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CFD Simulation of concentration profiles and velocity field. Application: in bioleaching process

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Abstract

In this study, some important variables in the bioleaching, such as ferric and zinc ions concentration in the liquid phase and velocity field around a single particle were simulated. Volume of fluid (VOF) method was used to predict the mentioned fields in a 3D geometry. Results show that VOF is a successful approach for prediction of velocity and concentration fields. The computational model has successfully captured the results observed in the previous works [1, 2]. Simulation results indicate that concentrations of species in a thin layer of liquid on the particle surface are very higher than their concentrations in the liquid bulk.

Keywords: Simulation; Velocity field; Concentration profile; Bioleaching process; Volume of fluid method

1. Introduction

Bacterial leaching is an important process used in the extraction of metals such as gold, copper and zinc from their ore and concentrate using microorganisms.

Bioleaching of sulfide minerals is based on the ability of the iron-oxidizing bacteria such as *Acidithiobacillus ferrooxidans* to oxidize ferrous iron (Eq. (1)). In the leaching of zinc concentrate with ferric iron, the zinc is dissolved, and the ferric iron is simultaneously reduced to ferrous iron (Eq. (2)).

$$2FeSO_4 + {}^1\!/_2\, O_2 + H_2SO_4 \xrightarrow{bacteria} Fe_2(SO_4)_3 + H_2O \tag{1}$$

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

$$S^0 + {}^3\!/_2\, O_2 + H_2O \xrightarrow{bacteria} H_2SO_4 \tag{3}$$

$$ZnS + {}^1\!/_2\, O_2 + H_2SO_4 \rightarrow ZnSO_4 + H_2O + S^0 \tag{4}$$

The pathway to a faster extraction is not obvious yet, because of the complex and poorly understood hydrodynamics and reaction kinetics involved in the extraction processes. 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 computer simulations. Computational Fluid Dynamic (CFD) has the potential to assist by improving understanding of the interaction between hydrodynamics and chemistry [3,4]. Recently, most studies [5-9] have been aimed at improving the understanding of bioleaching kinetics and hydrodynamics. Many models have been presented in order to predict velocity, concentration and temperature fields, but there is no scientific literature about the application of volume of fluid method as a modelling approach for the prediction of velocity and concentration fields in the bioleaching processes.

In the present attempt VOF method was used to predict the concentration profiles and liquid velocity field around a single sphalerite particle in a 3D geometry. To investigate the effect of inlet air velocity on the fluid velocity field two different inlet velocities for air were applied.

2. Mathematical modeling and numerical method

2.1. Governing equations

The following governing equations for unsteady, incompressible, Newtonian, two-phase flow were solved throughout the domain. It was assumed that the flow was under isothermal conditions, i.e., the flow was considered without temperature variation.

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

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

where $\boldsymbol{u}$ is the fluid velocity, p is the pressure, $\boldsymbol{g}$ is the gravity acceleration, and $\boldsymbol{F}$ stands for body forces. In the present work, the continuum surface force model (CSF), originally proposed by Brackbill et al. [10], was used to model the force due to surface tension acting on the gas-liquid interface.

The conservation equation for transport species takes the following form:

$$\rho(\frac{\partial y_i}{\partial t}) + \rho \nabla.(\boldsymbol{u} y_i) = -\nabla.\boldsymbol{J_i} + S_i \tag{7}$$

where y_i is the local mass fraction of i^{th} species, S_i is the source term for i^{th} species due to the reaction, and $\boldsymbol{J_i}$ is the diffusion flux of species *i*, which arises due to concentration gradients. Diffusion flux can be written as

$$\boldsymbol{J_i} = -\rho D_{i,m} \nabla y_i \tag{8}$$

here $D_{i,m}$ is the diffusion coefficient for species *i* in the mixture.

2.2. Numerical implementation

In this research GAMBIT 2.2 was used to create the geometry. To divide the geometry into discrete control volumes, more than 4×10^5, 3D tetrahedral computational cells and 9×10^4 nodes were used. Figure 1 shows the schematic of the computational domain, liquid entrance and particle grid.

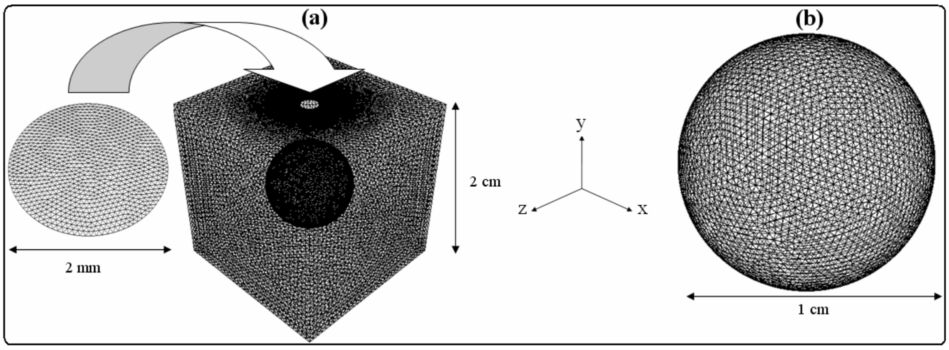

Fig. 1. (a) grid and dimensions of the computational domain and liquid entrance, (b) particle grid.

The VOF approach implemented in the commercial code for computational fluid dynamics, FLUENT, has been used for the simulations. Using the appropriate under-relaxation factors a reasonable rate of convergence was achieved. It is worth noting that refinement of the grids did not produce any significant differences in the results.

Liquid velocity at the entrance was set to 0.01 m/s. The inlet air velocities from the bottom side were 0.01 and 0.5 m/s. The initial concentrations of ferrous, ferric and zinc ions was set to 5, 0 and 0 g/l, respectively.

3. Results and discussion

The snapshots of the concentration profile of ferric ion in the liquid phase are illustrated in Fig. 2 (a-d). As Fig. 2 (b-c) shows the concentration of ferric ion due to the reaction (1) firstly was increased and again it was decreased because ferric ion consumed according to the reaction (2).

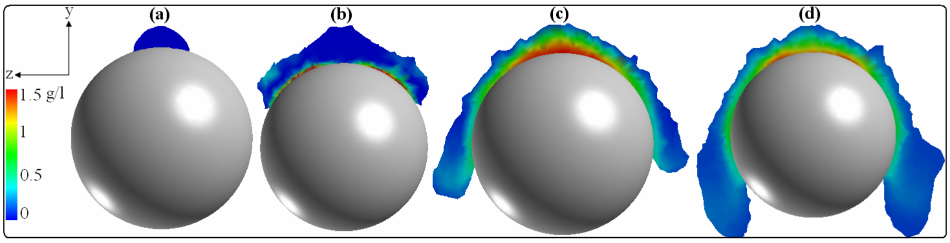

Fig. 2. Snapshots of the concentration profile of ferric ion. Realizations each separated by 0.01 s and the simulation was carried out for the inlet air velocity of 0.01 m/s.

Fig. 3 (a-d) illustrates the temporal evolution of the concentration profile of zinc ion on the surface of particle in the plane passing through its centre. The initial concentration of zinc ion according to Fig. 3 (a) is zero. As Fig. 3 (b) shows the concentration of zinc at the beginning of simulation is very low. The reason is that firstly zinc sulphate was produced by reaction (2). Sulphuric acid was generated by reaction (3) and its participation in the reaction (4) increased the zinc ion concentration as it can be seen in Fig. 3 (c-d).

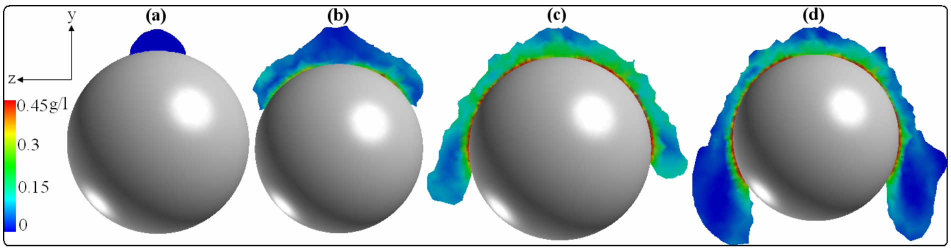

Fig. 3. Snapshots of the concentration profile of zinc ion on the surface of particle. Realizations each separated by 0.01 s and the simulation was carried out for the inlet air velocity of 0.01 m/s.

In Fig. 4 variations of concentration profiles of ferric and zinc ions from the surface of particle towards the liquid bulk have been shown in 2-D plots.

Concentration variations are considered in 1 mm layer of liquid. From 2-D plots it is clear that the concentrations of both species decrease dramatically in the thin layer of liquid. For example, maximum concentration of ferric on the surface is 1.5 g/l while it decreases to about 0.5 g/l at 0.5 mm from the surface. The ferric ions concentration, measured in the bulk of the liquid, differ significantly from the concentrations on the surface of sulphide mineral. Metodiev et al. [2] investigated the liquid velocity and ferric ions concentration profiles in the vicinity of *A. ferrooxidans*, attached to the surface of a sulphide mineral. In comparison our results are in good agreement with their results.

Fig. 5(a and c) shows the temporal evaluation of the liquid velocity field in the plane passing through the centre of the particle at inlet air velocities of 0.01 and 0.5 m/s respectively. In Fig. 5 snapshots were taken at $t = 2\times10^{-2}$ s. The results reported in this paper are in good agreement with the experiment results [1]. Simulations with high inlet air velocity, 0.5 m/s, represent two symmetric vortices (Fig. 5a). These structures could play an important role in the transport mechanism such as momentum dispersion [11]. These vortices may improve heat transfer, so the present simulation may open the possibility for developing a meaningful numerical model for the bioheap leaching where heat transfer is important.

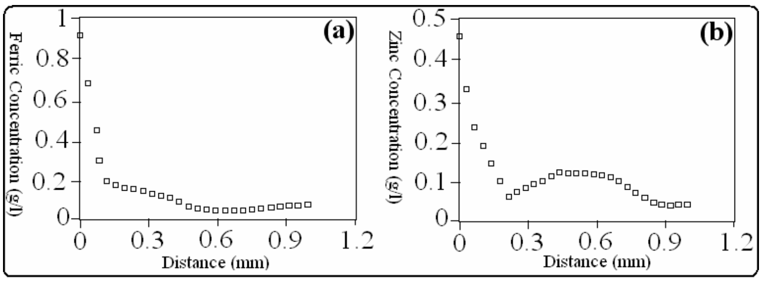

Fig. 4. 2-D plots for the variations of ferric (a) and zinc (b) concentration versus distance from the particle surface to the bulk of liquid

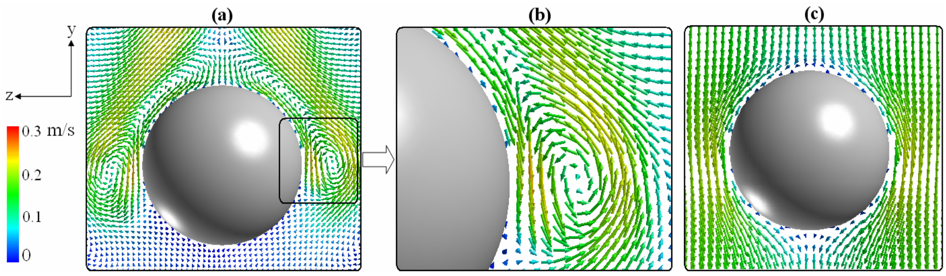

Fig. 5. Vector plot of liquid velocity field around single particle. Here the inlet air velocity is 0.5 and 0.01 m/s for parts a and c respectively. To obtain better visualization of flow field around the particle, the flow patterns marked in (a) is magnified and represented in (b).

4. Conclusion

In this study, computational fluid dynamics was performed to predict the liquid velocity field and ferric and zinc ions concentration profiles around a single particle, which are useful for the bioleaching. Results show that for prediction of concentration profiles and velocity field in the gas-liquid systems VOF method could be applied as an investigative tool. It provides good engineering descriptions, and can be used reliably for predicting the flow and concentration patterns in bioleaching process. It has been shown that due to the reactions, which was assumed occur on the surface, there is high local concentration of metal ions on the particle surface. Results show that the concentrations in a thin layer of liquid, less than 1 mm from the surface to the bulk, strongly decreased. Using inlet air velocity of 0.5 m/s some vortices around the particle were observed. This finding seems to have a significant impact in the design of efficient multi-phase reactors for the bioleaching process. These investigations have merit as a scientific tool and will have practical applications in the metal extraction.

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