Modelling and simulation of gold ore leaching

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A leaching model for gold ore that takes into account the impact of cyanide and oxygen concentrations as well as gold surface exposure on leaching performance is developed. Cyanide consumption is estimated by an empirical model that is a function of ore particles size distribution as well as cyanide, copper and sulphur concentrations. The proposed model has been validated by data from laboratory leaching tests on the Sleeping Giant gold mine ore.

Keywords: gold leaching, modelling, exposure surface.

Nomenclature

\( A_A \): Anodic surface area
\( A_C \): Cathodic surface area
\( [Au] \): Ore gold concentration
\( [Au_0] \): Ore gold concentration before cyanidation begins
\( [CN] \): Cyanide concentration in solution
\( [Cu] \): Ore copper concentration.
\( d_g \): Length of cubic gold grain sides
\( d_p \): Length of cubic ore particle sides
\( D_{CN} \): Cyanide diffusivity
\( D_{O_2} \): Oxygen diffusivity
\( K \): Constant factor used to approximate hindered transport through pores
\( K'_{O_2} \): Kinetic rate constant associated with oxygen-bearing minerals
\( K'_{Cu} \): Kinetic rate constant associated with copper-bearing minerals
\( K'_{S} \): Kinetic rate constant associated with sulphur-bearing minerals
\( M_{O_2} \): Gold molecular weight
\( m_{O_2} \): Mass of partially liberated gold
\( m_{Au} \): Mass of totally liberated gold
\( m_{Au,ag} \): Mass of gold in the liquid phase
\( m_{Au,ag} \): Mass of gold accessible through ore porosity
\( m_{CN} \): Mass of cyanide added to the leaching thank
\( m_{L} \): Total mass of liquid in the leaching thank
\( N \): Number of totally liberated gold grains
\( [O_2] \): Oxygen concentration
\( P_{O_2} \): Proportion of inaccessible gold grains
\( P_{Au} \): Proportion of totally liberated gold grains
\( P_{Au,ag} \): Proportion of gold grains accessible through ore porosity
\( P_{Au,ag} \): Proportion of gold grains accessible at the ore surface

\( R \): Oxygen efficiency
\( [S] \): Ore sulphur concentration.
\( S_{ag} \): Surface of gold particle available for chemical reaction
\( S_{ag} \): Surface of partially exposed gold grains
\( S_{Au} \): Surface of totally liberated gold grains
\( v_{Au} \): Molar rate of gold dissolution per unit of gold surface available to reaction
\( v_{Au,ag} \): Molar rate of gold dissolution for gold accessible through porosity per unit of gold surface available to reaction
\( x_{ag} \): Percentage of ore in class of average diameter \( d_p \)
\( u_g \): Mean of gold size distribution
\( \omega_{CN} \): Cyanide consumption per unit of time and mass of liquid
\( \phi_{CN} \): Molar diffusion rate of cyanide
\( \phi_{O_2} \): Molar diffusion rate of oxygen
\( \psi_{Au} \): Mass dissolution rate of partially liberated gold
\( \psi_{Au} \): Mass dissolution rate of totally liberated gold
\( \psi_{Au,ag} \): Mass dissolution rate of gold accessible through ore porosity
\( \sigma_0 \): Thickness of the boundary layer
\( \sigma_1 \): Distance between gold surface and bulk solution
\( \sigma_g \): Standard deviation of gold size distribution
\( \sigma_p \): Threshold distance from the ore surface above which gold grains are not accessible to chemical attack by cyanide.
\( \rho_{Au} \): Gold density

Introduction

Leaching by cyanide solution is widely used as a separation method to recover gold from ores. Different processes can be used to perform this chemical separation. Some rely on...
the exposure of gold surfaces to enhance dissolution kinetic. In this type of process, the ore is crushed and ground to expose the surface of gold grains to a chemical attack by cyanide in presence of oxygen. This chemical reaction produces a soluble complex of gold cyanide which is subsequently recovered by adsorption or cementation. Others use an approach, called heap leaching, which consists of spraying a cyanide solution on a roughly crushed ore pile. In this approach, cyanide and oxygen diffuse slowly through the pores and fractures of the ore to reach gold surfaces.

