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Controlled Random Search Applied to Parameters Estimation of the Longitudinal Solutes Transport Model for Rivers

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Abstract Numerical computations are presented for the longitudinal transport of passive, conservative solutes in an actual river with the inclusion of geometrical complexities of river channels. A special emphasis is put on the method of the identification of model parameters which is based on a specially designed optimisation procedure using random controlled search algorithm. Two different situations are considered namely a linear version in which one can assume that the mean velocity does not vary along the channel course and when the model parameters are constant and the nonlinear version implying channel nonuniformity (and variability of model parameters along the channel).

INTRODUCTION

Computational schemes for the simulation of the mass transport equations in cross-sectionally averaged form have been widely used for many years. A wide variety of schemes have been produced encompassing much of what is generally available in computational fluid dynamics: finite difference, finite volume and finite element methods for spatial discretization and explicit and implicit time stepping. Discussion of such methods in respect to the advection-dispersion equations but with the inclusion of temporarily storage zone is rather scarce in literature (Runkel and Chapra, 1993; Strauber 1995). In this paper we are concerned with the 1D solute transport equations, which are combined with the process of the exchange of mass between the mainstream and the existing in the flow areas that cause temporary storage of the solute.

The overall aim of the paper is to establish a robust and efficient scheme for modelling of solute transport in natural watercourses and to demonstrate its prediction capability. To achieve this goal a relevant procedure for identification of model parameters is proposed. The results of computations will be compared with selected experimental results obtained by means of a dye tracer test in a lowland river.

MATHEMATICAL MODEL OF LONGITUDINAL TRANSPORT OF SOLUTES

We will concern only one-dimensional conditions after a substance has become fully mixed across the depth and width of a river. In such case a model describing the processes of advection, longitudinal dispersion, i.e. the spreading relative to the cross-sectional averaged velocity and also temporary storage is suitable for the description of the spread of conservative, passive pollutants. The transient storage process describes water moving from the flowing stream channel into stagnant areas in which waters are well-mixed but not transported downstream. The detailed description of the transient storage model may be, for example, found in (Czernuszenko and Rowiński, 1997; Czernuszenko et al., 1998) and here we will just present the relevant partial differential equations.

Transport of the solutes in the main stream may be described by:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}-\frac{1}{A}\frac{\partial}{\partial x}\left(DA\frac{\partial C}{\partial x}\right)=\frac{\varepsilon}{T}\left(C_D-C\right) \tag{1}$$

where: x – longitudinal direction, t-time, C(x,t) –solute concentration, u(x)-cross-sectionally averaged velocity of water, D(x) – dispersion coefficient, A – cross-sectional area of the channel. It has been assumed that the hydraulic conditions in the channel are steady, i.e. parameters u, A, D do not change in time. $C_D(x, t)$ denotes the concentration of solute in the storage zone, parameters $\varepsilon(x)$ and T(x) denote the ratio of the volume of the storage zones to volume of the main stream for unit length and the penetration time of tracer into the storage zones, respectively. In many practical situations we may additionally assume that these parameters do not change along the channel and then the above equation is reduced to the following form:

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}-D\frac{\partial^2 C}{\partial x^2}=\frac{\varepsilon}{T}\left(C_D-C\right) \tag{2}$$

where U, D, ε and T are constant parameters.

The balance of mass in the storage zones is represented by:

$$\frac{\partial C_D}{\partial t}=\frac{1}{T}\left(C-C_D\right) \tag{3}$$

Equations (1) or (2) and (3) describe variations of the solute concentrations in both the main channel and the storage zones. The solution domain is the plane Oxt limited by inequalities $0\le x\le L$ and $t\ge 0$, where L is the length of the modeled channel reach. The model equations are complemented by the following:

- initial conditions:

$$C(x, t=0)=C_p(x) \qquad C_D(x, t=0)=C_{Dp}(x) \qquad \text{dla } x\in[0, L] \tag{4}$$

- and boundary conditions

$$C(x=0, t)=C_0(t) \qquad D\left.\frac{\partial C}{\partial x}\right|_{x=L}=0 \qquad t\ge 0 \tag{5}$$

where C_p i C_{Dp} are the initial distributions of solute concentration along the channel reach in both the main stream and the storage zones and C_0 describes the inflow of admixture at the initial cross-section.

