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Artificial neural network application for predicting soil distribution coefficient of nickel

Amin Falamaki*

Department of Engineering, Payame Noor University, PO Box 19395-3697, Tehran, Iran

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ABSTRACT

The distribution (or partition) coefficient (K_d) is an applicable parameter for modeling contaminant and radionuclide transport as well as risk analysis. Selection of this parameter may cause significant error in predicting the impacts of contaminant migration or site-remediation options. In this regards, various models were presented to predict K_d values for different contaminants specially heavy metals and radionuclides. In this study, artificial neural network (ANN) is used to present simplified model for predicting K_d of nickel. The main objective is to develop a more accurate model with a minimal number of parameters, which can be determined experimentally or select by review of different studies. In addition, the effects of training as well as the type of the network are considered. The K_d values of *Ni* is strongly dependent on *pH* of the soil and mathematical relationships were presented between *pH* and K_d of nickel recently. In this study, the same database of these presented models was used to verify that neural network may be more useful tools for predicting of K_d. Two different types of ANN, multilayer perceptron and redial basis function, were used to investigate the effect of the network geometry on the results. In addition, each network was trained by 80 and 90% of the data and tested for 20 and 10% of the rest data. Then the results of the networks compared with the results of the mathematical models. Although the networks trained by 80 and 90% of the data the results show that all the networks predict with higher accuracy relative to mathematical models which were derived by 100% of data. More training of a network increases the accuracy of the network. Multilayer perceptron network used in this study predicts better than redial basis function network.

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1. Introduction

The distribution (or partition) coefficient (K_d) is an applicable parameter for modeling contaminant and radionuclide transport as well as risk analysis. This parameter is usually obtained from laboratory experiments. The five general methods of published literature to measure K_d values, include: the batch laboratory method, the column laboratory method, field-batch method, field modeling method, and soil organic carbon/water partition coefficient (K_{oc}) method (EPA, 2004). The K_d values may cause significant error in predicting the impacts of contaminant migration or site-remediation options. Therefore, selecting appropriate K_d values for different conditions is very important to estimate the behavior of contaminants and radionuclides in soils for making an environmental safety assessment (International Atomic Energy Agency, 1994). In this regards, different researchers presented various models to predict K_d values. Some of the models that are used in predicting K_d are the constant partition coefficient models, the parametric models, the isotherm adsorption models and mechanistic adsorption models (EPA, 1999). These models are used in computer codes to update K_d during the modeling of contaminant transport (Goldberg, 1995; Davis and Runnells, 1987). A limitation of some of these models is heterogeneity of environment.

The constant partition coefficient (which is defined as the ratio of quantity of adsorbate i.e., metal or radionuclide, adsorbed per unit mass of solid to the quantity of the adsorbate remaining in solution at equilibrium) does not shows sensitivity to changing conditions (e.g., *pH* and solution ionic strength). In the practical parametric K_d model, the K_d value varies as a function of empirically derived relationships with aqueous and solid phase independent parameters. Thus, it has the distinct advantage that considers new K_d values for each environmental condition. The empirical predictor equations may be derived commonly by statistical analysis and take the form of a linear and nonlinear polynomial expression. Table 1 shows some of the relations between K_d values

* Tel.: +98 912 3792901; fax: +98 711 6222262.
E-mail addresses: a_falamaki@pnu.ac.ir, afalamaki@yahoo.com, falamaki@spnu.ac.ir.

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Table 1
Relations between K_d values and environmental condition in soils.

Relationship	Species	Reference	Comments
Log $K_d = 2.0 + 0.1$ [NaOH] $- 26.8$ [HEDTA] $- 153.4$ [HEDTA]^2	Americium	Delegard and Barney (1983)	
$K_d = -0.54 + 0.45$ (pH).	Cadmium	EPA, 1999	Different soils
Log (K_d) $= 1.2 + 1.0$ log (CEC)	Cesium	Akiba and Hashimoto (1990)	A large number of soils, minerals, and rock materials
K_d(ml/g) $= 1639 - 902.4$ (pH) $+ 150.4$ (pH)^2	Lead	Gerritse et al. (1982), Rhoads et al. (1992)	Different soils
$K_d = 284.6$ (DCARB) $+ 27.8$ (CLAY) $- 594.2$	Plutonium	EPA, 1999	Different soils
$K_d = 488.3$ (DCARB) $+ 29.9$ (CLAY) $- 119.1$ (pH) $- 356.8$ (EC)	Plutonium	EPA, 1999	Different soils
$K_d = 25.7$ (DCARB) $+ 12.14$ CLAY) $+ 2.41K_d < 767.5$ $K_d = 286.0$ (DCARB) $+ 21.3$(CLAY) $- 81.2K_d > 767.5$	Plutonium	EPA, 1999	Different soils
log (K_d) $= -0.13 + 0.69$ (pH).	Thorium	EPA, 1999	The pH range of 4–8
K_d (ml/g) $= 9550\ C^{-0.335}$	Lead	Rhoads et al. (1992)	Hanford soil at a fixed pH

C = The equilibrium concentration of lead (μg/l) DCARB = The Concentrations of Dissolved Carbonate of Soils CLAY = The Clay Content of Soils EC = Electrical Conductivity, HEDTA = N-(2-hydroxyethyl) ethylenedinitrilotriacetic acid.

and environmental condition in soils. The errors of these types of models are rarely suitable.

