IDENTIFICATION OF PARAMETERS OF ADSORPTION BY APPROXIMATION OF INVERSE RELATION AND USING ARTIFICIAL NEURAL NETWORKS

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1. Presentation of the problem

In our former papers ([1], [2]) we have solved an inverse problem related to the convection in porous media by approximation of an inverse relation and using Artificial Neural Networks to this end. In those papers we have identified a source intensity Q and its position, conductivity $\boldsymbol{k}$ and diffusivity $\boldsymbol{D}$ of the porous medium. Given data in this inverse problem are: known concentrations c and the hydraulic head h measured in few points of the porous body. The concentration field and average velocity $\boldsymbol{v}$ of a steady flow across a permeable stratum are the direct solution of the well-known equations (1), in which the sorption S has been, previously, neglected:

(1) $$\frac{\partial c}{\partial t}=\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(v_i c\right)-\frac{\partial S}{\partial t}+Q \quad \text{where: } v_i=-k_{ij}\frac{\partial h}{\partial x_j}$$

We are going now to illustrate the applicability of the proposed approach in the case of non steady problem. We complete thus the considered equation assuming adsorption of the migrating solute at the skeleton of the porous body. We solve the simplified equation (1), leaving only dispersion process and the advection on the wallets of the porous skeleton. In examples we limit ourselves to the one dimensional case of dispersion with adsorption. This can be easily interpreted as a well, a sand column in the ground. Some applications in biomechanics (drug delivery) are also possible. In environmental geomechanics identification of leakage from waste disposal basing on data from standard monitoring of the suspensions concentration in some piezometers can be interpreted as the problem formulated in the title. Amount of the adsorbed solute S is defined by a law of adsorption. We will consider here only isotropic, linear, isothermal process. In this paper we will try to deduce from the observed concentrations which type of description is applicable. In order to illustrate the method of inverse solution, we present here the adsorption models of Freundlich and Langmuir. In both cases the equation (1) can be reorganized in a standard way, replacing the constants by time depending coefficients in which appears so called "retardation factor" $\delta(c)$ expressed by (2_1) in the case of Freundlich and by (2_2) by the Langmuir model respectively.

(2) $$\delta_F\left(c\right)=1+a_m K\beta_d c^{\beta-1} \qquad\qquad \delta_L\left(c\right)=1+a_m\frac{K}{\left(1+Kc\right)^2}$$

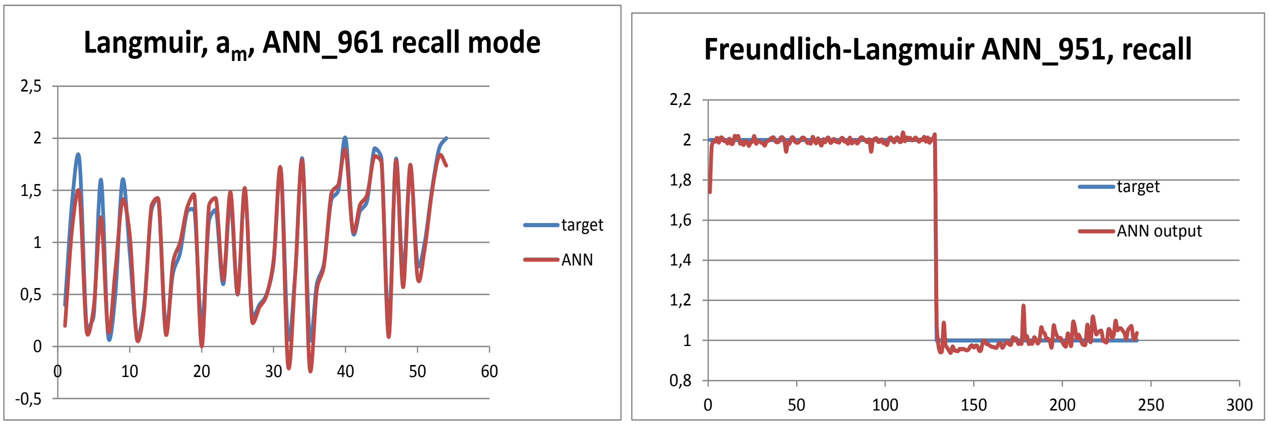
In eq. (2), K, a_m and β are some constitutive constants, the first one is the constant defining the equilibrium of the adsorption, the second – adsorption at the moment of formation of a single layers of molecules of the solute, the exponent β – empirical value less than 1,0. These constants will be found as solutions of the inverse problem associated with the direct problem (1).

2. Approximation of inverse relation with artificial neural networks

A direct relation is usually defined by direct solution of engineering problems and we assume that it is "easy" to find using one of the usual engineering methods. The inverse relation is a representation of the unknowns of the inverse problem (for example K, a_m and β , source parameters) by means of the observable variables (concentrations in few points and few time instances). The training of a suitable artificial neural network with observable data at the input and unknowns of the inverse problem at the output assure the best approximation of the inverse relation. ANN acts here as an universal approximator. The method is well known, we refer also to [1] for details.

3. Numerical examples

In the examples, the numerical experiment (instead of a real one) consists of observations of the concentration of not adsorbed solute. We decide to observe the concentration in two different points and in five different time instances in each. The chosen data of concentration will be used as the input of the ANN. We have obtained a satisfactory results of identification of all coefficients of Langmuir model, the case of Freundlich law allows us to illustrate some problems in obtaining the inverse solution and to show the ways to overcome these difficulties. In Figure 1a. the example illustrating the quality of approximation of a_m is shown. In Figure 1b. the suitably trained ANN discovers which adsorption law governs the process at hand.



a. b.

Figure 1. Examples of the identification, ANN with 9 nodes at the input, 5 or 6 hidden nodes and 1 node at the output. Explanation above, in the text.

4. Conclusions

We conclude thet the identification of parameters of adsorption by approximation of inverse relation with artificial neural networks can be successfully applied. We highlight, that numerical and analytical tools needed are limited to those that are usually used to obtain the solution of the corresponding direct problem. Thus the method is oriented toward some practical, engineering applications.

Obviously, in this approach artificial neural networks are crucial, however, no sophisticated developments are needed, on the contrary any commercial ANN code can be sufficient. We intentionally avoided the well-known special formulations like, for example Bayesian ANN or PCA-type preprocessing.

5. References

[1] D.P. Boso and M.Lefik (2012). *Inverse Problem: a Soft Solution*. W: Bytes and Science, Barcelona:International Center for Numerical Methods in Engineering (CIMNE), Barcelona 2012, s.271-288.

[2] M. Lefik, D.P. Boso, B.A. Schrefler (2012). *Identification of a steady-state flow in porous media using artificial neural networks*, Proceedings of the ASME 2012 11th Biennial Conference On Engineering Systems Design And Analysis ESDA2012 July 2-4, 2012, Nantes, France