NUMERICAL SOLUTION

Equations (2) & (3) may be solved analytically only by means of statistical moments (Czernuszenko and Rowiński, 1997) and therefore numerical methods are highly demanded. A finite difference method has been applied for the described case. The scheme is set up with a rectangular horizontal mesh. Equally spaced points along both the t- and x-axes are chosen with grid spacing Δt and Δx correspondingly, which makes the channel divided into N computational cross-sections and M temporal levels. A convention is used for which the cross-section denoted by 1 corresponds to $x = 0$, and by N to $x = L$. The Cranck-Nicholson differencing scheme has been used for the representation of (2)-(3) which reads:

$$\begin{aligned}&-\left(\frac{U\Delta t}{2\Delta x}+\frac{D\Delta t}{2\Delta x^2}\right)C_{j-1}^{i+1}+\left(1+\frac{U\Delta t}{2\Delta x}+\frac{D\Delta t}{\Delta x^2}+\frac{\varepsilon\Delta t}{2T+\Delta t}\right)C_j^{i+1}-\frac{D\Delta t}{2\Delta x^2}C_{j+1}^{i+1}=\\&=\left(\frac{U\Delta t}{2\Delta x}+\frac{D\Delta t}{2\Delta x^2}\right)C_{j-1}^{i}+\left(1-\frac{U\Delta t}{2\Delta x}-\frac{D\Delta t}{\Delta x^2}-\frac{\varepsilon\Delta t}{2T+\Delta t}\right)C_j^{i}+\frac{D\Delta t}{2\Delta x^2}C_{j+1}^{i}+\frac{2\varepsilon\Delta t}{2T+\Delta t}C_{D\,j}^{\ i}\end{aligned} \tag{6}$$

for cross-sections $j = 2, 3, \ldots N\text{-}1$ and

$$C_{D\,j}^{\,i+1} = \frac{\Delta t}{2T + \Delta t}\left(C_j^{i+1} + C_j^i\right) + \frac{2T - \Delta t}{2T + \Delta t} C_{D\,j}^{\,i} \tag{7}$$

for $j = 1, 2, \ldots N$. Approximation of boundary conditions at each temporal level leads to:

$$\text{for } j = 1 \qquad C_1^{\,i+1} = C_0(t_{i+1}) \tag{8}$$

$$\text{for } j = N$$

$$\begin{aligned} &-\left(\frac{U\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right) C_{N-1}^{i+1} + \left(1 + \frac{U\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2} + \frac{\varepsilon \Delta t}{2T + \Delta t}\right) C_N^{i+1} = \\ &= \left(\frac{U\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right) C_{N-1}^{i} + \left(1 - \frac{U\Delta t}{2\Delta x} - \frac{D\Delta t}{\Delta x^2} - \frac{\varepsilon \Delta t}{2T + \Delta t}\right) C_N^{i} + \frac{2\varepsilon \Delta t}{2T + \Delta t} C_{D\,N}^{\,i} \end{aligned} \tag{9}$$

Eq. (9) has been obtained from (6) with the assumption that

$$C_{N\text{-}1} = C_{N+1} \tag{10}$$

which is the consequence of the numerical approximation of (5).

In the case of the model in the form represented by (1) and (3) the situation is much more complex and the application of the Cranck-Nicholson differencing scheme has not led to satisfying results due to the generation of large errors in the process of computations. It has been assumed that the influence of three processes (advection, pure dispersion and transient storage) might best be computed separately as three stages in a three-stage difference scheme. Abbott and Minns (1998) suggest to think about such multi-staging as some processes are being “frozen” or “locked” while the other is implemented.

In the first stage a pure advection process has been considered:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{11}$$

In the second stage the results obtained from (11) are corrected by considering the dispersion process:

$$\frac{\partial C}{\partial t} = \frac{1}{A}\frac{\partial}{\partial x}\left(DA\frac{\partial C}{\partial x}\right) \tag{12}$$

Last stage concerns the existence of the storage zones by means of the following equations:

$$\frac{\partial C}{\partial t} = \frac{\varepsilon}{T}\left(C_D - C\right) \tag{13}$$

$$\frac{\partial C_D}{\partial t} = \frac{1}{T}\left(C - C_D\right) \tag{14}$$

An upwind scheme has been used for approximation of (11)

$$\text{for } j = 1 \qquad C_1^{\,i+1} = C_0(t_{i+1}) \tag{15}$$

$$\text{for } j = 2, 3, \ldots N$$

$$-\theta\frac{u_j \Delta t}{\Delta x} C_{j-1}^{i+1} + \left(1 + \theta\frac{u_j \Delta t}{\Delta x}\right) C_j^{i+1} = \left(1 - \theta\right)\frac{u_j \Delta t}{\Delta x} C_{j-1}^{i} + \left[1 - \left(1 - \theta\right)\frac{u_j \Delta t}{\Delta x}\right] C_j^{i} \tag{16}$$