Several authors studied gold dissolution kinetics. Some considered pore diffusion transport in heap leaching (Prosser1, Bouffard and Dixon2) while others addressed the leaching problem by the concept of gold surface liberation. In those conditions, experimental results showed a reduction of leaching kinetics as the chemical reaction advances. To model that behaviour, many authors (Brittan3, Nicol et al.4, Hodouin et al.5, Ling et al.6) proposed mathematical equations based on the evolution of leachable gold concentration. When it decreases, the chemical reactions rates slow down. Changes in the kinetic mechanisms are also proposed to explain the slowing down effect. The initial reaction may be governed by diffusion through boundary layers if pulp agitation is not sufficiently vigorous (Brittan5) while it is controlled by diffusion through ore porosity in the later stages. Habashi8 presented a gold dissolution model based on an electrochemical mechanism as well as cyanide and oxygen diffusivities through a boundary layer. Rubisov et al.9 applied that diffusion model to pure gold by adding a stoichiometric factor representing the number of leached gold moles per mole of consumed oxygen. Crundwell and Godorr10 proposed a model that considers the formation of a passivation layer of materials on the surface of gold particles as they dissolved. De Andrade Lima and Hodouin11 went one step further by including the effect of particle size in the kinetic model. This indirectly takes into account the liberation effect on leaching behaviour.

This paper proposes a kinetic model that takes into account the fast rate of dissolution of exposed gold surfaces and slower one of gold accessible through ore porosity. The reduction of leaching kinetic is explained by the disappearance of exposed gold surfaces as the reaction evolves. This approach first requires a geometrical model to describe the surface liberation phenomena. This model is presented and explained in Section 2. Section 3 introduces the leaching model, while Section 4 proposes an empirical cyanide consumption model. Finally, the model is calibrated and validated on batch leaching tests.

Golden grain surface accessibility to reagents

Depending on their degree of accessibility, gold grains have different leaching kinetics. When gold is directly exposed to the surrounding phase it has a fast leaching kinetic. On the other hand, gold attacked through ore porosity, like in heap leaching, exhibits slow dissolution kinetics. Figure 1 shows four different classes of gold, each one having a different leaching behaviour. One can see that gold can be totally liberated, accessible at the ore surface or through pores. The fourth class contains inaccessible gold which cannot be leached. The differences in leaching behaviour of totally liberated gold and exposed gold at the ore surface is due to the fact that the first one offers more accessible surface to cyanide. The slow kinetics of gold accessible through ore porosity is related to the hindered transport of cyanide to the reaction site.

Gold liberation (or accessibility) has an important impact on leaching kinetics; therefore, it is interesting to be able to characterize it. Many authors have developed mathematical models for the liberation of minerals such as those proposed by Wiegel and Li12, King13, 14, Barbery15, Gay16. Stamboliadis17 modified King’s14 model by adding an empirical term that accounts for the fraction of leachable gold that is not directly exposed to cyanide. Wen et al.19 developed a cubic exposure model to predict the proportion of exposed inclusive gold. This section proposes a simple geometric model to characterize the proportions of free gold grain, exposed inclusive gold as well as inclusive leachable gold through ore fractures or porosity.

Based on simple geometrical assumptions for gold grains and ore particle shape size and distribution, it is possible to approximate the gold surface degree of exposure and its accessibility through ore porosity. Those assumptions are:

- Ore particle shape is approximated by cube of side \( d_p \)
- Gold grains are approximated by cubes of side \( d_g \)
- Gold grain orientation is the same as the ore particle orientation; therefore the cubes edges are parallel
- The space distribution of gold grain centres inside ore particles is uniform
- Gold is unbreakable, therefore fragmentation is intergranular
- Total liberation of gold grains occurs when at least 50% of the volume of gold is out of an ore particle
- Gold grains positioned farther than a threshold distance \((r_p)\) from the ore surface are not accessible to chemical attack by cyanide.

