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CFD simulation of mass transfer and flow behaviour around a single particle in bioleaching process

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ABSTRACT

The pathway to reach a certain target in many processes such as bioleaching, due to the complex and poorly understood hydrodynamics, reaction kinetics, and chemistry knowledge involved is not apparent. An investigation of the interactions between the parameters in bioleaching process can be applied to optimize the rate of metal extraction from sulphide minerals. Such investigations can be carried out with the aid of numerical simulations. In this study, a computational fluid dynamics (CFD) model was developed to better understand the mass transfer phenomenon and complex flow field around a single particle. The commercial software FLUENT 6.2 has been employed to solve the governing equations. Volume of fluid (VOF) method was used to predict the fluid volume fraction in a 3D geometry. The computational model has successfully captured the results observed in the experiments. Simulation results indicate that concentrations of species in a thin layer of liquid on the particle surface are much higher than their concentrations in the liquid bulk and significant gradients in the ion concentrations between the surface of the particle and the liquid bulk were observed.

1. Introduction

Bioleaching refers to the mobilization of metal ions from insoluble ores by biological oxidation and complexation. The application of bacterial leaching to metal recovery from mineral ores has progressed steadily in the last 20 years. Heap bioleaching involves stacking the ore to form a heap, and applying acidified leaching solution to the top of the heap. This technique is used to treat mostly low grade ore, and copper is the primary targeted metal, although it is also considered for zinc, cobalt and nickel recovery. It is also used for the pre-treatment of refractory gold ores.

Bioleaching of sulphide minerals is based on the ability of the iron-oxidizing bacteria such as *Acidithiobacillus ferrooxidans* or *Leptospirillum ferrooxidans* to oxidize ferrous ion (Eq. (1)) [1–3]. In the leaching of zinc concentrate with ferric ion, the zinc is dissolved, and the ferric ion is simultaneously reduced to ferrous ion (Eq. (2)). The elemental sulphur produced in Eq. (2) may also be re-oxidized to sulphuric acid (Eq. (3)) in the presence of sulphur-oxidizing microbes such as *Acidithiobacillus thiooxidans* and *Acidithiobacillus caldus* [4]. The actual role of bacteria in the bioleaching process has not been completely resolved [5–8]; albeit Sand et al. [5] suggest that the oxidation of sulphide minerals occurs mainly via the chemical attack from ferric ion and/or sulphuric acid (Eqs. (2) and (4)), which are generated as a results of bacterial action. Pyrite is often found with sphalerite in practice, and so leaches by reacting with ferric ions to release ferrous ions and acid (Eq. (5)):

$$2FeSO_4 + \tfrac{1}{2}O_2 + H_2SO_4 \xrightarrow{\text{bacteria}} Fe_2(SO_4)_3 + H_2O \tag{1}$$

$$Fe_2(SO_4)_3 + ZnS \rightarrow 2FeSO_4 + ZnSO_4 + S^0 \tag{2}$$

$$S^0 + \tfrac{3}{2}O_2 + H_2O \xrightarrow{\text{bacteria}} H_2SO_4 \tag{3}$$

$$ZnS + \tfrac{1}{2}O_2 + H_2SO_4 \rightarrow ZnSO_4 + H_2O + S^0 \tag{4}$$

$$FeS_2 + 7Fe_2(SO_4)_3 + 8H_2O \rightarrow 15Fe(SO_4) + 8H_2SO_4 \tag{5}$$

Despite the present widespread use of bioleaching in industry, the process is still plagued by low recoveries, long extraction times, and high operation costs. Hence there is a need to optimize process

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operations. The complexity of the fluid dynamics problem makes it difficult or impossible to exactly solve for equations of an object in a flow. Approximate solutions can be obtained by construction and measurement of prototypes placed in a flow, or by use of a numerical simulation. Since usage of prototypes can be prohibitively time-consuming and expensive, many have turned to simulations to provide insight during the engineering process. In this case the simulation setup and parameters can be altered much more easily than one could with a real-world experiment.

Investigation of the interactions between the physical, chemical and biological processes provides knowledge that can be applied to solve the problems. Such investigations can be carried out with the aid of numerical models. CFD as powerful tool has the potential to assist by improving understanding of the interaction between hydrodynamics and chemistry.

The application of computational fluid dynamics to the design of hydrometallurgical plants is still in its infancy. The gap between the complexity of the physics and the appropriateness of the numerical models is gradually getting smaller through advances in commercially available computational fluid dynamics software and faster computers.

In the recent years, CFD has been considered as a powerful tool to incorporate many of the important heap phenomena [9–12]. CFD models have been significantly enhanced and calculation speeds have greatly increased, so that CFD has been used to simulate hydrodynamics in complex flows such as two-phase flow in packed beds [12,13], bubble columns [14] or fluidized beds [15]. This numerical tool is now widely used and its advantages and limitations are more clearly identified.

Recently, most studies [16–19] have been aimed at improving the understanding of bioleaching kinetics and hydrodynamics. Many models have been presented for the reactors, bioreactors and bioheap reactors under batch and continuous operations in order to predict velocity, concentration and temperature fields, but there is no scientific literature about the application of volume of fluid (VOF) method as a multiphase modelling approach in the bioleaching processes.