The Cranck-Nicholson differencing scheme could be applied for the dispersion equation which resulted in the following:

$$\text{for } j = 1 \qquad C_1^{\,i+1} = C_1^{\,i} \tag{17}$$

$$\text{for } j = 2, 3, \ldots N\text{-}1$$

$$-\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+A_jD_j\right)C_{j-1}^{i+1}+\left[1+\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)\right]C_j^{i+1}+$$

$$-\frac{\Delta t}{4\Delta x^2 A_j}\left(A_jD_j+A_{j+1}D_{j+1}\right)C_{j+1}^{i+1}=\frac{\Delta t}{4\Delta x^2 A_j}\left(A_jD_j+A_{j+1}D_{j+1}\right)C_{j-1}^{i}+ \tag{18}$$

$$+\left[1-\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)\right]C_j^{i}+\frac{\Delta t}{4\Delta x^2 A_j}\left(A_jD_j+A_{j+1}D_{j+1}\right)C_{j+1}^{i}$$

and for $j = N$

$$-\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)C_{j-1}^{i+1}+$$

$$+\left[1+\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)\right]C_j^{i+1}= \tag{19}$$

$$=\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)C_{j-1}^{i}+$$

$$+\left[1-\frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1}+2A_jD_j+A_{j+1}D_{j+1}\right)\right]C_j^{i}$$

It is important to note that in the second stage the input for computations is taken from the first process and not from the actual preceding time level. Equations of the last stage are solved by means of the fourth-order Runge-Kutta method. Let's denote:

$$y_1 = C \qquad y_2 = C_D \tag{20}$$

$$f_1(t,\mathbf{y})=\frac{\varepsilon}{T}(y_2-y_1) \qquad f_2(t,\mathbf{y})=\frac{1}{T}(y_1-y_2) \tag{21}$$

which allows us to present the problem (13) - (14) as ordinary differential equation that reads

$$\frac{d\mathbf{y}}{dt}=\mathbf{f}(t,\mathbf{y}) \tag{22}$$

A single step of this method may be represented as:

$$\mathbf{k}_1=\Delta t\mathbf{f}\left(t_i,\mathbf{y}^i\right) \qquad \mathbf{k}_2=\Delta t\mathbf{f}\left(t_i+\frac{\Delta t}{2},\mathbf{y}^i+\frac{\mathbf{k}_1}{2}\right) \tag{23}$$

$$\mathbf{k}_3=\Delta t\mathbf{f}\left(t_i+\frac{\Delta t}{2},\mathbf{y}^i+\frac{\mathbf{k}_2}{2}\right) \qquad \mathbf{k}_4=\Delta t\mathbf{f}\left(t_{i+1},\mathbf{y}^i+\mathbf{k}_3\right) \tag{24}$$

$$\mathbf{y}^{i+1}=\mathbf{y}^i+\frac{1}{6}\left(\mathbf{k}_1+2\mathbf{k}_2+2\mathbf{k}_3+\mathbf{k}_4\right) \tag{25}$$

It is proposed that the described method of taking individual consistencies over to component differential forms and adding these differential component forms to obtain a resultant differential form which brings correct results.

IDENTIFICATION OF PARAMETERS – PROBLEM FORMULATION

A real problem arises at the level of the identification of model parameters. A number of estimation methods have been elaborated in literature such as physically based empirical method of Pedersen (1977); fitting of the theoretical slope of the Laplace transformed solution

for the concentration of the flow zone to the observed slope (Czernuszenko *et al.* 1998), moments matching procedure (Lees *et al.* 2000) or even visual determination of the set of parameters yielding the best fit to the concentration data (Bencala, Walters 1983). An obvious element is the relating the computed solute concentrations to some experimentally obtained curves. In the present study the results obtained by means of the dye tracer test in the Wkra River have been used and the time-concentrations distributions $C_m(x_k, t)$ ($k = 1, 2, ...$) at a few selected cross-sections in the main stream have been used for comparisons. As for the boundary condition at the inflowing cross-section the measurements taken in the first cross-section $C_m(x_1, t)$ have been taken. The measurements in the remaining cross-sections have been used for the determination of parameters with the objective function taken as:

$$\min_{u,D,\varepsilon,T}\left\{F\left[u,D,\varepsilon,T\right]=\sum_{k=2}^{K}\int_{0}^{T_H}\left[C_m\left(x_k,t\right)-C\left(x_k,t\right)\right]^2 dt\right\} \tag{26}$$

where F is the criterion function, T_H – the optimization time horizon, K number of measuring cross-sections. The wetted cross-section has been determined from the mass balance under steady stated conditions given by:

$$Q = u\left(x\right)A\left(x\right) \tag{27}$$

where Q is the given discharge.

