Estimation of longitudinal dispersion and storage zone parameters

P.M. Rowiński, T. Dysarz & J.J. Napiórkowski
Institute of Geophysics, Polish Academy of Sciences, Warsaw, Poland

ABSTRACT: Numerical computations are presented for the longitudinal transport of passive, conservative solutes in an actual river channel with the inclusion of its geometrical complexities. Only one-dimensional conditions after a substance has become fully mixed across the depth and width of the river are concerned. In such case a model describing the processes of advection, longitudinal dispersion, and also temporary storage is suitable for the description of the spread of admixture. 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 control search algorithm. The algorithm is one of the random global optimisation techniques and particularly its realization by means of the CRS2 method. 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). The results of tracer tests carried out in the selected reach of the Wkra river in Central Poland have been used in the analyses. 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.

1 INTRODUCTION

Various versions of the storage-zone models have become increasingly popular for the calculation of the longitudinal dispersion of a solute in a river with irregular cross-sections (e.g. Czernuszenko & Rowiński 1997; Czernuszenko et al. 1998; Manson 2000; Thackston & Schnelle 1970, etc.). On top of the mixing processes (advection and dispersion) this model is the reflection of the existence in the rivers of stagnant zones of water that are stationary relative to the faster moving waters near the center of the channel. It constitutes a kind of a compromise between data consuming two-dimensional models and the simpler one-dimensional approach. Mathematically similar approach may pertain to the exchange between the streaming water and the subsurface bed sediment, namely to hyporheic exchange causing the retardation of the solute transfer (e.g. Packman & Bencala 2000; Fernald et al. 2001; Jonsson 2003). As is usually the case in physically based models the main difficulty is the estimate of the proper values of the parameters occurring in the model. All those parameters have relatively clear physical interpretation and as such should assume logical values. It should be noted that even in the much simpler case of the application of the Fickian type advection-dispersion equation, the evaluation of the dispersion coefficient constitutes an important problem since usually the information necessary for its estimate is rather scarce. The methods of its evaluation are disputable (Deng et al. 2002; Sukhodolov et al. 1998; Rowiński et al. 2003). It is then not very surprising that a number of methods, often leading to different results, are proposed in respect to the dead-zone types of models. Recently Seo & Cheong (2001) discussed different methods for the estimates of the parameters of the storage zone model and they concluded that the parameters obtained by the methods of moments are in good agreement with the measured parameters, whereas the fit by the maximum likelihood method as well as the existing literature approaches are not. A number of other 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.

Estimation of the parameters has to obviously be proceeded by a proper formulation of the computational procedure. 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 & 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. This study is just a first stab and the performance of the model is demonstrated against the measured data from one dye tracer field study in Central Poland. The emphasis is rather put on the elaborated mathematical approach.

2 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:

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

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:

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

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

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

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

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:

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

- and boundary conditions:

$$C(x = 0, t) = C_0(t), \quad D\frac{\partial C}{\partial x}\bigg|_{x=L} = 0, \quad t \ge 0 \qquad (5)$$

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.

The effects of simple shift in time and dissipation in traditional Fickian-type advection – dispersion transport are well known. The source term that occurs in Equations 1 and 2 causes additional effects of pollutant decrease and accumulation (Figure 1). The intensity of the exchange of mass between storage zones and the main stream depends on the difference in concentrations. At the beginning the storage zones accumulate the pollutants which causes the decrease of the admixture concentration in the main stream. However, the stored mass is given back to the channel when the concentration in the main stream is lower than in the storage zone. This process may

