Estimation of parameters of models of pollutant transport in rivers depending on data availability

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Abstract

Different approaches allowing the prediction of pollutant transport in rivers have attracted a great deal of attention among scientists throughout the world. Unfortunately, the prerequisite for running most of the proposed models is the detailed information about the hydraulic and morphometric conditions of the considered river. Even when the simplest advection-diffusion model is planned to be used, identification of its parameters is usually based on specially designed experimental studies performed in the reach under consideration. In practice however, an unexpected spillage of pollutant may occur in an ungauged river in which no tracer tests had been performed in the past and the model is expected to provide some evaluation of the pollution fate. Managers and decision makers, who have just a modelling tool at their disposal and the basic information about the stream, are supposed to derive some conclusions about the admixture pattern in the stream after its release at some location. In the present paper the outline of methods based on artificial neural networks for estimation of parameters of two pollutant transport models is presented. As the key issue is the question of availability of hydraulic and morphometric data for particular site, three different possible cases are considered, which differ in a number of information at the user's disposal. If the concerned river reach is sufficiently well-recognized, the artificial neural network based method of estimation of transient storage zone model parameters is suggested. When little information is available, only parameters of advection-diffusion equation may be estimated. In such a case two versions – the simple one and the requiring more information are discussed. Clearly the pollutant transport prediction error increases significantly with the decrease of available information about the river reach. The significance of proper estimation of water velocity is indicated as crucial for the correct prediction in every case.

Introduction

Relatively complex models that require advanced knowledge from their users are used to describe the constituent transport in rivers. Such models are usually fed with substantial amount of hydraulic and morphometric data specific for the considered

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river reach. The constructed models are usually validated and/or calibrated based on the results of in-situ tracer tests and they suffer from low level of confidence when applied to river reaches without such detailed recognition. But even in such cases various users expect that such models should provide reliable results. Therefore a detailed discussion on how to deal with situations when not enough data is available, seems to be very useful and it constitutes the main objective of this paper. This discussion is based upon authors' experience and their studies of numerous cases.

Pollutant transport modelling

Let us consider the situations when the pollution concentration distribution in vertical and lateral directions more or less equalizes so one may focus on the concentrations averaged over the cross-section, i.e. on one-dimensional models. Among the variety of the pollutant transport models two are of special interest due to their popularity, relative simplicity and physical background (Rutherford, 1994). The simplest and the most popular in practice is modelling based on the Fickian advection–dispersion equation (ADE) as follows :

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}=\frac{1}{A}\frac{\partial}{\partial x}\left(AE_x\frac{\partial C}{\partial x}\right) \tag{1}$$

where C (g/L) is the concentration in a river cross-section A (m^2), t (s) is time, U (m/s) is cross-sectional averaged water velocity, x (m) is longitudinal axis and E_x (m^2/s) is the longitudinal dispersion coefficient. Two model parameters (U and E_x) have to be evaluated.

In natural streams concentration distributions very often become much more skewed than the ones produced by (1) and therefore so-called Transient Storage Models (TSM) were introduced in literature (e.g. Nordin and Troutman, 1980; Czernuszenko and Rowinski, 1997). Their main advantage is that they account for the exchange of mass between the existing storage zones and the main stream. The model equations are the following:

$$\begin{aligned}&\frac{\partial C_m}{\partial t}+U\frac{\partial C_m}{\partial x}-K_f\frac{\partial^2 C_m}{\partial x^2}=\frac{\varepsilon}{T}(C_d-C_m)\\&\frac{\partial C_d}{\partial t}=\frac{C_m-C_d}{T}\end{aligned} \tag{2}$$

where C_m (g/L) is the area-averaged concentration in the main stream, U (m/s) is the area-averaged mean stream velocity which is assumed constant along the given sub-reach, C_d (g/L) is the concentration in the dead-zone, K_f (m^2/s) is the constant longitudinal dispersion coefficient in the main stream, and T (s) and ε are additional constant coefficients, representing an exchange parameter related to the residence time in the storage zones and the ratio of volume of stagnant areas to volume of mainstream for unit length of a river reach, respectively. Both concentrations C_m and C_d are usually normalized by the total mass of the solute discharged into the river.

Although TSM is clearly advantageous, it requires four parameters (namely K_f, T, ε and U) to be estimated. The models like (1) or (2) may be further extended over the terms governing the chemical reactions and exchange of mass with bed sediment (Rowinski et al. 2008), but it increases the number of parameters to be estimated. Therefore we will limit our considerations to conservative, passive substances only.
The best situation is when a few tracer tests are performed in the considered river reach at different flow conditions (Q). Then the model parameters may be fitted to measurements and, if necessary, estimated for actual Q from the found nonlinear relationships. Real problems appear when no tracer tests were performed, or when the flow conditions significantly differ from the ones noted during an accidental spillage. In this study we discuss how to deal with such situations.