Special constraints have been put on the sought parameters or functions:

$$X_{\min} \le X\left(x\right) \le X_{\max} \tag{28}$$

where $X_{\min}$ i $X_{\max}$ are the lower and upper bounds for $X(x)$.

Te computations of the values of the objective function for the estimated (by the described method) parameters u, D, ε, T have been realized through the simulations of the transport of solutes and the comparisons of the concentration distributions $C(x_k, t)$.

In case of the identification of parameters of the model (1)-(3) to lower the dimensionality of the problem a linear approximation of the sought parameters has been assumed. The longitudinal variations of $u(x)$, $D(x)$, $\varepsilon(x)$, $T(x)$ have been determined based on their values in the same cross-sections where the solute concentrations had been measured.

CONTROLLED RANDOM SEARCH METHOD

The optimisation problem (26) was solved by means of the global random search procedure (Price, 1987) namely the following version of Controlled Random Search (CRS2) described in details in Dysarz and Napiórkowski (2002). The algorithm is one of the random global optimisation techniques. Its basis is well known simplex method used in non-linear optimisation. The set of points from n-dimensional space is processed in following iterations. In each step, new solution is generated by reflection of a simplex vertex. One of a few well known versions of the method was used, namely CRS2.

The algorithm starts from the creation of the set of points, many more than $n + 1$ points in n-dimensional space, selected randomly from the domain. The optimal quantity of set was taken as suggested by Price (1987), equal to $10(n + 1)$. Let us denote the set as S. After evaluating the objective function for each of the points, the best x_L (i.e. that of the minimal value of the performance index) and the worst x_H (i.e., that of the maximal value of the performance index) points are determined and a simplex in n-space is formed with the best point x_L and n points ($x_2, x_3, \ldots, x_{n+1}$) randomly chosen from S. Afterwards, the centroid x_G of points $x_L, x_2, \ldots, x_n$ is determined. The next trial point x_Q is calculated as the reflection of x_{n+1}, that is $x_Q = 2x_G - x_{n+1}$ (Niewiadomska-Szynkiewicz et al., 1996). Then, if the last derived

point x_Q is admissible and "better" it replaces the worst point x_H in the set S. Otherwise, a new simplex is formed randomly and so on.

If the stop criterion is not satisfied, the next iteration is performed. This part of the algorithm was formed in different way then in the Price original concept. The experiments showed that following condition may be taken as the stop criterion

$$F_{ave} - F\left(x_L\right) < \varepsilon \tag{29}$$

where F_{ave} is the mean objective function value in the set, $F(x_L)$ the objective function value in the best point x_L and ε is the expected accuracy determined empirically (Dysarz and Napiórkowski, 2002).

NUMERICAL COMPUTATIONS VERSUS EXPERIMENTAL RESULTS

The results of a tracer test carried out in the selected reach of the Wkra River have been used in the analyses. Three different experimental tests (the discharge Q was 4.18, 3.97 and 4.32 m^3/s) performed over a 6 kilometers river reach with 5 measuring cross sections are taken into account. As an initial condition for computations a lack of dissolved solutes in the channel was assumed:

$$C_p(x) = C_{Dp}(x) = 0 \qquad \text{dla } x \in [0, L] \tag{30}$$

The time horizon for simulations was taken as 4h. Time step is taken as Δt = 20 s and the spatial one Δx = 20 m.

Admissible range for model parameters is given in Tab.1. Since the differences in the values of the sought parameters are large, a normalization was necessary and it was performed by projecting of the admissible set on the unit cube in R^n by means of expression:

$$\alpha = \frac{X - X_{\min}}{X_{\max} - X_{\min}} \qquad 0 \le \alpha \le 1 \tag{31}$$

Examples of simulations of the transport of solutes are shown in Figures 1 and 2. These figures show the measured and computed concentration distributions at five cross-sections.

