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Application of artificial neural networks to predict pyrite oxidation in a coal washing refuse pile

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HIGHLIGHTS

- ▶ We predict the pyrite oxidation applying artificial neural networks (AANs).
- ▶ In comparison to classical techniques, fewer parameters are needed for prediction.
- ▶ Unlike mathematical models, ANN makes no prior assumptions about data distribution.
- ▶ Pyrite content remained within the waste particles increases gradually with depth.

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ABSTRACT

This paper presents a neural network model to predict the pyrite oxidation in the spoil of the Alborz Sharghi coal washing refuse pile, northeast Iran. Spoil depth, annual precipitation, effective diffusion coefficient and initial amount of pyrite in the spoil particles were used as inputs to the network. The output of the network was the amount of pyrite remained in the spoils at different depths. Feed-forward artificial neural network with back-propagation learning algorithm with 4-7-4-1 arrangement was found capable to predict the rate of pyrite oxidation. The network was used to predict the amount of pyrite remained at different depths of three trenches over the refuse pile. Simulated values obtained by the network were very close to the experimental results. The correlation coefficient (R) value was 0.99821 for training set, and in testing stage the R value was 0.99007, 0.9958 and 0.99898 for trench 1, trench 2 and trench 3 respectively which shows the model prediction was quite satisfactory.

1. Introduction

Acid mine drainage (AMD) is the most important environmental concern relating to mining operations and areas having sulphide rich waste dumps. AMD is often characterised by low pH, with high concentrations of iron, sulphates and heavy metals of varying composition dependent upon the originating mineral deposit types [1]. Oxidation of sulphide minerals, in particular pyrite, as the most abundant sulphide mineral, resulting from the exposure of these minerals to both oxygen and water [3], is the most important factor in producing AMD. So, the first step in an environmental survey of an area including sulphide rich waste-dumps is to evaluate the proportion of sulphide minerals especially pyrite and their oxidation.

Previously, several mathematical models have been developed to predict the pyrite oxidation and AMD generation (e.g., [4–9,11,12]).

A one-dimensional model for oxidation and leaching processes was developed by Cathles and Apps [4]. Temperature dependence, oxygen balance and air convection effects were the parameters used for this model of which air convection was assumed to be the main mechanism of oxygen transport through the dump to oxidise ferrous ion in the presence of iron oxidising bacteria.

Jaynes et al. [5] developed a one-dimensional finite difference model called POLS for simulation of AMD in a reclaimed strip mine. Direct molecular oxygen oxidation and ferric iron oxidation were included in the model and it was assumed that pyrite oxidation is controlled by first-order kinetics and the rate of diffusion of oxidant into the reaction particle. The model further assumes that the oxidation products are removed from the reclaimed strip mine by percolating surface water. The role of groundwater in transporting the oxidation products was neglected [12].

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Davis and Ritchie [7] presented a one-dimensional mathematical model for pyrite oxidation within the White's overburden dump at Rum Jungle, Australia, where diffusion of oxygen to the reaction sites is the rate-limiting factor. The modelling was carried out in a two-stage approach with: first, the diffusion of oxygen into the pore space of the dump, and second, a shrinking core model to describe the diffusion of oxygen into the individual particles through the oxidised coating that forms around the unreacted core of the particles.

The numerical model developed by Elberling et al. [8] can be used to simulate pyrite oxidation in tailings. The model was formulated by combining the effect of oxygen diffusion to a depth where oxidation takes place with first-order kinetics with respect to oxygen. The rate of pyrite oxidation in the model is based on the continuity relationship for oxygen with both oxygen transport through the tailings and the consumption of oxygen at the surface of the sulphide minerals grains.

Gerke et al. [15] modelled the impact of physical and chemical heterogeneity on solute leaching in pyritic overburden mine spoils. The major processes considered consist of variably saturated water flow, oxygen diffusion, shrinking core kinetics of pyrite oxidation, multicomponent reactive solute transport and geochemical equilibrium reactions between aqueous and mineral components.

Doulati Ardejani et al. [11] presented a combined mathematical-geophysical model for prediction of pyrite oxidation. Effective diffusion coefficient, pyrite fraction, bulk density of spoil, molar density of pyrite within particle, surface area of pyrite per unit volume of spoil, diameter of particles, first-order rate constant for oxygen, diffusion coefficient of oxygen in water, recharge value and waste column depth were considered in their simulation.