The main objective of this study was to simulate the mass transfer and flow behaviour around a single sulphide particle, as a simplified example for bioleaching process, using VOF method in a 3D geometry. CFD was used to predict the concentration profiles and liquid velocity field. To investigate the effect of inlet air velocity on the fluid velocity field two different inlet velocities for air were applied.

2. Materials and methods

2.1. Ore sample characteristics

In this study a zinc–lead sulphide ore supplied by Kooshk lead and zinc mine (Yazd, Iran) was used. Chemical analysis of the sample revealed: 22.8% S; 8% Fe; 9.32% Si; 8.9% Zn; 2.9% Pb; 2.3% CaO and less than 0.2% Cu. X-ray diffraction analysis of the ore showed sphalerite (ZnS) (13%); pyrite (FeS_2) (14%), and quartz (SiO_2) (18%) as the major components and calcite ($CaCO_3$) (5%) and galena (PbS) as the minor ones. Chalcopyrite ($CuFeS_2$) was present in trace amounts.

2.2. Microorganism and medium

A strain of *Acidithiobacillus ferrooxidans* isolated from chalcopyrite concentrate of Sarcheshmeh copper mine (Kerman, Iran) was used throughout these experiments. The microorganism was grown and maintained on 9 K medium [20]. The cultures of bacteria were incubated in 500 ml Erlenmeyer flasks each containing 200 ml of the 9 K medium and 10% (v/v) inoculum, on a rotary shaker at 180 rpm at constant temperature of 33 °C. The initial pH of the cultures was adjusted to 1.5 using 1 N H_2SO_4.

2.3. Apparatus and procedure

The experiments were carried out in a simple mini column reactor, as shown in Fig. 1. The column was 3 cm high with an internal diameter of 3 cm. A perforated support plate was placed allowing air to be injected below the plate and dispersed uniformly over the ore in the column. The column was fed with the bacterial solution using a peristaltic pump. The leach solution was passed over the particle by gravity and re-circulated through a side loop with a peristaltic pump. A container with a capacity of 1 L collected the pregnant liquid solution (PLS) draining from the column. When the system reached a steady state condition, a sample was taken from the collecting container. Zinc and total iron concentrations in the sample solutions were measured by an atomic absorption spectrophotometer (German, model AAS 5EA) after the filtration of the suspension through a 0.22 μm membrane filter to remove biomass. The ferric ion concentration in the solution was determined by sulphosalicylic acid spectroscopy method (Varian Techtron UV–vis spectrophotometer, model 635) [21]. The ferrous ion concentration was ascertained by a volumetric method by titration with potassium dichromate [22]. The pH of the cultural suspension and zinc extractive solution were monitored at room temperature with a pH meter (Metrohm, model 691) and calibrated with a low pH buffer.

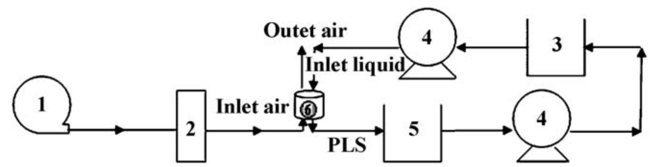

Fig. 1. Schematic diagram of experimental setup; 1—Air pump; 2—Air flow meter; 3—Feed solution; 4—Peristaltic pump; 5—PLS container; 6—Single particle.

3. Mathematical modelling and numerical method

3.1. Governing equations

In this study, the system is defined as a volume comprises of a solid phase, a liquid phase (stagnant and flowing leaching solution, which contains dissolved solutes) and a gas phase. The governing conservation equations (continuity, momentum and species transport) for unsteady, incompressible, Newtonian, two-phase flow are solved throughout the domain. It was assumed that the flow was under isothermal conditions, i.e., the flow was considered without temperature variation. The resulting fields (velocity and pressure) are shared among the phases. The momentum equation, shown below, is dependent on the volume fractions of all phases through the properties ρ and μ.

$$(\nabla.\boldsymbol{u}) = 0 \tag{5}$$

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}.\nabla\boldsymbol{u}\right) = -\nabla p + \mu\nabla^2\boldsymbol{u} + \rho\boldsymbol{g} + \boldsymbol{F} \tag{6}$$

where **u** is the fluid velocity, p is the pressure, **g** is the gravitational acceleration, and **F** represents any external body forces acting on the fluids. The local averaged density, ρ, and viscosity, μ, are evaluated from the local distribution of the phase indicator, f, which is governed for two-fluid flows by Eq. (12). For the local average density and viscosity, linear weighing of the densities and viscosities of phases, Eqs. (14) and (15), are used.

The effects of surface tension along the interface between each pair of phases and wall adhesion play an important role and it could be included in the VOF model. In the present work, a widely used surface tension model, the continuum surface force model (CSF), originally proposed by Brackbill et al. [23], was used to model the force due to surface tension acting on the gas–liquid interface. In this model the surface tension is modelled as a body force, **F**, that is non-zero only at the interface and is given by the following equation:

$$\boldsymbol{F} = \sigma\kappa\nabla f(x, y, z, t) \tag{7}$$

where κ is the local mean curvature of the interface.

$$\kappa = -\nabla.(\boldsymbol{n}/|\boldsymbol{n}|) \tag{8}$$