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Forecasting solute breakthrough curves through the unsaturated zone using artificial neural networks

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Summary Effective groundwater management requires precise forecasting of the amount of contaminants intruding into groundwater from the surface. In this study, solute breakthrough curves throughout the unsaturated zone were predicted using artificial neural networks (ANNs), through numerical tests and through laboratory experiments. In the numerical tests, the applicability of the ANN model to the prediction of breakthrough curves was evaluated using synthetic data generated by a groundwater flow and transport model in a variably saturated media, HYDRUS-2D. The use of two ANNs, one for solute arrival times and the other for solute mass breakthroughs after the solute arrival time, was suggested in order to reduce the prediction error. The results showed that the network building process was essential in ANN model applications. The best ANN model gave a correlation coefficient value between target and output values of over 0.98. The sensitivity analysis of data forms for the network training demonstrated that regular breakthrough curves that contain a peak value can train the ANN model effectively. Then, the ANN model was verified using laboratory data obtained by tracer infiltration tests in a sand column. The overall results demonstrate that the ANN model can be an effective method for forecasting solute breakthrough curves through the unsaturated zone when hydraulic data are available.

Introduction

Groundwater begins to be polluted when surface contaminants infiltrate the unsaturated zone and reach the groundwater table. Thus the characterization of contaminant transport in the unsaturated zone is important for effective groundwater management. The unsaturated zone is often a highly heterogeneous medium with water contents varying substantially in space. There have been many attempts to describe the mechanisms of water and solute movement through unsaturated zones (Butters et al., 1989; Tseng and Jury, 1994; Simunek et al., 2002; Skaggs et al., 2004).

One of the most common approaches is to apply conventional physical models for solute transport through the unsaturated zone which are governed by the convection

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dispersion equation (CDE) with several assumptions. These models use constant parameters for the CDE, which are valid only after solute mixing is complete throughout a volume of soil in which non-uniform velocities occur. Due to this limitation, there are models that are intended to be used only for the cases when either water velocity is relatively uniform or when substantial time has elapsed since the solute was introduced into the soil (Jury et al., 1991; Tseng and Jury, 1994).

Transfer functions have been used as an alternative approach (Jury, 1982; Jury and Sposito, 1986; White et al., 1986; Butters and Jury, 1989; Skaggs et al., 1998). The transfer function model initiated by Jury (1982) follows the concept of Black Box model based on a linear relationship between inputs and outputs. It represents solute transport in soil without an explicit description of the physical transport processes, using a probability density function of the solute travel time through the unsaturated zone.

Recently, the application of artificial neural networks (ANNs) as an approach to forecasting water resource variables is growing (Zealand et al., 1999; Sharma et al., 2003; Jain et al., 2004). The ANN is a flexible mathematical structure patterned after a biological nervous system and is considered the standard computational tool for nonlinear problems in a variety of fields. However, the building process of an ANN is not standardized and it is difficult to assess whether ANN results are optimal or not. Therefore it is important to discover the optimal network architecture and network parameters for a given system (Maier and Dandy, 2000). For solute transport problems, ANN applications have been used to predict the transport parameters and solute distribution in groundwater (Morshed and Kaluarachchi, 1998; Almasri and Kaluarachchi, 2005). Morshed and Kaluarachchi (1998) conducted numerical tests for the unsaturated flow and solute transport. They considered various parameters for properties of the medium and contaminant including grain size, hydraulic conductivity, dispersivity, solute sorption and decay, and the boundary condition including various water fluxes on the surface. They successfully predicted four key parameters of the breakthrough curve in typical groundwater remediation problems, which were breakthrough time, time to reach MCL, time to maximum concentration, and maximum concentrations.

In farmlands, it is necessary to spread solutes on the surface such as fertilizers and pesticides. For preventing the groundwater contamination, an optimal application method of surface contaminants including their concentration and application time should be suggested. As a preliminary work to this problem, the solute transport through the unsaturated zone under various surface boundary conditions should be predicted. Moreover, it is necessary to predict the solute transport with respect to elapsed time, both for accurate predictions of the mass of solutes reaching the groundwater table and for coupled simulations of solute transport in the unsaturated zone and groundwater. In this study, the applicability of ANN models for predicting solute transports throughout the unsaturated zone was investigated. We considered constant values of hydraulic parameters and non-reactive solute transports, which were simpler cases for the medium and contaminant than Morshed and Kaluarachchi (1998)'s. Instead we focused on predicting breakthrough curves under various boundary conditions including water flux, injected solute concentration and duration of solute injection. These considerations of boundary conditions on the surface will be useful for the management of water resources in agricultural areas. In this study, for accurate prediction of breakthrough curves, a dual ANN model was suggested in numerical tests and verified by laboratory experiments.

Artificial neural network (ANN)

In general, ANNs are composed of input, hidden and output layers, and each layer contains nodes. The basic comprehensive information on ANNs is presented in the following literatures (Hagan et al., 1996; Maier and Dandy, 1996; Mehrotra et al., 1997). For the construction of an ANN framework, a feed forward network with one hidden layer and a back propagation algorithm was used in this study.

Feed forward network

A feed forward network is one of the most common neural nets. In this network, nodes in one layer are connected to nodes in the next layer successively. Fig. 1 represents the conceptual diagram of a feed forward network. Mathematical descriptions of a feed forward process are as follows

$$s_j^J = \sum_i w_{ji}^{JI} x_i^I + b_j^J \tag{1a}$$

$$x_j^J = f_J(s_j^J) \tag{1b}$$

$$s_k^K = \sum_j w_{kj}^{KJ} x_j^J + b_k^K \tag{2a}$$

$$x_k^K = f_K(s_k^K) \tag{2b}$$

where superscripts I, J and K indicate the input, hidden and output layers, respectively, subscripts i, j and k mean the nodes of I, J and K layers, respectively, x denotes the nodal value, w denotes the weight between two nodes, b denotes the nodal bias, s denotes the weighted summation of nodal values in the previous layer with a nodal bias, and

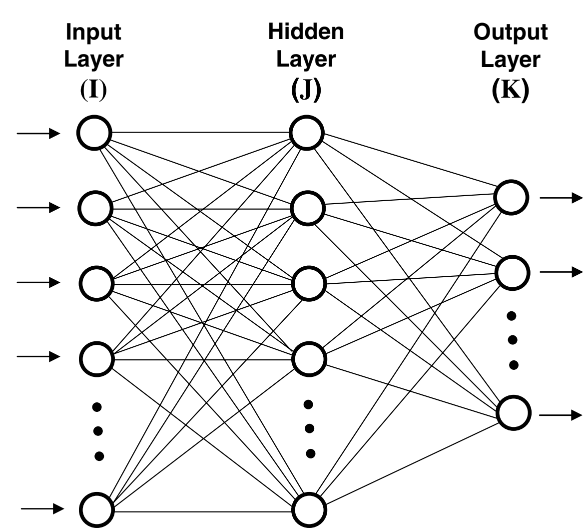

Figure 1 Conceptual diagram of a feed forward network with one hidden layer.