Estimation of the model parameters depending on data availability
In principle TSM reproduces pollutant concentration distributions in a more accurate way than ADE but unfortunately it requires four parameters to be optimized. There is also a problem with the uniqueness of the obtained parameters, e.g. the decrease of the storage zone area may be counterbalanced by the increase in the residence time in the storage zone, what can make the parameters estimated for different rivers incoherent. Literature is rich in various methods of the empirical estimation of TSM parameters (e.g. Pedersen, 1977; Cheong et al., 2007 and Camacho and Gonzales, 2008) but the quality of the results is still insufficient. Rowinski and Piotrowski (2008) experimented upon the use of neural networks for the estimation of three TSM model parameters (excluding U) and they concluded that although much improved, the results are still of moderate quality, especially when T is concerned – see Figure 1. Error in estimation of T in extreme situations may reach almost one order of magnitude.
Note that in the above-mentioned studies, including neural network approach, the detailed data from the considered river reaches were required such as bed shear velocities, mean depth, width and the water velocity, whereas often the results are expected in situations when such data is not available. Camacho and Gonzales (2008) proposed power law relationships among different TSM parameters and the flow only but it seems that there is too little information to justify such hypothesis. At the moment no reliable method exists to use the TSM approach in river reaches where no detailed field measurements were done.
When due to insufficient information one cannot rely on TSM approach, much simpler ADE method should be considered. A great number of regression-based empirical formulae have been proposed for the estimation of longitudinal dispersion coefficient (Wallis and Manson, 2004). Among them relationships provided by Seo and Cheong (1998) and Deng et al. (2001) are probably of best overall performance. Most of the proposed regression-based equations required again the detailed data from the considered river reach. Another disadvantage was that part of those relationships were created for specific types of rivers only (Wallis and Manson, 2004) and no variable connected with river meandering was included.
The performance of various expressions designed for the estimation of the longitudinal dispersion coefficient differs significantly (Deng et al. 2001, Wallis and Manson, 2004), but all of them are outperformed by multi-layer perceptron neural

networks, applied for the first time by Kashefipour et al. (2002). The neural network based on data composed of the mentioned four input variables was able to provide the value of the longitudinal dispersion coefficient for selected river reach with reasonable accuracy.

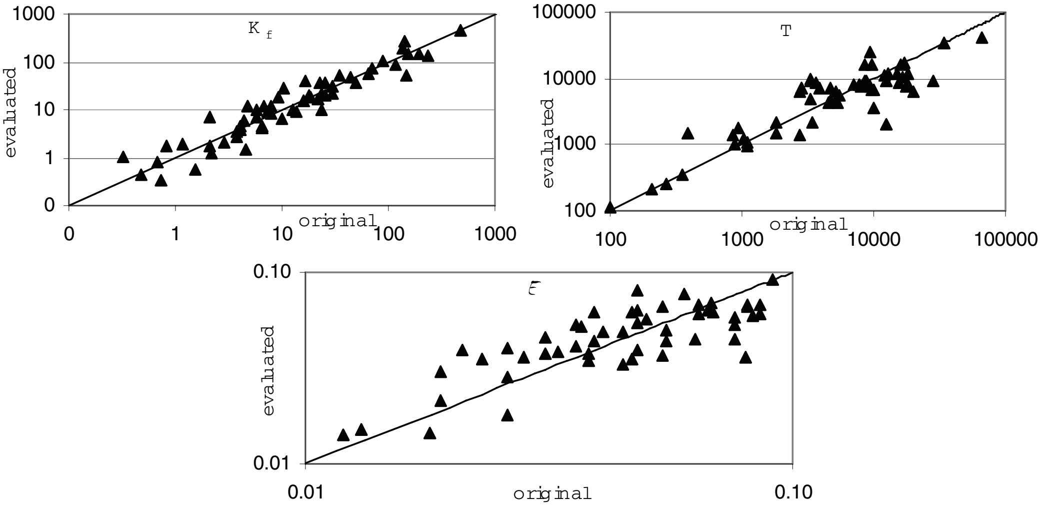

Figure 1. Comparison of TSM parameters fitted to measurements and evaluated from multi-layer perceptron neural network – logarithmic scale (after Rowinski and Piotrowski, 2008).

