International Journal of Heat and Mass Transfer 85 (2015) 390–400

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

A 3D coupled model of turbulent forced convection and diffusion for heat and mass transfer in a bioleaching process

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ARTICLE INFO

Article history:
Received 16 June 2014
Received in revised form 27 January 2015
Accepted 29 January 2015

Keywords:
Bioleaching pile
Numerical simulation
Biochemical reactions
Self-heating
Bio-hydrometallurgy

ABSTRACT

The bioleaching unlike the leaching is a process catalyzed by bacteria. Generally, the mine material containing is previously agglomerated to build piles. A three dimensional mathematical model to describe the fluid mechanics, mass and heat transport that consider inside the pile source terms for oxidation reaction, biological kinetic, and oxygen depletion due to methanogenic bacteria (15–45 °C), is presented. The Reynolds average equation with the κ–ε turbulence model was considered for the air surround it. An experimental leaching pile of tailing agglomerated was performed and built in order to obtain data with which to compare the numerical results. The results of computational simulations using the proposed mathematical model and the finite volume method were successfully validated comparing it with those experimental results. The numerical simulation allows to describe the internal effect of the bacteria on temperature, oxygen concentration and acid evaporation for a pile in field with bioleaching process.

1. Introducction

The bioleaching is a leaching process catalyzed by microorganisms and applied to copper sulfate minerals to improve the dissolution kinetic. The bacteria involved in the process are generally autotrophic, aerobic and chemosynthetic and resistant to extreme acid and high metal concentration media. The copper extraction from minerals such as chalcocite (Cu_2S) and covellite (CuS) by bioleaching is practiced commonly in mines around the world. The thermophilic bacteria are the most studied due to the advantages in bio-hydrometallurgy processes. In order to reach maximum copper extraction from the pile, in the range between 80% and 90%, a time period of 250–350 days of process is required [1]. The oxidation reactions are exothermic thus allowing self-heating of the pile which improves the copper extraction and consequently the acid depletion.

Ojumu et al. [2] made a review of the rate equations proposed for microbial ferrous-iron oxidation. Ogbonna [3] proposed a dimensional mathematical model of agglomerate scale phenomena in heap bioleaching solved by using the finite difference method. The numerical simulations have been applied to bioleaching piles by finite difference methods [4–7], finite element methods [8,9] and finite volume methods [8,10]. A mathematical model for the self-heating in piled material introduced by Sidhu et al. [11] was modified [12–14] to include the oxidation kinetic being catalyzed by thermophilic microorganisms in the bioleaching pile. This model has the particularity of combining the effect of the growth of microorganism colonies in a parametric equation, comparatively simple compared to classical equations of biologic kinetic. The oxidation reaction of the organic matter can be described by an Arrhenius type equation [11]. In order to predict the solute flow in soil one equation that considers the advection (Darcy law), diffusion (Fick law) and hydrodynamic dispersion have been developed [15]. This equation considers that solute is diluted in water thus flowing with it [15]. The three dimensional resulting mathematical model is solved by the classical finite volume method [16].

The objective of this paper is to describe a novel mathematical model for heat and mass transfer inside a bioleaching pile and in the surrounding air by using finite volume method simulations. In this paper a coupled three dimensional mathematical model for oxygen flow, thermal energy and acid solution inside a bioleaching pile and for temperature, acid solution and turbulent fluid mechanics in the surrounding air is proposed. In the mathematical model the chemical and biological reactions that occur in the pile are

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.01.135
0017-9310/

Nomenclature

A_1	pre-exponential factor for the oxidation [1/s]
A_2	pre-exponential factor for the inhibition of biomass growth [–]
C	concentration [kg/m^3]
$C_{p,T}$	coefficient dependent on geometric, thermal and material property values [J/kg K]
C_{H^+}	acid concentration [kg/m^3]
D	diffusion coefficient [m^2/s]
E	activation energy [J/mol]
k	thermal conductivity [W/m K]
H	head pressure [m]
K_I	cell inhibition constant [cell/l]
K	inhibition constant [mol/l]
K_d	distribution coefficient [m^3/kg]
G'''	volumetric heat generation density [W/m^3]
Q	exothermicity of the biomass growth reaction [J/kg]
N	microbial population [cells/l]
R	ideal gas constant [J/K mol]
R_f	retardation factor [–]
T	time [d]
T	temperature [K]
tp	total number of experimental points [–]
S	source term [–]
s	adsorption [–]
x	cartesian axis direction [m]
y	Cartesian axis direction [m]
z	cartesian axis direction [m]