According to those assumptions, Figure 2 shows the different zones where gold grains centres can be positioned. The centre position influences the degree of gold leachability, a property related to gold surface accessibility to reagents.
From geometrical considerations, it is possible to obtain the proportion of inaccessible \( P_{\text{ina}} \) and totally liberated gold grains \( P_{\text{lib}} \):

\[
P_{\text{ina}} = \frac{d_g^3 + 2.25d_g^2(d_p - d_g)}{d_p^3}
\]  

\[
P_{\text{lib}} = \frac{(d_p - d_g - 2\sigma_p)^3}{d_p^3}
\]  

The proportion of gold grains accessible through ore porosity \( P_{\text{por}} \) is obtained by subtracting the unreachable volume from the unexposed one:

\[
P_{\text{por}} = \frac{(d_p - d_g - 2\sigma_p)^3}{d_p^3}
\]  

Finally, the proportion of gold grains accessible at the ore surface \( P_{\text{surf}} \) represents the non-liberated gold present in the exposed volume of ore, and then is obtained by:

\[
P_{\text{surf}} = \frac{3d_g^2(d_p - d_g)^2 + 0.75d_g^2(d_p - d_g)}{d_p^3}
\]  

### Gold leaching model

The dissolution model is based on the basic electrochemical and diffusion mechanisms proposed by Habashi. It is modified to account for possible loss of oxygen efficiency, as proposed by Rubisov et al. who used a stoichiometric factor representing the number of moles of leached gold per moles of oxygen consumed, assuming that oxygen is consumed by an intermediate reaction producing peroxide. According to Habashi, the anodic reaction is:

\[
Au + 2CN^- \rightarrow [Au(CN)_2]^- + e^-
\]  

while the cathodic reactions are:

\[
\frac{1}{2}O_2 + e^- + H_2O \rightarrow OH^- + \frac{1}{2}H_2O
\]

\[
\frac{1}{2}H_2O_2 + e^- \rightarrow OH^-
\]

The overall reaction mechanism assumes that 0.25 mole of oxygen is required to dissolve one mole of gold. The oxygen efficiency is then maximal. However, if peroxide is not completely used to subsequently produce OH\(^-\), its efficiency is reduced and oxygen consumption increases.

Then, the overall cathodic reaction is given by:

\[
\frac{1}{4R}O_2 + \frac{1}{2R}H_2O + e^- \rightarrow OH^- + \left(\frac{1}{2R} - \frac{1}{2}\right)H_2O_2
\]  

where \( R \) is the oxygen efficiency.

According to Habashi's model, which considers that the chemical reaction is much faster than the reagent diffusion rate, and Fick's law of diffusion applied to a boundary layer, the oxygen and cyanide molar diffusion rates \( \phi ) \) at the exposed gold surface are:

\[
\phi _{o} = \frac{D_o A_o [O_2]}{\sigma _o}
\]

\[
\phi _{CN} = \frac{D_{CN} A_C [CN]}{\sigma _o}
\]

where \( A_o \) and \( A_C \) are the surface areas of anodic and cathodic reaction, respectively \( D_{CN} \) and \( D_o \) are the diffusivities of cyanide and oxygen in the pulp phase, and \( \sigma _o \) is the thickness of the boundary layer, which is considered as dependant on impeller rotation speed.

The dissolution kinetic of exposed gold surfaces can then be calculated as a function of the oxygen efficiency:

\[
\phi _{o} = \frac{1}{4R} \phi _{CN}
\]

Then, the rate of gold dissolution (in moles per unit of time and gold surface available to the reaction) is given by:

\[
\nu _{o,n} = \frac{4RD_{CN} [CN]D_o [O_2]}{\sigma _o (D_{CN} [CN] + 8RD_o [O_2])}
\]

Where the gold surface available to the reaction is given by (Habashi):

\[
S_{o,n} = A_o + A_C
\]

Equation [12] is adapted in the following sections to the three classes of leachable gold grains.

#### Totally liberated gold grains

Since gold grains are approximated by cubes of side length \( d_g(t) \) at any time of reaction, the overall surface of totally liberated gold in a batch of ore can be calculated by:

\[
S_{o,n}(t) = 6N d_g^2(t)
\]

where \( N \), the number of totally liberated gold grains, is obtained by:

\[
N = \frac{m_{\text{tot}}(0)}{\rho d_g^3(0)}
\]

where \( \rho \) is the gold density.

Equation [1] can be used to approximate the proportion of totally liberated gold grains and therefore the mass of material attributed to that class of gold at the beginning of the reaction \( m_{\text{tot}}(0) \). Finally, using Equations [12], [14] and [15], one can approximate the dissolution rate of totally liberated gold \( \psi_{o,n} \) expressed in mass of leached gold per unit of time.
where is the molecular weight of gold.