Rowinski et al. (2005) showed that inclusion of the sinuosity indices of river reaches improved the results significantly – see Figure 2. Left figure concerns the estimation of longitudinal dispersion coefficient when sinuosity index is included as one of the neural network inputs whereas in right figure it is neglected in computations. The use of other, more complex so-called intelligent methods, such as radial-basis, fuzzy neural networks and generalized regression neural networks, did not improve the results (Piotrowski et al., 2006; Toprak and Cigizoglu, 2008).

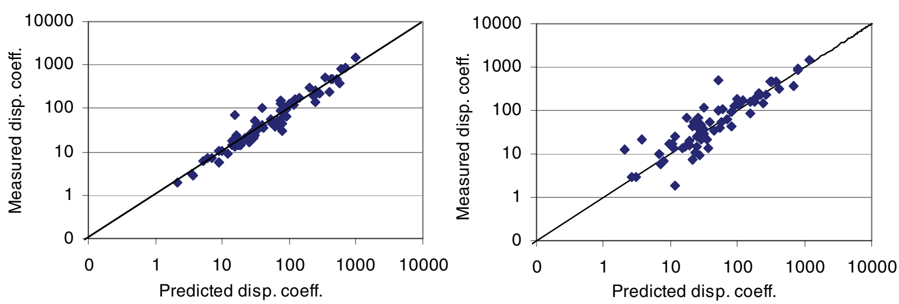

Figure 2. Comparison of ADE longitudinal dispersion parameter fitted to measurements and evaluated from multi-layer perceptron neural network when sinuosity index is considered (left) or when it is not considered (right) – logarithmic scale.

To summarize – when enough data is available the approach proposed in Rowinski et al. (2005) is advisable. It was for example successfully applied to estimate the longitudinal dispersion coefficient in different reaches of extensively-studied Murray Burn creek in Edinburgh, UK (Wallis et al., 2007). Researchers continuously try to evaluate the dispersion coefficients with much smaller amount of data. Such trial was made by Tayfur (2006) who based his considerations upon given flows only but that approach led to the overestimated lower dispersion values by as much as 1000%.
It has been recently investigated (Piotrowski et al., 2009) whether the prediction of pollutant transport is possible when data includes only the discharge and the water velocity at the injection site, and also the river bed slope and the sinuosity index. In such case the procedure is the following. At first the water velocity averaged over the river reach of interest is estimated with use of a multi-layer perceptron neural network based on the given data. Then the estimated value of the mean water velocity is used, with other input data, to compute the sought longitudinal dispersion coefficient. Note that the importance of the proper evaluation of water velocity is often neglected in literature, although it has profound impact not only on the proper timing of breakthrough curve but also on its shape and peak noted at a given cross-section. In case of a long river reach it should be divided into relatively homogenous reaches for which both water velocity and the longitudinal dispersion coefficient should be estimated separately. Assuming instantaneous release of contaminant the analytical solution of ADE is used within the initial reach.

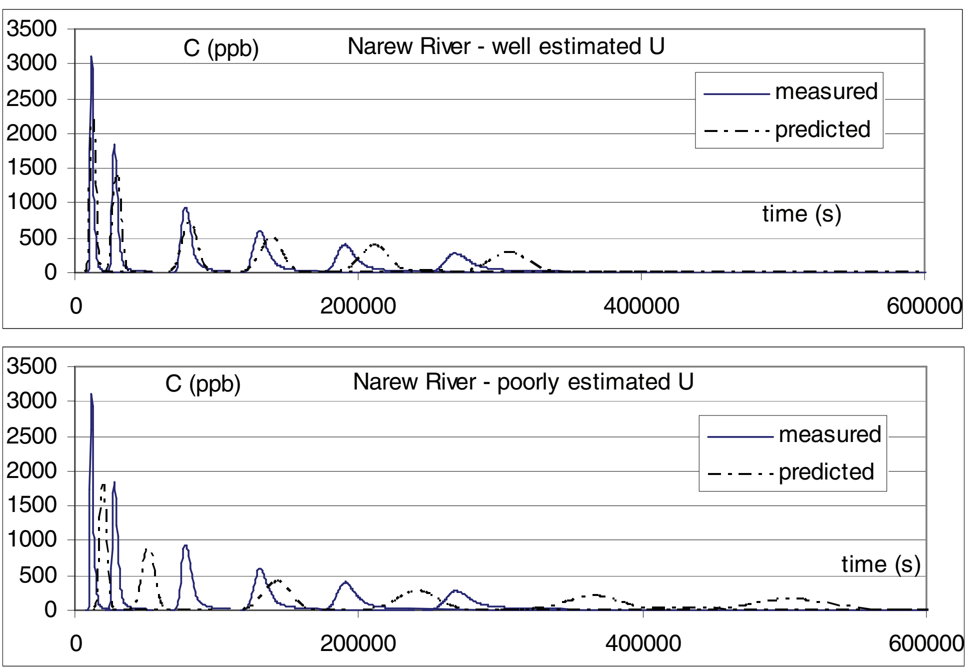

Figure 3. Predicted and measured breakthrough curves for Narew River (Poland) when little information about the considered river is available.

