Verification of numerical modeling results using analytical solution for oxygen diffusion process in sulfide waste dump

AHMAD ARYAFAR* , FARAMARZ DOULATI ARDEJANI* 
*Faculty of Mining Engineering, Oil and Geophysics  
Shahrood University of Technology  
Shahrood, Iran, P.O.Box. 36155-316

Abstract: Weathering of pyrite-containing rocks causes the well-known problem of acid rock drainage. Depending on the rate of pyrite oxidation, availability of water and oxidants and buffering capacity of surrounding rocks and sediments, the pH of the drainage is often very low[1]. When the pyrite or other sulfide mineral exposure by the atmosphere and water, the acid mine drainage was generated. Oxygen can be transported into the waste deposit by three mechanisms: (1) advective transport with water, (2) free ore forced air convection and (3) diffusion in the gaseous and aqueous phases through pores in waste material[2]. In generally, the pyrite oxidation and acid generation were controlled by oxygen diffusion. So, in this research was attempted that variation of oxygen concentration in waste dump depths was investigated and the analytical and numerical models results (obtained using PHOENICS software)[3] were compared. The obtained results can use for controlling and reducing the environmental impacts.

Keywords: Numerical modeling- Analytical model- Oxygen diffusion- Waste dump- Sulfide mineral- PHOENICS software

1 Introduction

Open pit mines involve the mobilization of large amounts of overburden that need to be disposed in waste rock dumps. If pyrite is present, acid drainage may result[4]. There are various environmental problems that may be associated with mining, such as surface water acidification and the discharge of heavy metals to surface and groundwater these problems are due to the fact that mine waste often contains different sulfide minerals containing iron and heavy metals, where pyrite is the predominant sulfide mineral.

The waste dump environments is a complex system of coupled physical and biogeochemical processes which can be divided into primary processes (e.g. water infiltration, water-saturation, oxygen diffusion, sulfide oxidation) and secondary processes (e.g. microbial activity, secondary precipitates, complexation, surface run off)[5].

Both oxygen and water are required for the continual oxidation of sulfide minerals. If only oxygen is available, the mineral will still oxidize, but the oxidation products will not be transported away from the sulfides, since water is necessary to dissolve and transport the oxidation products. Oxygen also supports the production of ferric iron; witch is another oxidant of sulfide minerals. If there is no oxygen supply, sulfide oxidation reactions will be prevented[2]. It has been shown that the important parameters affecting pyrite oxidation are: PH, concentration of oxygen, presence of bacteria, concentration of ferric iron, temperature, and specific surface area of the mineral.

Oxygen can be transported into the waste deposit by three mechanisms: (1) advective transport with water that contains oxygen, (2) free or forced air convection through the top layer of the waste dump and (3) diffusion in the
gaseous and aqueous phases through pores in the waste dump. The last mechanism is the dominant mechanism for transporting the atmospheric oxygen from the surface of the dump to the depth where the oxidation takes place. For importance of this problems, in this research was attempted the oxygen concentration profile in waste dump using analytical and finite volume numerical model was compared. Such results can be used for waste management in order to control of pyrite oxidation.

2 Analytical equations of oxygen diffusion and obtained results

By many researchers, oxygen diffusion process within waste dump in stead/non-steady state condition was formulated. Oxygen diffusion mechanism in either gas or water phase may be treated as one-dimensional, and can then be approximated by Fick’s first law as following:

\[ F_{O_2} = -D_{eff} \frac{C}{\theta_a} \frac{d}{dz} \]  

Where \( F_{O_2} \) is the mass flux of oxygen (mass flux per unit area per unit time), \( \theta_a \) is air-filled porosity (volume per volume), \( D_{eff} \) is the effective diffusion coefficient (for air \( 1.8 \times 10^{-5} \) m²s⁻¹ for water \( 2.2 \times 10^{-11} \) m²s⁻¹), \( C(t) \) is concentration at time \( t \) (mass per volume) and \( z \) is depth of dump (m). In dumps \( D_{eff} \) is a function of the diffusion coefficient for oxygen in air and a factor that depends on the percentage of gas-filled pores (related to the volumetric moisture content) and a tortuosity factor characterization of the soil.