**Exposed gold at the ore surface**

The kinetic behaviour of gold exposed on the ore surface is similar to the one of completely liberated gold grains. The major difference between the two classes of gold, is that the accessible surface of partially liberated gold is much smaller. The area of these surfaces follows a distribution dependent on the position of gold grain centers in the ore particle. However, to simplify modelling equations and simulations algorithms, this surface is approximated by:

\[
S_{\text{da}}(t) = N d_g(0) \lambda \sigma(t)
\]

Figure 3 shows an accessible gold grain at the surface of an ore particle. It points out that, at the beginning of the reaction, the reagents need to diffuse through the thickness of the boundary layer and, as the reaction progresses, the distance between the bulk solution and the gold grain surface increases. Considering that the dissolution of gold is uniform on the exposed surface, it is possible to approximate this distance by:

\[
\sigma(t) = d_g(0) \left[ 1 - \frac{m_{\text{exp}}(t)}{m_{\text{tot}}(0)} \right]
\]

where is the mass of exposed gold at the ore surface at the beginning of the reaction and obtained using Equation [4]. The rate of dissolution for partially exposed gold grains expressed in moles per unit of time and gold surface area is given by:

\[
v_{\text{da}} = 4R D_0 \sqrt[4]{\text{CN}(t)} d_g(0) \left[ \sigma(t) + d_g(0) \left( 1 - \frac{m_{\text{exp}}(t)}{m_{\text{tot}}(0)} \right) \right]
\]

Expressed in mass of leached gold per unit of time, it becomes:

\[
\psi_{\text{da}} = \frac{m_{\text{da}}(0)}{\rho_g d_g(0)} v_{\text{da}} M_g d_g(t) \lambda \sigma(t)
\]

**Gold accessible through ore porosity**

To dissolve gold accessible through ore porosity, reagents have to cross the boundary layer and diffuse on a certain distance within the ore pores. Diffusivity coefficients of cyanide and oxygen differ in these two zones. The transport through ore porosity is hindered and therefore is slower than through the boundary layer. Figure 4 shows the process of lixiviation for the third class of gold.

By considering that both diffusivities of reagent are proportionally reduced by a constant factor while travelling trough pores and that there is a uniform consumption of gold along the grain face parallel to the nearest particle face, it is possible to obtain the molar diffusion rates of cyanide and oxygen.

\[
\psi_{\text{co}} = KD_0 A \left[ Q(t) \right] \frac{4 R D_0 \sqrt[4]{\text{CN}(t)} d_g(0)}{K (\sigma(t) + \alpha(t)) + \sigma(t)}
\]

\[
\psi_{\text{co}} = KD_0 A \left[ CN(t) \right] \frac{4 R D_0 \sqrt[4]{\text{CN}(t)} d_g(0)}{K (\sigma(t) + \alpha(t)) + \sigma(t)}
\]

Based on reaction stoichiometry, the molar kinetics of gold dissolution per unit of surface can then be expressed as:

\[
v_{\text{da}} = \frac{4 R D_0 \sqrt[4]{\text{CN}(t)} d_g(0)}{K (\sigma(t) + \alpha(t)) + \sigma(t)} \left[ Q(t) \right] \left[ \text{CN}(t) \right] \left[ \text{O}_2(t) \right]
\]

Finally, by considering an average accessible surface, one can characterize the behaviour of gold accessible through ore porosity expressed in mass of gold per unit of time.

\[
\psi_{\text{arer}} = \frac{m_{\text{arer}}(0)}{\rho_g d_g(0)} v_{\text{arer}} M_g d_g(t) \lambda \sigma(t)
\]

where is the mass of gold accessible through ore porosity at the beginning of the reaction and obtained by Equation [3].