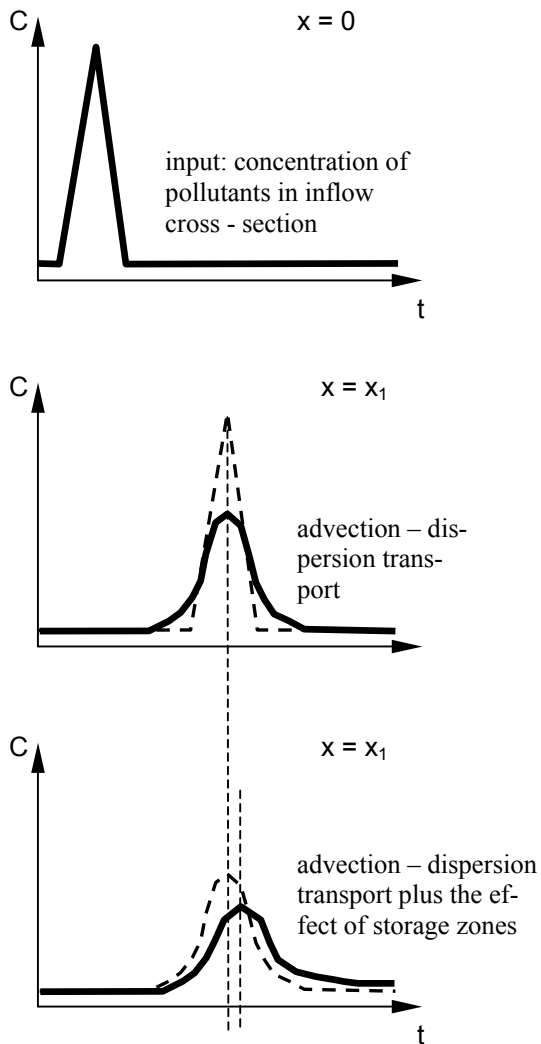even cause the shift in time of the peak of concentration temporal distribution (Figure 1).

Figure 1. Schematic representation of advection, dispersion and storage zones processes.

3 NUMERICAL SOLUTION

Equations 2 & 3 may be solved analytically only by means of statistical moments (Czernuszenko & 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 Equation 2-3 which reads:

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

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

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

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

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

for $j = N$

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

Equation 9 has been obtained from 6 with the assumption that

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

In the case of the model in the form represented by Equations 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. The procedure as described in details below may be schematically presented as in Figure 2.

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:

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

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

An upwind scheme has been used for approximation of Equation 11

for $j = 1$ $\quad C_1^{i+1} = C_0(t_{i+1})$ (15)

for $j = 2, 3, \dots N$

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

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

The Cranck-Nicholson differencing scheme could be applied for the dispersion equation which resulted in the following:
for $j = 1$

$$C_1^{i+1} = C_1^i \tag{17}$$

for $j = 2, 3, \dots N-1$

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

$$+\left[1 + \frac{\Delta t}{4\Delta x^2 A_j}\left(A_{j-1}D_{j-1} + 2A_j D_j + A_{j+1}D_{j+1}\right)\right]C_j^{i+1} + \tag{18}$$

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

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

and for $j = N$

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

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

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

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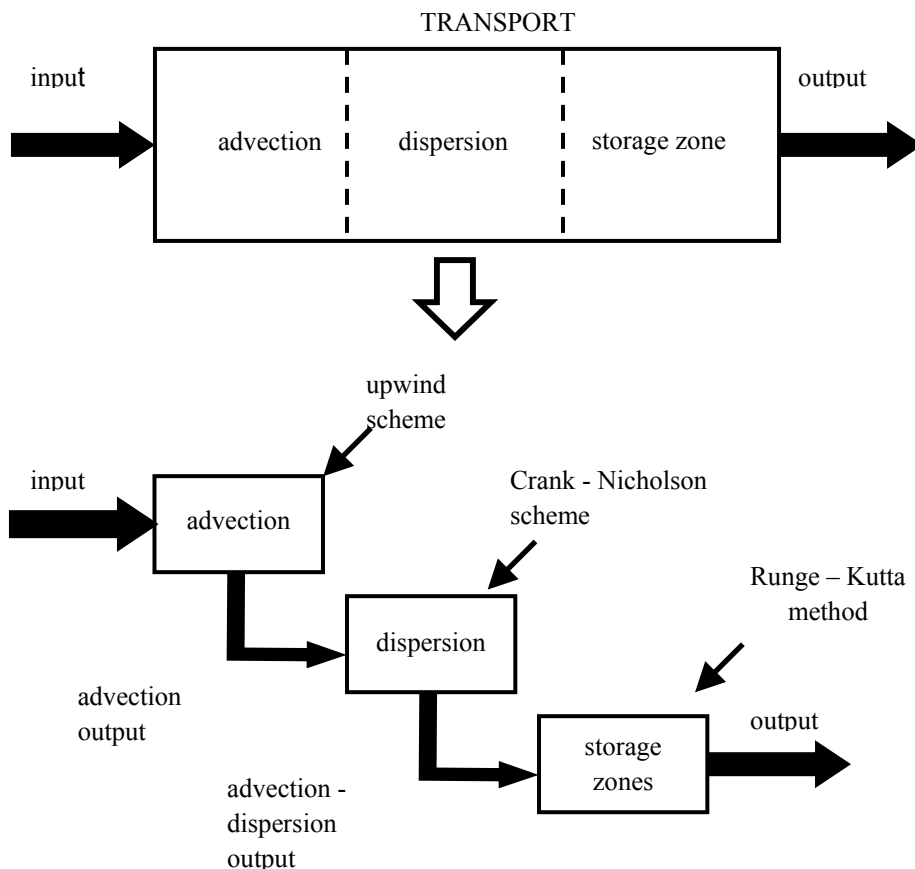

Figure 2. Schematic representation of the applied splitting technique

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:

$$y_1 = C, \quad y_2 = C_D \tag{20}$$

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

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:

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

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

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

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.

4 FIELD STUDY - DYE TRACER TEST IN THE WKRA RIVER

The presented model has been verified based on the tracer test performed in the lowland river reach in Central Poland, namely the Wkra River. The flow rate as well as other hydraulic and topographic characteristics in respect to all the measuring cross-sections are shown in tables 1a, 1b, 1c. The measurements were repeated three times in the same river reach. A variety of different irregularities along the river banks were observed. The creation of wakes behind the sand waves as well as the areas on the insides of bends with small radius of curvature most likely causing that the flow "overshoots" the bend could be expected and therefore one may assume the existence of different storage zones in the considered river reach.

The method of instantaneous injection of the tracer was applied and it did not require the complex dosing facilities and allowed to obtain high initial concentrations of the tracer. The dye release consisted of 10 liters of alcoholic solution of a fluorescent red dye (Rhodamine). This dye was released at three points at the cross-section just downstream of the stage of fall which speeded up the cross-sectional mixing of the admixture. Concentrations were measured at five cross-sections as indicated in Table 1. First cross-section was established at a distance at which 1D conditions were supposed to be achieved. During the early stages of a test the dye was visible to the naked eye, which facilitated sample collections. The dye was detected by using the field fluorometer Turner Design with continuous flow cuvette system on the one hand and also water samples were collected at sampling points.

Table 1a Hydraulic and topographic characteristics – Wkra River (case 1)

Characteristic	Cross-section				
Mean flow [m³/s]	4.18				
Mean water surface slope [‰]	0.318				
	P-1	P-2	P-3	P-4	P-5
Distance from release point [m]	600	1460	2450	3480	4780
Cross-section area [m²]	8.07	9.72	9.19	10.15	10.35
Width at the surface level [m]	9.82	10.23	9.69	8.89	11.18
Mean velocity [m/s]	0.518	0.430	0.455	0.412	0.404
Mean depth [m]	0.82	0.95	0.95	1.14	0.93
Wetted perimeter [m]	0.77	0.89	0.81	1.01	0.88
Manning roughness [m^{-1/3}s]	0.03	0.0413	0.0370	0.0472	0.0419

Table 1b Hydraulic and topographic characteristics – Wkra River (case 2)

Characteristic	Cross-section				
Mean flow [m^3/s]	3.97				
Mean water surface slope [‰]	0.318				
	P-1	P-2	P-3	P-4	P-5
Distance from release point [m]	600	1460	2450	3480	4780
Cross-section area [m^2]	7.82	9.36	8.81	9.80	10.02
Width at the surface level [m]	9.73	10.1	9.57	8.77	11.07
Mean velocity [m/s]	0.508	0.424	0.451	0.405	0.396
Mean depth [m]	0.80	0.93	0.92	1.12	0.91
Wetted perimeter [m]	0.75	0.87	0.79	0.99	0.86

