1-Dimensional numerical modelling of unsaturated water flow and oxygen diffusion in overburden material column using hydrus 1-D

Jarwinda1, A Badhurahman2, G J Kusuma2,3 and R S Gautama2,3
1 Department of Mining Engineering, Industrial and Production Technology, Institut Teknologi Sumatera, Indonesia
2 Centre of Research Excellence in Mining Environment and Mine Closure (CoRE MEMC), Faculty of Mining and Petroleum Engineering, Institut Teknologi Bandung, Indonesia
3 Department of Mining Engineering, Institut Teknologi Bandung, Indonesia
*Corresponding author’s e-mail: jarwinda@ta.itera.ac.id

Abstract. Coal mining activities, especially overburden material dumping can cause a negative impact into the environment, i.e., acid mine drainage. Acid mine drainage is characterized as low pH water with high sulphate and metal content produced from sulphidic-bearing overburden material with oxygen and water. In unsaturated condition, both of gaseous and water phases exist, acid mine drainage is generated. This study aims to characterize and model the water content in unsaturated condition and diffusion of oxygen of overburden material using the Hydrus 1-D software in a laboratory-scaled column. Laboratory-scaled column is initially filled with 75-cm height of dry overburden material and subjected into 5-cm constant head water level at the top of the column with free-flow condition at the bottom of column. The modelling result shows the water content of overburden material varies within depth and time elapsed and is saturated between 32400 minutes and 36000 minutes after initial wetting. Diffusivity of oxygen is linearly correlated with the water content of the overburden material at any given time and depth that varies between $1.34 \times 10^{-7}$ m$^2$/s and $8.80 \times 10^{-12}$ m$^2$/s. Water content and diffusivity of oxygen is expected to affect the generation of acid mine drainage in the overburden material.

1. Introduction
Coal mining activities, especially dumping activity of overburden material can pose a negative impact into the environment[1]. One of the negative impacts is acid mine drainage[2], which is characterized as low pH water with high sulphate and metal content which produced from sulphidic-bearing overburden material with oxygen and water[2,3].

To inhibit the acid mine drainage generation on a mine site, the process of acid mine drainage formation in overburden is essential[4]. Chemical process of acid mine drainage in overburden dumping site is affected by its physical condition of overburden material. Pores in overburden material can be not only filled with air which consist of nitrogen, oxygen and other gases but also fill with water. In unsaturated condition, in which both gaseous and water phases are exist, the acid mine drainage is generated[5,6].

Previous studies in modelling of water content in unsaturated condition and their relationships with oxygen diffusion in mine tailing are abundant[5,6], but the study using overburden material from coal
mine is still limited. Indonesia as the 1st exporter of coal and produces more than 500 million ton of coal in 2020 [7] is expected to face acid mine drainage problems from coal mines in the foreseeable future. Thus, the processes of acid mine drainage generation from overburden material of coal mine affected by water content and oxygen diffusion are essential to be studied in order to manage and minimize the negative impact of the environment. This study aims to characterize and model the water flow in the unsaturated zone and diffusion of oxygen of overburden material using Hydrus 1-D software as a preliminary study of further study in the laboratory in term of explaining the effect of water content and diffusion of oxygen into the generation of acid that may drainage from coal overburden material.

2. Materials and Methods

2.1. Material
Material used in this study is an overburden material from coal mine, which characterized as potentially acid forming material with high probability of producing acid mine drainage through oxidation of pyrite and dissolution of iron-bearing sulphate mineral. Particle size distribution of material is shown in Figure 1.

Based on the particle size distribution analysis, the overburden material consists of 21.39% clay-sized material, 43.41% silt-sized material and 35.20% sand-sized material. Plot of the ternary diagram of soil texture (United States Department of Agriculture) in Figure 2 shows that the overburden material is classified as clay loam which yields moderately permeability of water.

![Figure 1. Particle size distribution](image1)

![Figure 2. Ternary diagram of soil texture](image2)

2.2. Methods
The water flow modelling is conducted using Hydrus 1-D software[8]. Hydrus 1-D is developed to simulate one dimensional water flow in incompressible, porous and unsaturated media, both in transient and steady-state regime using discretization and numerical modelling of Richards equation, which requires geometry information and discretization, boundary condition, initial condition, material hydraulic properties as its inputs[9].

Water flow in unsaturated material is governed by Richard’s equation[10] as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K \left( \frac{\partial \theta}{\partial z} + 1 \right) \right]$$  (1)
Where h is water pressure head, θ is water content of soil, K is the hydraulic conductivity, which is varies in different θ value, t is time-related reference and z is spatial coordinate, usually depth. The model uses van Genuchten equations to set the water retention curve θ(h), which relates the volumetric water content in pressure potential to the hydraulic conductivity curve K(h) as follow[11]:

\[ \theta(h) = \theta_r + \frac{\theta_s - \theta_r}{1 + |\theta h|^{\alpha}} \gamma, \text{for } h < 0 \]  
\[ \theta(h) = \theta_r \text{, for } h \geq 0 \]  

Where, α, β = van Genuchten parameters, γ is equal to 1 - \frac{1}{\beta} or assumed as 0.5, \theta_r is residual water content of material, \theta_s is saturated water content of material. Hydraulic conductivity of unsaturated material is further calculated using equation as shown below[12,13]:

\[ K(\theta) = K_s r S_e \left[ 1 - \left( 1 - S_e^{1/m} \right)^m \right]^2 \]  
\[ S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \]  

Where m = 1 - (1/n), n > 1 and Ks is the saturated hydraulic conductivity, Se is the effective saturation, and r-is the pore connectivity saturation, and is assumed as 0.5.