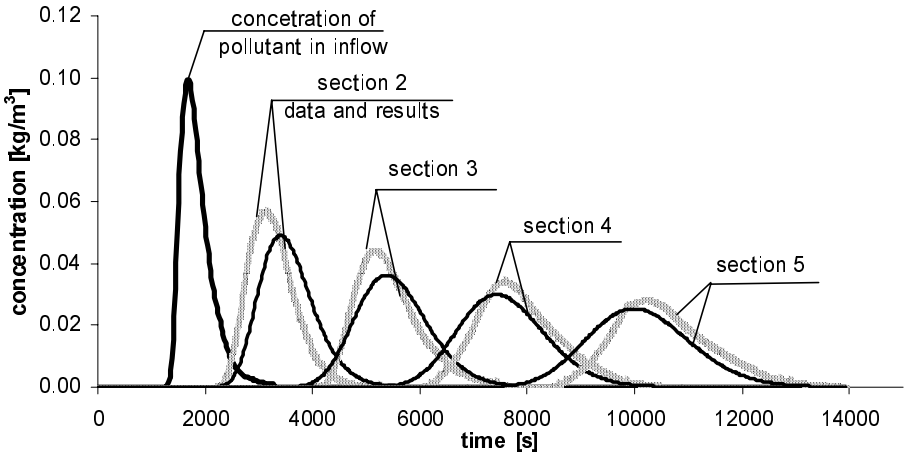

Fig.1 Measured solute concentrations and that obtained by means of linear model

Performance of both linear and nonlinear models is presented. Table 2 provides the mean values of the objective function as well as the values of standard deviation obtained by means of the expression:

$$\sigma_{\%} = \frac{1}{\overline{X}} \sqrt{\frac{\sum_{i=1}^{N} \left(X_i - \overline{X} \right)^2}{N-1}} 100\% \qquad (32)$$

where X_i is the single sample from a series of N samples having the mean value $\overline{X}$. It is readily seen that the agreement with the measuring data is much better in case when the variability of model parameters along river channel is taken into account, i.e. in case of eqs. (1) and (3). Mean values of the criterion function varied in the range from 0.005 to 0.01 in this case while those values were ten times larger in case of eqs. (2) and (3). The values of standard deviation in both cases did not exceed 5% of mean value. However, the increase in the accuracy of results has been obtained at much larger computational cost of parameters' identification. Mean value of the number of runs was 131.4 in case of linear model and it was as large as 4377.6 for the nonlinear model. Table 3 and Fig.3 provide mean values and the standard deviations for each determined parameter for both presented models. The values of the storage zone parameters reflects the relatively simple geometry of the considered channel of Wkra river. Discussion of the performance of these parameters may be, for example, found in (Czernuszenko et al., 1998).

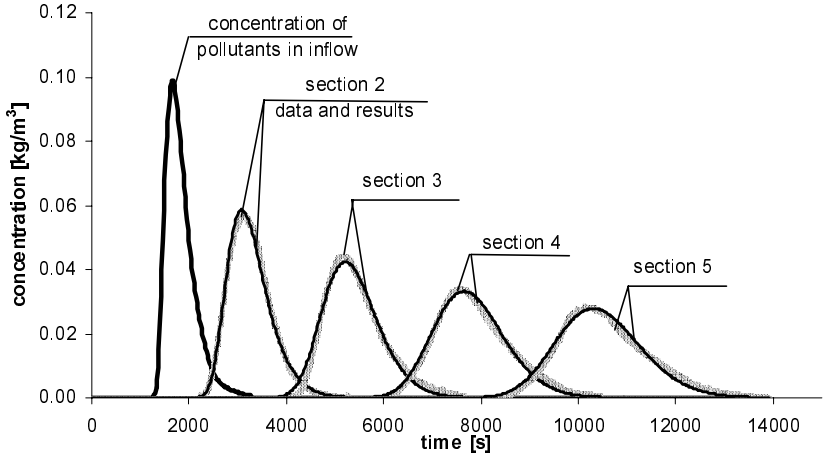

Fig.2 Measured solute concentrations and that obtained by means of nonlinear model

Tab. 1 Constraints for the sought parameters

Parameter	Steady flow			
	Uniform – Eqs. (2) i (3)		Nonuniform– Eqs. (1) i (3)	
	min	max	min	max
u [m^3/s]	0,3	0,7	0,4	0,8
D [m^2/s]	0,5	10,0	3,8	9,0
ε [-]	0,0	0,2	0,0	0,2
T [s]	0,001	200,0	0,001	200,0