In the frame of suggested approach the neural networks were trained based on the part of data collected from the works of Nordin and Sabol (1974), Godfrey and Frederick (1970), Sukhodolov et al. (1997) and Rowinski et al. (2004). Contrary to previous studies both the optimal longitudinal dispersion and the water velocity were obtained by the same criteria. The testing set consisted of the remaining part of the experimental data from the above-mentioned papers and additionally from the data of Burke (2002) and Rowinski et al. (2008). The considered river reaches significantly varied in size and morphometric conditions. The length of the experimental reaches start from a few kilometers and they extend towards much over 100 kilometers. Examples of the verification of the obtained breakthrough curves are shown in figures 3 and 4.

The performance of the method depends significantly on the results of the evaluation of water velocity – even relatively low errors in its prediction may have crucial impact on the results. It is particularly evident when the errors are of the same sign for consecutive reaches and consequently they accumulate – e.g. compare the cases of the Narew River (Figure 3) and the Antietam Creek (Figure 4). Water velocity is rarely estimated sufficiently correctly, but if this is the case, the results (noted as "well estimated U") may be satisfying having in mind limited number of available information about the considered reaches. When the estimation of mean water velocity is far from reality, the obtained breakthrough curve may be of poor quality.

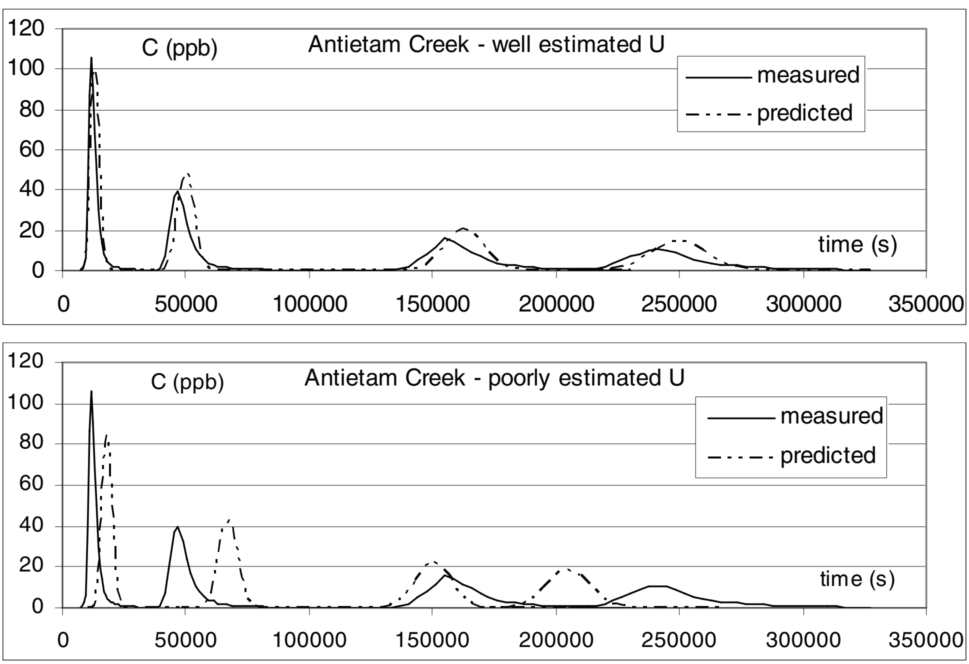

Figure 4. Predicted and measured breakthrough curves for Antietam Creek (USA) for which little information is available.

Conclusions

An outline of methods based on artificial neural networks for the estimation of parameters of two pollutant transport models is presented in this paper. The key issue discussed is the usefulness of the methods depending on the availability of hydraulic and morphometric data. Three different cases were considered, which differ in a number of information at user's disposal. If a considered river reach is sufficiently well-recognized, the method based on the artificial neural networks applied for the estimation of transient storage zone model parameters is suggested. When the information about the river reach is scarce, only parameters of the classical advection-diffusion equation may be estimated. In such a case two versions – the simple one and the one requiring more information are discussed. Clearly the pollutant transport prediction error increases significantly with the decrease of available information about the river reach. The significance of the proper estimation of water velocity is indicated as crucial for the correct prediction in every case.

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