**Cyanide consumption model**

Cyanide is consumed by several minerals to form a variety of complexes. Copper sulphides and other minerals are highly soluble in aqueous cyanide solutions and can form a variety of complex ions with coordination numbers between one and four (De Andrade Lima and Hodouin[11]). More generally, sulphide minerals are large consumers of cyanide because they form very stable complexes (Marsden and House[20]).
It is difficult to develop a rigorous cyanide consumption model due to the impressive variety of complexes that can be formed with cyanide. De Andrade Lima and Hodouin proposed a pseudo-homogenous empirical model to describe the cyanide consumption process. Their model takes into account cyanide concentration and ore particle size. This section introduces a model which takes into account these two variables as well as the copper and sulphur concentrations in the ore. Cyanide consumption per unit of time and mass of liquid for ore particles of size $d_p$ is given by:

$$
\omega_{CN}(d_p) = K_{CN}^1 \left[ CN \right]^1 \left[ Cu \right]^1 + K_{CN}^2 \left[ CN \right]^1 \left[ S \right]^1 + K_{CN}^3 \left[ CN \right]^{\alpha_3} \left[ d_p \right]^{\beta_3} \frac{d_p}{d_p^3}
$$

The first term roughly corresponds to the dissolution of copper-bearing minerals (mainly chalcopyrite in the studied example), the second one to the sulphur-bearing minerals which produces sulphur-cyanide complexes, and the third one to all other cyanide consumption assumed to be diffusion controlled and particle size sensitive. Cyanide consumption by copper and sulphide is also related to the extent of surface accessibility and therefore are particle size sensitive. This is considered in the following relationships for estimating dissolution rate constants:

$$
K_{CN}^1 = \frac{K_{CN}^1}{d_p - K_{CN}^1} \left( 1 + \frac{[Au]}{[Au_0]} \right)^{\alpha_1}
$$

$$
K_{CN}^2 = \frac{K_{CN}^2}{d_p - K_{CN}^2} \left( 1 + \frac{[Au]}{[Au_0]} \right)^{\alpha_2}
$$

These equations also contain a slowing down effect that models the reduced leaching rate related to disappearance of easily accessible cyanide surfaces. As this effect is difficult to quantify, it is empirically correlated to gold dissolution extent, where $[Au]$ is the ore gold concentration and $[Au_0]$ is the gold concentration prevailing before cyanidation begins. The coefficients $K_{CN}^1$, $K_{CN}^2$, $K_{CN}^3$, $K_{CN}^4$, $\alpha_1$, $\alpha_2$, $\alpha_3$, $\beta_1$, $\beta_2$, $\lambda_1$, $\lambda_2$, $\theta_1$, $\theta_2$ and $\theta_3$ are parameters to be estimated from experimental data.

### Application to batch leaching

Batch leaching tests were performed with the Sleeping Giant gold mine ore. Twelve tests were performed on a pre-aerated and ground ore (50% passing 38 micrometers). Leaching was carried out at pH 11, at 50% solid, with a 600 ppm initial cyanide concentration and a saturated oxygen concentration maintained by constant injection of $O_2$. Liquid samples were regularly collected to dose cyanide and gold concentrations. After each liquid sampling, cyanide was added to the leaching tank for maintaining cyanide concentration near its initial value. Figure 5 summarizes the twelve tests performed at four different agitation speeds, and their initial conditions.

The equations presented in earlier sections are written for a unique dimension of gold grain size ($d_g$). If the gold grain size distribution is known, these equations can be extended to a multigrain distribution. The mineralogical properties of the Sleeping Giant ore used for the leaching tests were characterized and 307 gold grains were identified. Figure 6 shows the density distribution in numbers of gold grains according to their diameter as well as an approximation of it by a gamma distribution. This distribution coupled with the liberation and leaching equations is used to calibrate the model parameters.

Batch leaching simulation equations are obtained by writing species mass balance equations. Using the kinetic expressions for the three classes of gold (liberated, exposed and accessible through pores) in the solid phase, one obtains:

$$
dm_{Au}(t) = \frac{6M_{Au}m_{Au_0}(t)^{1/3}}{\rho_{Au}d_p(t)} \cdot \frac{dm_{Au}(t)^{2/3}}{dt}
$$

$$
dm_{CN}(t) = \frac{M_{CN}m_{CN_0}(t)^{1/3}}{\rho_{CN}d_p(t)^2} \cdot \frac{dm_{CN}(t)^{2/3}}{dt}
$$

$$
dm_{CN}(t) = \frac{M_{CN}m_{CN_0}(t)^{1/3}}{\rho_{CN}d_p(t)^2} \cdot \frac{dm_{CN}(t)^{2/3}}{dt}
$$