Three frequently used adsorption isotherm models are the Langmuir, Freundlich, and Dubinin–Radushkevich models that are used in situations where the amount of contaminant loaded on the available adsorption sites is too large. The isotherm models consider dependency of the partition coefficient on only the solution concentration of the contaminant of interest and do not consider dependence on other solid and solution parameters that can influence adsorption. Finally, the mechanistic models emphasize the dependency of K_d values on contaminant concentration, competing ion concentration, variable surface charge on the adsorbent, and solute species solution distribution. The mechanistic models are rarely applied to complex natural soils because the surfaces of natural mineral are very irregular and difficult to characterize.

Some of the models include several parameters, however, some studies tried to make simplified model with the lowest parameters because of the complexity of the soil and environmental behavior. In recent times, Sauve' et al. (2000), Vandenhove et al. (2009) and Gil-Garcia et al. (2009) presented simple models that predict K_d for Nickel with respect to pH variation.

The idea of application of ANNs for prediction of K_d was presented by Shariatmadari et al. (2004) for the first time. They used ANNs to predict the variation of the partition coefficient with variation of environmental components. However, limited data were used for their study. In this study, ANNs is used to present simplified model for predicting K_d. The main objective is to develop a more accurate model with a minimal number of parameters, which can be determined experimentally or select by review of different studies. In addition, the effects of training as well as the type of the network are considered. This study focuses on the prediction of K_d of nickel. US Department of Energy considers the Ni radioisotopes for a radiological performance assessment analysis of a low-level waste disposal facility (DOE, 1996). Vandenhove et al. (2009) demonstrated that ^{59}Ni and ^{63}Ni have half-lives of 76,000 and 100.1 years, respectively, and are components of radioactive waste. It has been showed that K_d of Ni is strongly dependent on pH by several studies. Therefore, pH is considered to be the most important parameter affecting Ni availability (Sauve' et al., 2000; Weng et al., 2001, 2003; Staunton et al., 2002; Staunton, 2004).

1.1. Modeling with neural networks

Work on artificial neural networks has been motivated right from its inception by the recognition that the brain computes in an entirely different way from the conventional digital computer (Haykin, 1994; Ghiassian et al., 2006; Shariatmadari et al., 2004). The steps for solving a problem are as follows: (1) selection of the proper network architecture for the problem; (2) collecting and preprocessing data for network training and testing; (3) design, train, and test the network model; and (4) deploy the network to the end user (Shi et al., 1998). In this research, two kinds of ANNs models are used to predict K_d values reported in literature, Multilayer perceptrone network (MLP) and redial basis function network (RBF). A complete description of these networks is beyond the scope of this paper and can be found in other publications (e.g. Haykin, 1994; Zurada, 1992; Fausett, 1994).

2. Material and methods

Sauve' et al. (2000), Vandenhove et al. (2009) and Gil-Garcia et al. (2009) verified different functional relationships between sorption characteristics and pH for nickel. Some of these functions are summarized in Table 2.

Two latter equations of Table 2 are used to verify that ANNs models may predict more accurate relative to these equations. For verifying the proposed ANNs models, analysis of statistical parameters may be used to evaluate model performance. These parameters are the standard error (SE), maximum error (ME), root mean square error ($RMSE$), coefficient of determination (CD), modeling efficiency (EF), and coefficient of residual mass (CRM) which have been used in this paper. The mathematical expressions of these statistics can be written as follows (Zarei et al., 2009)

$$SE = \sqrt{\frac{1}{n-2}\left[\sum_{i=1}^{n}(M_i-\overline{M})^2 - \frac{\left[\sum_{i=1}^{n}(S_i-\overline{S})(M_i-\overline{M})\right]^2}{\sum_{i=1}^{n}(S_i-\overline{S})}\right]}$$

Table 2
Sorption - pH functions (Vandenhove et al., 2009).

Study	Function	No. of data	R^2
Sauve' et al. (2000)	log $K_d(Ni) = +0.72$ (±0.05) $+ 1.75$ (±0.36) pH	139	0.58
Vandenhove et al. (2009)	log $K_d(Ni) = -0.30$ (±0.22) $+ 0.42$ (±0.04) pH	143	0.51
Gil-Garcia et al. (2009)	log $K_d(Ni) = -0.1$ (±0.3) $+ 0.34$ (±0.05) pH	58	0.46

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