The air-filled porosity, \( \theta_a \), can be related to the degree of saturation, \( S_r \), where \( \theta_a \) is the total porosity, according to equation (2): \[ \theta_a = \theta_t (1 - S_r) \]

The oxygen diffusion rate in the unsaturated zone is high, relative to the saturated zone, since the oxygen diffusion rate is 10000 times faster in air than in water [6]. Therefore, in the unsaturated zone, the sulfide oxidation rate may be relatively rapid, since the potential availability of both water and oxygen is large. Below the groundwater table, oxygen diffusion is heavily reduced, and the oxygen content is limited to its solubility in water, which results in that sulfide oxidation should occur slowly below the groundwater table.

Since, the oxygen concentration within dump varies by time, so equation (1) is not appropriate. The analytical equation of oxygen diffusion in transient state can be expressed as below:

\[ \frac{\partial C}{\partial t} = D_{eff} \frac{\partial^2 C}{\partial z^2} \]  

To solve the equation (3) the input and output boundary condition were considered as below:

- Boundary condition for input of model \( C(z=0,t)=C_0=0.21 \)  
- Initial condition \( C(z,0)=0 \)

Solution of equation (3) by considering above boundary and initial condition was obtained as below:

\[ C(z,t) = C_t + (C_0 - C_t) \text{erfc} \left( \frac{z}{\sqrt{4D_{eff}t}} \right) \]  

As a case study, oxygen concentration for a waste dump under below conditions was calculated:

- Waste dump type: sulfide
- Mineral type: chiefly pyrite
- Dump depth: 5 (m)
- Time steps for modeling: 6, 9, 12, 24 (month)

The oxygen concentration profile for 6, 9, 12, 24 (month) time steps was illustrated in the Figs. 1, 2.
Consequence, the role of effective diffusion coefficient in oxygen diffusion process was investigated and the result was depicted in Fig.3.

The obtained results from analytical solutions, show, and the increase of effective diffusion coefficient affect more the oxygen flux on top layers. Results express the oxygen flux in deeper depth decrease such that the pyrite oxidation stops or diminishes. Another point, since the erfc function values by interpolation must be obtained, so it is not possible to gain the accurate values for oxygen concentration.

3 Numerical modeling for oxygen diffusion within waste dump using PHOENICS software

Airflow and ARD production in waste dump is a complex process involving multiphase flow (gas and water), chemical reactions, heat transfer, and mass transfer in the liquid phase (infiltration) and in the gas phase (advection, diffusion). Numerical simulation is needed to handle all those processes and understand their interactions. Only few numerical models are currently available to represent the physical processes acting within waste dump.

In the present research, PHOENICS that is a computational fluid dynamic (CFD) code was used. PHOENICS is adapted for modeling of oxygen diffusion and acid rock drainage, especially in waste dump. In this code, the
governing equation was solved based on finite volume numerical model. For a detail description of this numerical simulator, the reader is referenced to CHAM (2007) [3]. In this research, the oxygen diffusion process in waste dump for time interval 6, 9, 12 and 24 month was illustrated. Obtained results from both analytical and numerical model have been compared in Fig.4.

Obtained results from numerical modeling show the oxygen concentration decrease from surface to depth of dump, and by increase in effective diffusion coefficient, the oxygen flux will increase.

4 Conclusions
Pyrite oxidation and acid rock drainage are the most important environmental problems in mining environments. One of the effective factors in generation of AMD in waste dump is oxygen concentration. By modeling of effective factors in pyrite oxidation and using of obtained results can reduce or eliminate the environmental impacts of oxidation that is named the waste dump management. In this research, the oxygen diffusion process both analytical and numerical models, were simulated and was indicated that the effective diffusion coefficient has an important role in oxidation and pollution production. Because of approximation estimation in analytical modeling, the obtained results is less reasonable relative to numerical modeling, consequence by considering of reaction kinetic for both analytical and numerical models, the oxygen diffusion process was simulated.

References:

