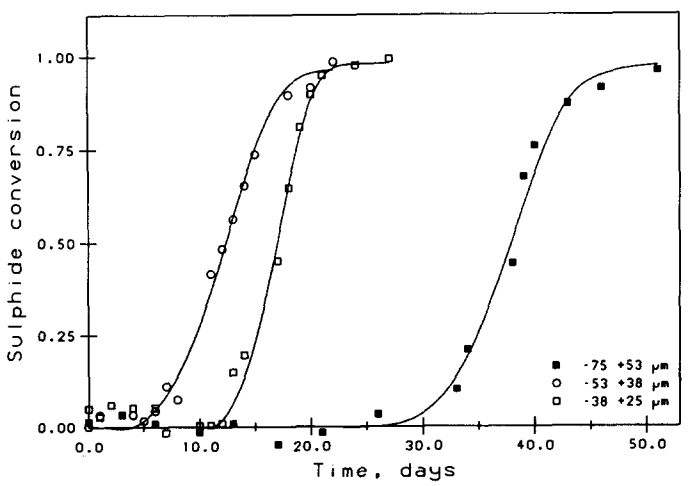

Fig. 2. The bacterial leaching of a gold-bearing pyrite concentrate in a batch reactor. The data are from Miller [28,29] and the lines represent the solution to the model, given by Eq. (23). The parameters for Eq. (23) are given in Table 2.

Table 2
Parameters for bacterial leaching obtained from the batch data

Parameter	Size class		
	−75+53 μm	−53+38 μm	−38+25 μm
k_B (−)	14.79	14.79	14.79
k_D (μm/day)	1.074	1.074	1.074
k_{MAX} (−)	0.0052	0.0063	0.0044
$k_{MAX}A_0$ (m^2/L)	0.0329	0.0329	0.0329

The population-balance model, given by Eq. (7), was used to describe the dissolution of the pyrite particles. This model requires an expression for $R(l)$, the rate of change of the size of the particles. This is obtained from Eq. (23) and is given by:

$$R(l) = \frac{k_D}{3}\frac{M}{M_0}\left(1 - \frac{k_{MAX}A_0M}{M_0A}\right) \tag{24}$$

The solution of Eq. (7) with Eq. (24) and using the boundary condition that $R(l)n(l) \rightarrow 0$ as $l \rightarrow \infty$ gives the number density of the pyrite particles leaving the reactor, $n(l)$. The conversion of pyrite is obtained from the number density using Eq. (9).

The simultaneous solution of Eqs. (20) and (21) indicates that a pseudo-stoichiometry between the bacteria and the conversion of pyrite exists, that is, the increase in the number of bacteria is proportional to the increase in conversion. The number of bacteria in the reactor is obtained from the solution of Eqs. (20) and (21) and is given by:

$$\frac{M}{M_0} = 1 + \frac{F_f}{F_0}k_BX \tag{25}$$

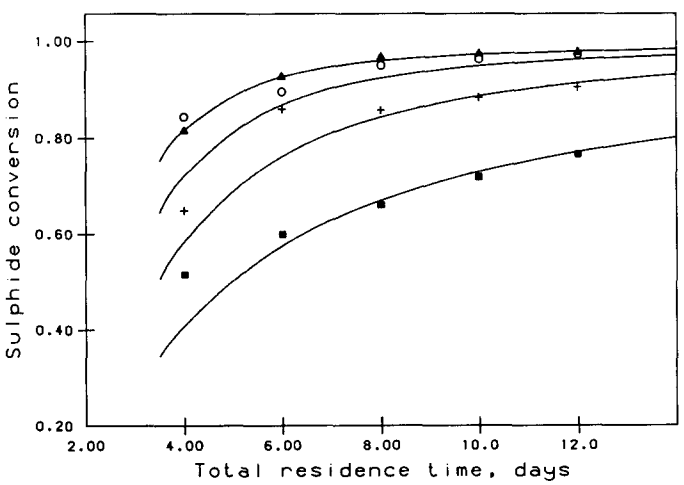

Fig. 3. The bacterial leaching of a gold-bearing pyrite concentrate in a series of continuous reactors. The data are from Miller [28,29] and the lines represent the model, given by Eqs. (7), (24) and (25). The parameters for the model were those determined from the batch experiments and are given in Table 2.

where F_f is the molar concentration of pyrite in the feed to the reactor. It has also been assumed in writing this equation that the bacteria are equally distributed over the available surface area of the mineral particles. This assumption is reasonable, since the bacteria are mobile, and will seek the easiest access to the energy source that is available.

The solution to this model of the continuous plant using the values of the parameters obtained from the batch experiments is shown in Fig. 3. The figure indicates that the model prediction and the plant data are in good agreement, suggesting that this model has accounted for the most important phenomena occurring during bacterial leaching.

6. Conclusions

This communication has indicated that significant advances have been made in the both the conceptual development of mathematical models for leaching and in the application of these models to operating plants.

The relationship between the previous models of leaching reactors was discussed, and it was shown that these models are related by the conditions of micro-mixing that occur in the reactor. It is suggested that the population-balance is the most appropriate approach for the mathematical modelling of leaching reactors.

The population-balance model has been used to describe the continuous operation of a pressure reactor and of a bacterial leaching plant. Both these models used values of the parameters that have been obtained from the evaluation of the batch experimental data, and are therefore predictions of the operating plant. For both these plants, the predictions based on the mathematical model and the actual plant data are in good agreement.

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