Tab. 2 Mean values of criterion function and standard error

test	1		2		3	
Flow	Linear model	Nonlinear	Linear model	Nonlinear	Linear model	Nonlinear
Mean value	0.1258	0.0049	0.1724	0.0104	0.1216	0.0052
Standard error. %	1.529	4.483	1.671	2.677	2.639	2.830

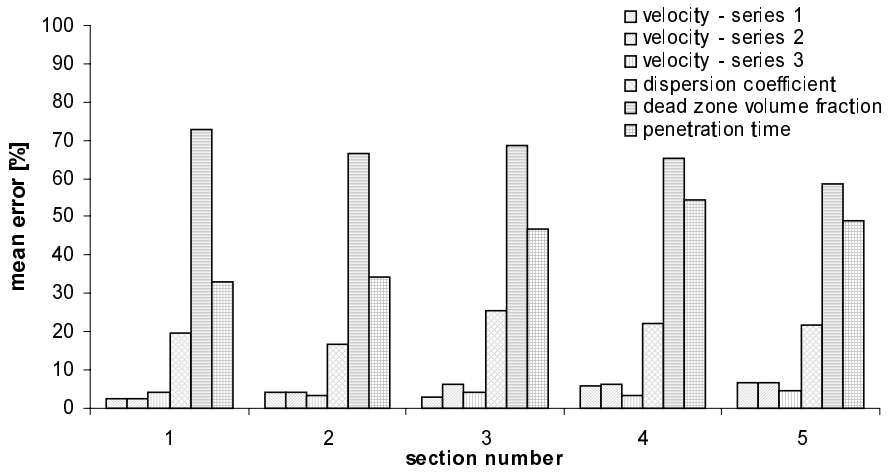

Fig.3. Standard deviations for each determined parameter for nonlinear model

Tab. 3 Mean values of the determined parameters and the standard errors – uniform flow conditions

Parameter	u [m/s]			D [m^2/s]	ε [-]	T [s]
	Test 1	Test 2	Test 3			
Mean value	0.5592	0.5546	0.5480	4.76127	0.1186	147.9942
Standard deviation %	4.313	3.835	3.105	37.086	31.239	23.480

CONCLUSIONS

In the study a special procedure was designed for the identification of the parameters of the model of longitudinal transport of pollutants in rivers with the inclusion of the phenomenon of transient storage. A model taking into account the changes of model parameters along river channel proved to provide better results when compared to the experimental data but the parameter identification in such case is computationally much more expensive.

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Literature

Abbott, M.B., Minns, A.W., 1998. Computational Hydraulics, Ashgate, Aldershot, 557.

Bencala, K.E., Walters, R.A. 1983. Simulation of solute transport in a mountain pool-and-riffle stream: a transient storage model. *Water Resources Research*, 19(3), 718-724.

Czernuszenko, W., Rowiński P.M., 1997. Properties of the dead-zone model of longitudinal dispersion in rivers, *Journal of Hydraulic Research*, 35,4, 491-504.

Czernuszenko, W., Rowiński, P.M., Sukhodolov, A.N., 1998. *Journal of Hydraulic Research* 36,2, 269-280.

Dysarz, T., Napiórkowski, J.J., 2002. Determination of reservoir decision rules during flood, *Acta Geophysica Polonica*, 50,1, 135-149.

Lees, M.J., Camacho, L.A., Chapra, S., 2000. On the relationship of transient storage and aggregated dead zone models of longitudinal solute transport in streams. *Water Resources Research*, 36(1), 213-224.

Niewiadomska-Szynkiewicz, E; Malinowski, K.; & Karbowski, A. 1996. Predictive Methods for Real-Time Control of flood operation of a Multireservoir System: Methodology and Comparative Study, Water Resources Research, Vol. 32, No. 9, 2885-2895.

Pedersen, F.B. 1977. Prediction of longitudinal dispersion in natural streams. Series Paper 14, Institute of Hydrodynamics and Hydraulic Engineering, Technical University of Denmark, Lyngby, Denmark.

Price, W.L., 1987. Global optimization algorithms for CAD Workstation, J. Optimiz. Theory Appl., 55(1), pp. 133-146.

Runkel, R.L., Chapra, S.C., 1993. An efficient numerical solution of the transient storage equations for solute transport in small streams, *Water Resources Research*, 29, 1, 211-215.

Strauber, G., 1995. Modified box schemes for pollutant transport in rivers with dead zones, *International Journal for Numerical Methods in Fluids*, 21, 12, 1123-1135.