Diffusivity of oxygen in unsaturated overburden material is calculated using a proposed simple predictive equation as follow[14]:

\[ D_e = \frac{1}{n^2} \left[ D_a \theta_a^{3.4} + H D_w \theta_w^{3.4} \right] \]  

Where De is effective diffusivity of oxygen, Da is diffusion coefficient of oxygen in air (≈ 1.8 × 10^{-5} m^2/s), Dw is a diffusion coefficient of oxygen in water (≈ 2.5 × 10^{-9} m^2/s), H is Henry equilibrium constant of (H ≈ 0.03 at 20º C for oxygen)[15].

Material is mounted into an acrylic column with diameter of 15cm and length of 100cm, which is only 75cm of column length is filled with overburden material. Bottom side of the column is connected into water-filled syphon pipe to prevent air flow from below. Upper side of column is filled with constant head of water (5cm) in order to provide water fluxes from above, as show in Figure 3.

Figure 3. Schematic of overburden-filled column
3. Result and Discussion

3.1. Unsaturated Water Flow Modelling

Further laboratory testing is conducted to determine the parameters needed for modelling. Hydraulic properties, i.e. hydraulic conductivity of saturated overburden is determined using falling head permeameter. In the other hand, Van Genuchten parameters for determining soil water characteristic curve is using neural network prediction based on physical parameters of material provided by Hydrus 1-D software[8][9]. Hydraulic properties of overburden material are shown in Table 1. Input parameter based on laboratory condition of overburden column is presented in Table 2:

| Table 1. Material hydraulic properties of Hydrus-1D model |
|----------------------------------------------------------|
| Hydraulic properties                                    |
| θr (cm³/cm³)    | 0.056 |
| θr (cm³/cm³)    | 0.2166 |
| α               | 0.0291 |
| β               | 1.1613 |
| γ               | 0.5   |
| Ks (cm/min)     | 0.00018 |

| Table 2. Input parameters of Hydrus-1D model |
|---------------------------------------------|
| Parameter                               | Values                |
| Geometry Information                    |                        |
| Depth (cm)                               | 75                     |
| Mesh Size (cm)                           | 0.75                   |
| Number of Nodes                         | 101                    |
| Number of Layer                         | 1                      |
| Time Information                         |                        |
| Simulation Time (minutes)                | 36000                  |
| Time Step (minutes)                      | 1                      |
| Print Time (minutes)                     | Increment of 3600      |
| Boundary Condition                       |                        |
| Water Flow                               |                        |
| Upper Boundary Condition                 | Constant Pressure Head |
| Lower Boundary Condition                 | Free Drainage          |
| Initial Condition                        |                        |
| Water Pressure Head at z=0 (cm)          | 5                      |
| Water Pressure Head at z ≠0 (cm)         | -10⁴ (dry material)     |

The soil water characteristic curve (SWCC) based on hydraulic properties presented in and Van Genuchten equation for overburden material is shown below (Figure 4). The SWCC is further is used to model soil water profile along abovementioned time increment as shown in Figure 5 as a result of modelling using Hydrus 1-D.

![Figure 4. Soil water characteristic curve (SWCC) of the overburden material based on van Genuchten equation](image-url)
It is evident that water content varies within depth and time elapsed. The overburden material of 75 cm depth is expected to be saturated between T10 and T11, i.e. between 32400 and 36000 minutes. The propagation of the soil moisture and water fronts takes place through the column upon the application of a constant head and a free drainage boundary at the inlet and outlet, respectively. The simulation using same soil type (loam soil) [16–18] with different hydraulic results shows longer time for saturated condition obtained (> 12 hours opposed to 9 – 10 hours in this study) since the flow in unsaturated materials are directly governed by their hydraulic properties[10,19]. The material used in this study is semi-compacted, thus reduce the porosity and saturated water content.

3.1.1. Diffusivity of Oxygen inside Overburden Column
Diffusivity of oxygen is calculated using equation 5 and the result is presented on Figure 6. It is evident that diffusivity of oxygen is linearly correlated with water content of the overburden material at any given time and depth, and varies between $1.34 \times 10^{-7}$ m$^2$/s and $8.80 \times 10^{-12}$ m$^2$/s. This result is also predicted in different porous medium[14].
4. Conclusion
From the abovementioned results, water content varies within depth and time elapsed and affecting linearly the effective oxygen diffusivity of overburden material.

It is evident that the diffusivity of oxygen in saturated overburden material is much smaller than that in dry overburden material by a factor ten-thousands, thus redox condition inside overburden column is expected to be shifted from oxic into anoxic condition as the effective diffusivity of oxygen decreased and oxygen availability/content inside overburden material is shrinking.

Further study using laboratory-scaled physical model is imperative to calibrate the numerical modelling of water content and oxygen diffusion in the overburden material. Coupling the unsaturated flow model in the overburden material with geochemical modelling will provide a clearer explanation on processes of acid mine generation in the laboratory which can be applied in the field to minimize its negative impact.

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