Special characters

ρ	density [kg/m^3]
$\rho_{s,b}$	bulk density [kg/m^3]
θ	volumetric water content [–]
F	function [–]
μ_{mox}	reaction velocity for the mass oxidation [m^3/kg s]
μ_{mgr}	reaction velocity for the biomass growth [1/s]
υ	viscosity [–]
κ	turbulent kinetic energy [m^2/s^2]
ε	dissipation of turbulent kinetic energy [m^2/s^2]
ξ	tortuosity [m]
E	porosity [–]
λ	dispersivity [kg/m^3 d]
λ^*	degradation constants for a chemical reaction of zero order [kg/m^3 d]
v	porous mean velocity [m/d]
ϕ	variable [–]
δ	first order degradation constant [–]

Subscripts

B	biomass
eff	volumetric effective expression
Fe	ferrous
Fl	fluid phase
in	inlet
irr	irrigation
m	mass
max	maximum
mgr	mass growth
Ox	oxygen
p	pile
s	solute
sf	sulfur
T	temperature
t	turbulent

included. Outside the pile the Reynolds average equation, in terms of the κ–ε model, besides the unsteady convective diffusive temperature and solute equations are used to describe the turbulent air flow around the pile. An experimental leaching pile of tailing agglomerated was performed and built to obtain measured data to compare with the numerical results. Analytical results are contrasted with numerical results for reactive solution transport. Experimental data or analytical results against numerical results were compared to validate the algorithm accuracy. A study case of a bioleaching pile allows the calculation of the variation in time for the internal spatial distribution of the turbulent kinetic energy, rate of dissipation of the kinetic energy, temperature and solute evaporation in the air flow around the pile, and temperature, oxygen depletion and solute transport including the biochemical self-heating reaction inside. The results showed that is possible to predict the solute flow and the water transport in the agglomerated material and quantify the surface effects of the air around it.

2. Mathematical model

2.1. General physical arrangement of the bioleaching pile in fields

Due to the big size and the extreme acidic conditions of the bioleaching pile, their disposal is generally in field under ambient conditions. This generates an important challenge to control the biochemical process conditioned by external ambient variables that cannot be controlled. These ambient variables must be considered coupled with the internal process to achieve good predictions. The mathematical model considers the transient coupled three-dimensional transport of momentum and thermal energy in the air around of the pile, as well as the diffusion of heat, oxygen and solute concentration in the agglomerated material, being treated as a porous medium. These are the main variables that must be taken into account in field to control the process. The physical general configuration is schematically shown in Fig. 1, and corresponds to a pile with the agglomerated material disposal in field. The size of the physical domain used in the calculations is $xl = 200$ m, $yl = 30$ m and $zl = 70$ m. The physical situation described in Fig. 1 is used in Section 4.2 to validate the numerical results for the water flow, and to calculate temperature, reactive flows and oxygen concentration in Section 4.3. The soil below the pile is assumed to be impermeable with a constant uniform temperature. Air at ambient temperature is forced into the calculation domain with a constant velocity. Symmetric boundary conditions in the other planes were considered.

The solution strategy includes a turbulent unsteady convective 3D model for the air flow around the pile. The κ–ε turbulent convective model is not activated inside the pile. Here, only heat and mass transfer by diffusion are considered and hence temperature, oxygen and solute concentration are calculated within the pile. The mathematical model includes the heat generation, oxygen and solute source terms inside the leaching pile. The turbulent heat and mass transfer convective model for the surrounding air flow and the heat and mass diffusion model inside the leaching pile are solved in a conjugated way as described in Section 2.3, respectively. The details of the boundary conditions incorporated in the mathematical model are included in Section 2.4.

The dependent variables calculated in the air outside of the pile are the three time averaged velocity components $\overline{u}$, $\overline{v}$, $\overline{w}$, the turbulent kinetic energy κ, the dissipation of turbulent kinetic energy