Gold mass balance in the liquid phase is therefore obtained by:

$$
\frac{dm_{Au}(t)}{dt} = \frac{dm_{Au}(t)}{dt} + \frac{dm_{Au}(t)}{dt} + \frac{dm_{Au}(t)}{dt}
$$

where $m_{Au}(t)$ is the mass of gold in the liquid phase at time $t$. Cyanide balance equation is obtained using the consumption model for five ore sizes ($d_p$) (<38 μm, 38–45 μm, 45–75 μm, 75–150 μm and >150 μm):

$$
\frac{d[CN(t)]}{dt} = - \sum \omega_{CN}(d_p) x_{d,p} \cdot \frac{m_{CN}(t)}{m_{Au}}
$$

![Figure 5. Leaching tests initial conditions](image)

![Figure 6. Density distribution gold grains for the Sleeping Giant gold mine ore](image)
where \( \omega_{dp} \) is the mass fraction of ore in class of average diameter \( d_{dp} \), \( m_{CN}(t) \) is the mass of cyanide added to the reactor at time \( t \) and \( m_{liq} \) is the mass of liquid in the leaching tank.

**Model calibration**

The model parameters were estimated using the data obtained for batch tests as well as the above simulation and liberation equations. The results of only nine tests were used, keeping the others for validation: the two leaching tests at 1500 rpm as well as the 1-hour and 4-hour tests at the three other agitation speeds. The twenty-four parameters characterizing the equations are estimated by a non-linear least square regression method minimizing the sum of squared differences between the gold and cyanide concentrations obtained experimentally and by simulation. In total, 164 measurements are used to approximate the parameters. Figure 7 summarizes the methodology used to calibrate the model. The model parameter estimates are presented in Table I. D is the product of two parameters (\( \mu_m \) and \( \sigma_0 \)). As it can be seen in the leaching kinetic equations, those two parameters cannot be estimated independently. \( \mu_g \) and \( \sigma_g \) are respectively the mean and standard deviation of the beta distribution used to approximate the gold size distribution. The variation of sigma zero with the impeller rotation speed confirms that external diffusion is a dominant kinetic mechanism. Figures 8 and 9 respectively compare the gold and cyanide concentrations in the liquid phase obtained by simulation to the experimental data for the tests at 1200, 1350, 1500 and 1650 rpm. One can see that simulated behaviours are reasonably fitting the measured values. The saw tooth behaviour of the cyanide consumption model is caused by punctual addition of cyanide in the leaching tank.

**Model validation**

To validate the proposed model, the three 2-hour length cyanidation tests at 1200, 1350, 1500 and 1650 rpm are simulated with the calibrated parameters. Since those three tests were not used to calibrate the model, the simulations results are considered as predictions. Figures 10 and 11 respectively compare the results predicted by the model with the measured liquid concentrations of gold and cyanide. The agitation speed of the stirrer influences the dissolution rate of gold but not the overall gold leachability. The large difference in final gold liquid concentration at 1600 rpm and other agitation speeds is due to the different initial concentrations of gold (see Figure 5) and their respective proportion of inaccessible gold grains.

From those results, one can see that the calibrated model can be used to predict the leaching behaviour of a gold ore based on its gold grain size distribution and a geometric liberation model.

**Conclusions**

This paper proposed a leaching model based on gold surfaces accessibilities and controlled by reagent diffusivities to the reaction site. The model allows an adequate prediction of gold dissolution and cyanide consumption for the studied ore. The integration of the model in a steady state simulator allows to predict the leaching behaviour of a gold ore based on its gold grain size distribution and a geometric liberation model.

<table>
<thead>
<tr>
<th>Parameters related to the liberation model</th>
<th>Parameters related to the cyanide consumption model</th>
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Table I. Numerical values of estimated parameters

Figure 7. Methodology used to approximate models parameters
Figure 8. Comparison between simulated and experimental gold liquid concentrations
(a) Results at 1200 RPM, (b) Results at 1350 RPM
(c) Results at 1500 RPM, (d) Results at 1650 RPM

Figure 9. Comparison between simulated and experimental cyanide concentrations
(a) Results at 1200 RPM, (b) Results at 1350 RPM
(c) Results at 1500 RPM, (d) Results at 1650 RPM
would allow studying the effectiveness of different cyanidation flowsheets in order to minimize cyanide consumption and maximize gold dissolution. This study will be presented in a subsequent paper.

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