Table 1c Hydraulic and topographic characteristics – Wkra River (case 3)

Characteristic	Cross-section				
Mean flow [m^3/s]	4.32				
Mean water surface slope [‰]	0.323				
	P-1	P-2	P-3	P-4	P-5
Distance from release point [m]	600	1460	2450	3480	4780
Cross-section area [m^2]	8.41	9.87	9.22	10.24	10.49
Width at the surface level [m]	9.93	10.29	9.69	8.92	11.22
Mean velocity [m/s]	0.514	0.438	0.469	0.422	0.412
Mean depth [m]	0.85	0.96	0.95	1.15	0.93
Wetted perimeter [m]	0.79	0.90	0.82	1.01	0.89

Measuring data were stored on graphical registers in the form of concentration distributions and then digitized to obtain relevant concentration time series. Concentration temporal distributions as obtained in the measurements are seen in Figures 3 and 4.

5 IDENTIFICATION OF PARAMETERS – PROBLEM FORMULATION

Model calibration problem is formulated as optimization problem

minimize $F(\mathbf{x})$ with respect to $\mathbf{x} \in D \subset R^n$

where $F: R^n \rightarrow R$ is scalar objective function and D is admissible domain with potential solutions $\mathbf{x}$. Many different methods were used to solve such kind of problems, but no one of them may be recommended if we do not know the features of the objective and constraints in the given problem. The most important features are the convexity of function $F(\mathbf{x})$ as well as the convexity of domain D.

The form of constraints guarantees that the set of admissible solutions is compact and convex. However, the described problem is a practical and a very complex task. So, we have expected that the calibration criterion may not be convex. This preliminary assumption was confirmed by further numerical tests.

In such case the global optimization techniques should be preferred. These methods have been developed and investigated for several decades and they have been treated as alternative algorithms for problems with many local optimal points. Originally they have constituted the combination of random global search, i.e. Monte Carlo method, and local accurate procedure. Another kind of methods has become very popular during last 30 years. They are based on natural selection and evolution of wild species such as genetic algorithms, evolutionary strategies or evolutionary programming. One of the first descriptions of genetic algorithms was given by Holland (1975). At the same time non-evolutionary methods of global optimization were developed, and among them the methods based on natural and artificial physical and chemi-

cal processes. Simulated annealing (Kirkpatrick et al. 1983; Dekkers & Aarts, 1991) and particle trajectory method (Griewank 1981) are well known examples in this area. Current knowledge of optimization and classic methods for convex function was the basis for developing new global techniques, i.e. Price (1983), Ali & Storey (1994).
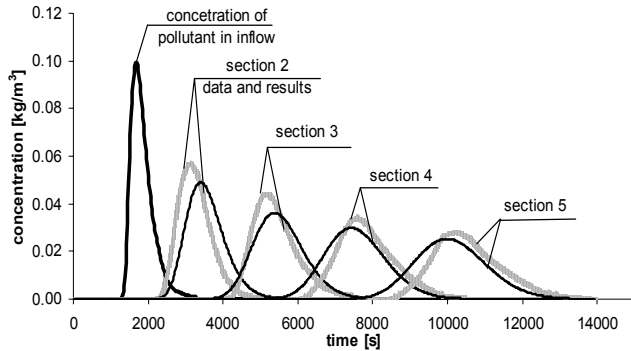

Figure 3. Measured solute concentrations and that obtained by means of linear model.
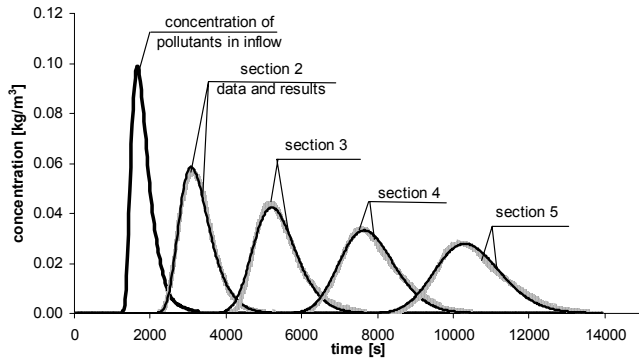