The multiplicity of the factors that affect the pyrite oxidation complicates the model development using classical techniques. In other words, in these classical techniques, it is necessary to obtain a variety of different factors to develop the model which take a long time and of course, so many experiments, which are needed to measure these factors, increase the probability of having more errors in the calculations. In addition, in these classical methods some data distributions and boundary conditions must be assumed which are not necessarily true in the nature. In contrast, approximation models such as artificial neural networks (ANNs) provide a very powerful and reliable tool for accurately predicting the non-linear behaviour of pyrite oxidation process. Unlike other modelling techniques, the artificial neural networks make no prior assumptions concerning the data distribution [26].

Artificial neural network is an empirical modelling tool, which is analogous to the behaviour of biological neural structures [27]. Artificial neural networks are basically a family of massively parallel architectures that solve difficult problems via the cooperation of highly interconnected but simple computing elements (or artificial neurons) [23]. The applications of artificial neural networks are finding their use in ecological and environmental sciences since 1990s [19]. Colosanti [28] recommended the utilisation of ANN for ecological modelling. The use of such networks is rapidly growing in different studies especially in process modelling, simulation and predictions (e.g., modelling the greenhouse effect [25], simulation N_2O emissions from a temperate grassland ecosystem [22]. Prediction of spontaneous heating susceptibility of coals [23]). These works have shown that the use of ANNs is so easier and more reliable.

In this research we applied artificial neural network to predict the pyrite oxidation process within the spoils of a refuse pile produced by the Alborz Sharghi active coal washing plant, northeast Iran. For this purpose, MATLAB software was used. In the presence of oxygen, pyrite is oxidised to form Fe^{2+}, SO_4^{2-} and H^+ and the amount of the pyrite within the spoil decreases subsequently. According to this fact we measured the amount of pyrite remained in the spoils at different depths to investigate the rate of pyrite oxidation.

2. Area description

2.1. Pyrite oxidation and AMD generation

The chemical reaction describing pyrite oxidation by O_2 is expressed by the following equation:

$$FeS_2 + 7/2\ H_2O \ \rightarrow\ Fe^{2+} + 2\ SO_4^{2-} + 2\ H^+ \tag{1}$$

Fe^{2+} which is produced by the pyrite oxidation (Eq. (1)) forms Fe^{3+} during the following reaction:

$$Fe^{2+} + 1/4\ O_2 + H^+ \ \rightarrow\ Fe^{3+} + 1/2\ H_2O \tag{2}$$

Fe^{3+} will be used by the reaction between pyrite and Fe^{3+}, generating more Fe^{2+}, SO_4^{2-} and H^+ according to the following equation [13]:

$$FeS_2 + 14\ Fe^{3+} + 8\ H_2O \rightarrow 15\ Fe^{2+} + 2\ SO_4^{2-} + 16\ H^+ \tag{3}$$

In presence of the lithotrophic bacteria "*acidithiobacillus ferrooxidans*", this reaction has an important role in pyrite oxidation. Fig. 1 shows a schematic diagram describing pyrite oxidation and subsequent pollutants leaching from a waste dump. Fig. 1 identifies oxygen diffusion, pyrite oxidation in waste materials, surface recharge, chemical reactions and the transport of oxidation products through coal waste materials [11].

2.2. Site description

Alborz Sharghi coal field consists of sandstone, thin bedded coaly shale of Shemshak formation and alluvial deposits. The extracted coal from the region, are washed in Alborz Sharghi coal washing company which is located northeast of Damghan and 57 km from Shahrood [24]. Extracted coals are washed either using jig machine or in a flotation process and wastes of each method is dumped separately. In the present study, samples were cut out of jig machine refuse pile. The location of study area and a schematic view of pile are shown in Fig. 2. As it is shown in the Fig. 2, samples were collected from three different points.

3. Materials and methods

3.1. Sampling and measuring the pyrite amount

Five samples were collected from trench 1 and six samples were collected from each one of two other trenches (total of 17 samples). Samples are extracted from different depths of trenches. For all points (trenches) the total depth of sampling was 2.0 m and the sampling interval was 0.4 m. First sample of trench 1 was cut out of the depth of 0.4 m and for two other trenches the first sample was taken from surface. Samples were oven dried at 105 °C for 72 h in the mineral processing laboratory at Amirkabir University of technology. Then grinding process was done applying jaw crusher, cone crusher and roll crusher respectively. For measuring the pyrite content remained in the spoils of different depths, a method presented by ASTM [16], was employed. For this purpose, we needed to achieve the maximum grain size of 0.00074 m (200 Mesh), therefore sieve analysis was done using five sieves with different sizes (30, 60, 100, 140, 200 Mesh). After obtaining the required grain size of samples (powders under the sieve No. 200 Mesh), Hydrochloric Acid (HCl) was used to dissolve sulphates and then the pyrite was extracted from the remained acid aqueous solution using Nitric Acid (HNO_3). An AA-670 Shimadzu atomic absorption at Shahrood University of technology was used to