Figure 4. Measured solute concentrations and that obtained by means of nonlinear model

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 measurement results from the first cross-section $C_m(x_1, t)$ have been taken. The measurements at the remaining cross-sections have been used for the determination of parameters with the objective function taken as:

$$\min_{u,D,\varepsilon,T} \left\{ F[u,D,\varepsilon,T] = \sum_{k=2}^{K} \int_0^{T_H} \left[C_m(x_k,t) - C(x_k,t) \right]^2 dt \right\} \quad (26)$$

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:

$$Q = u(x) A(x) \quad (27)$$

where Q is the given discharge.

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

$$X_{min} \leq X(x) \leq X_{max} \quad (28)$$

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

6 CONTROL 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 by Dysarz & 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 $(x_2, x_3, ..., x_{n+1})$ randomly chosen from S. Afterwards, the centroid x_G of points $x_L, x_2, ..., x_n$ 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.

Table 2. Constraints for the sought parameters

Parameter	Steady flow			
	Uniform – Equations 2 and 3		Nonuniform– Equations 1 and 3	
	min	Max	min	max
u [m³/s]	0.3	0.7	0.4	0.8
D [m²/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

The experiments showed that following condition may be taken as the stop criterion

$$F_{ave} - F(x_L) < \varepsilon \qquad (29)$$

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

7 NUMERICAL COMPUTATIONS VISA 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

Table 3. Mean values of criterion function and standard error.

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

Table 4. Mean values of the determined parameters and the standard errors – uniform flow conditions.

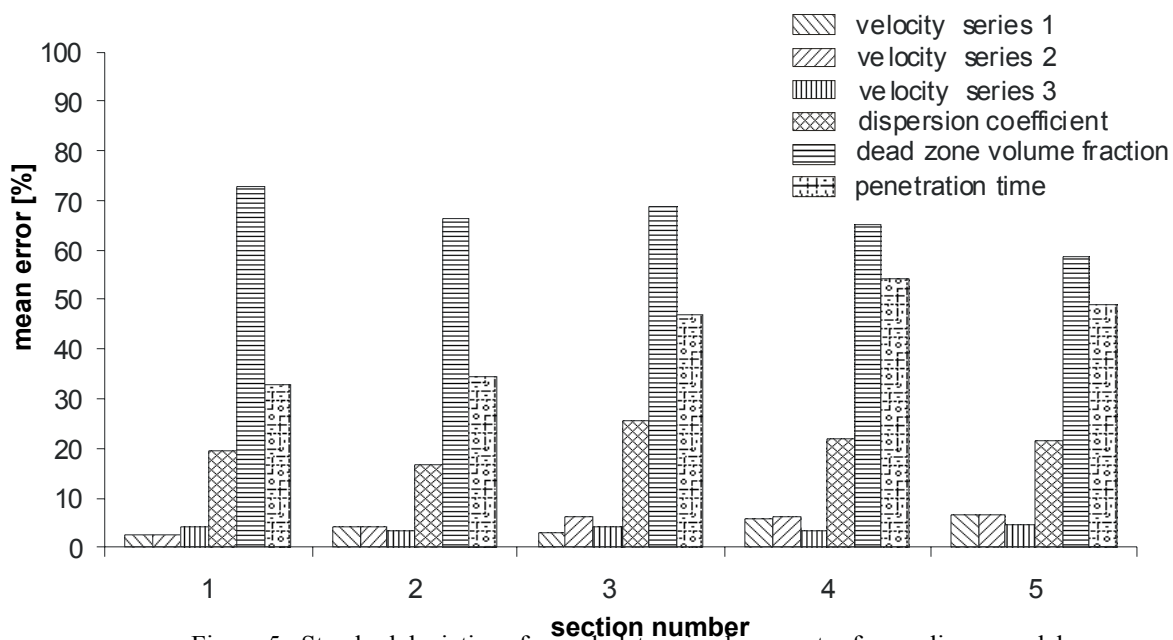| Parameter	u [m/s]			D [m²/s]	ε [-]	T [s]
	Test 1	Test 2	Test 3			
Mean value	0.5592	0.5546	0.5480	4.76127	0.1186	147.99
Standard deviation %	4.313	3.835	3.105	37.086	31.239	23.480

Figure 5. Standard deviations for each determined parameter for nonlinear model.

(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:

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

The time horizon for simulations was taken as 4h. Time step is taken as $\Delta t = 20$ s and the spatial one $\Delta x = 20$ m.

Admissible range for model parameters is given in Tab.2. 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:

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

Examples of simulations of the transport of solutes are shown in Figures 3 and 4. These figures show the measured and computed concentration distributions at five cross-sections.

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 Equations 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 Equations 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 Figure 5 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).

8 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.

REFERENCES

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

Ali M.M. & Storey C. 1994. Modified controlled random search algorithms. *Intern. J. Computer Math.*, 53: 229-235.

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. Experimental and numerical validation of the dead-zone model. *Journal of Hydraulic Research,* 36(2): 269-280.

Dekkers, A. & Arts, E. 1991. Global Optimization and Simulation Annealing. *Mathematical Programming*, 50: 367–393.

Deng, Z.Q., Begtsson, F., Singh, V.P. & Adrian, D.D. 2002. Longitudinal dispersion coefficient in single-channel streams. *Journal of Hydraulic Engineering*, ASCE, 128(10): 901-916.

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

Fernald, A.G., Wigington, P.J. & Landers D.H. 2001. Transient storage and hyporheic flow along the Willamette River, Oregon: Field measurements and model estimates. *Water Resources Research*, 37(6): 1681-1694.

Griewank, A.O. 1981. Generalized Descent for Global Optimization. *J. Optimiz. Theory Appl.*, 34(1): 11-39.

Holland, J.H. 1975. *Adaptation in Natural and Artificial Systems*. University of Michigan Press, Ann Arbor.

Jonsson, K. 2003. Effects of hyporheic exchange on conservative and reactive solute transport in streams. Model assessments based on tracer tests. *Acta Universitatis Upsaliensis. Comprehensive Summaries of Uppsala*

Dissertations from the Faculty of Science and Technology 866, Uppsala.

Kirkpatrick, S., Geatt, C.D. & Vecchi, M.P. 1983. Optimization by Simulated Annealing. *Science*, 220: 671-680.

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.

Manson, J.R. 2000. Predicting stream transient storage zone characteristics from tracer data. *Water Resources Research*, 36(2): 629-631.

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*,. 32(9): 2885-2895.

Packman A.I. & Bencala K.E. 2000. Modeling surface-subsurface hydrological interactions. In J.B. Jones, R.J. Mulholland (Eds.), *Streams and Ground waters*, Academic Press, 45-80

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 1983. Global optimization by controlled random search. *J. Optimiz. Theory Appl.*, 40(3): 333-348.

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

Rowiński, P.M., Piotrowski, A. & Napiórkowski J.J., 2003. Are artificial neural networks techniques relevant for the estimates of longitudinal dispersion coefficient in rivers?, submitted for publication.

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.

Seo, I.W. & Cheong, T.S. 2001. Moment-based calculation of parameters for the storage zone model for river dispersion, *Journal of Hydraulic Engineering*, ASCE, 127(6): 453-465.

Sukhodolov, A.N., Nikora, V.I., Rowiński P.M. & Czernuszenko W. 1997. A case study of longitudinal dispersion in small lowland rivers, *Water Environment Research*, 69(7): 1246-1253.

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.

Thackstone, E.L. & Schnelle, K.B. 1970. Predicting effects of dead zones on stream mixing. *Journal of Sanitary Engineering Division*, ASCE, 96(2), 319-331