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Dispersion Processes in Wetlands - Application of Data Based Mechanistic and Transient Storage Models

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Abstract

To better understand solute-transport processes, a fluorescent dye-tracer study was performed under steady-state flow conditions on a 16.8 km reach of an anastomosing section of the Upper Narew River. A known quantity of Rhodamine WT solution was instantaneously injected into a stream and the variation in tracer concentration observed as it moved downstream. The paper describes the results of applying Data Based Mechanistic and transient storage models. The observed breakthrough curves for the chosen cross-sections are compared with those simulated with 95% confidence bounds.

1. Introduction

The present study has been motivated by the need to understand the dynamics of the spread of pollutants in a unique river system situated within the Narew National Park. The Narew River reach chosen for the study has recently been identified as an anastomosing river, which is regarded as a separate group to braided, meandering and straight rivers.

A widely accepted method to understand the fate of solutes in streams is to perform a tracer study, in which a known mass of usually conservative solutes is released into the stream. The study consists of an examination at downstream stations of concentration versus time curves of the artificially released dye and of fitting appropriate models.

The first model considered was advection-dispersion with dead zones that can adequately describe the process of transport of pollutants in single-channel river with multiple storages. As an alternative to that transient storage model, the Data Based Mechanistic (DBM) approach introduced by Beer and Young (1983) was tested. In this approach the model is identified and the parameters are estimated from the collected time series data using system identification techniques (Young, 1984).

2. Description of the experiment and case study

The present paper is based on a tracer test performed in a unique multi-channel system of the Narew River reach within the Narew National Park in northwest Poland (Figure 2.1). A description of the experiment is presented in Rowiński et al. (2003a, b). The dye consisted of 20 liters of 20% solution Rhodamine WT injected at cross-section 0-N. Concentrations were measured in the Narew River at five transects, 2-N, 3-N, 5-N, 6N and 7N corresponding to flow distances of 5.75 km, 8.34 km, 10.62, 13.58 km, and 16.83 km respectively. The dye was detected using the field fluorometer Turner Design with a continuous flow cuvette system. Water samples were also collected at sampling points.

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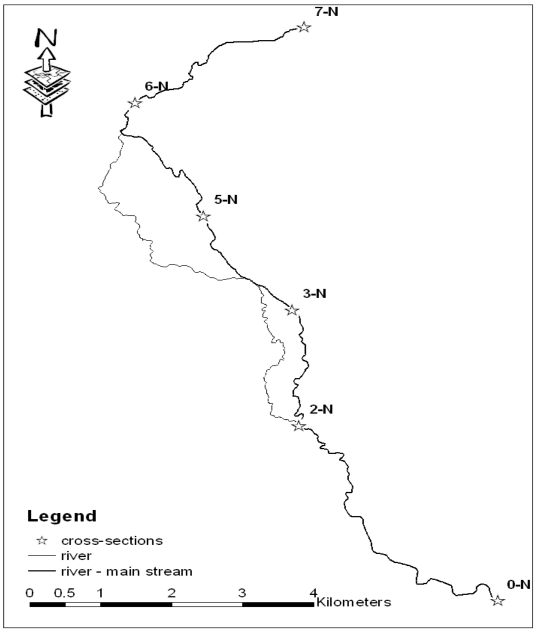

Figure 2.1: Map of the experimental reach of Upper Narew River

3. Distributed transient storage model

The transport of a conservative soluble pollutant along a uniform channel is usually described by the well-known Advection-Dispersion Equation. To apply this equation to a practical scenario, the dispersion coefficient for the reach is required. Since dispersion coefficients cannot be measured *in situ* directly from a simple individual measurement, they have to be estimated (optimized) on the basis of available experimental data. The One-dimensional Transport with Inflow and Storage model (OTIS) introduced by Bencala and Walters (1983) was applied in this study. The OTIS model is formed by writing mass balance equations for two conceptual areas: the stream channel and the storage zone. The stream channel is defined as that portion of the stream in which advection and dispersion are the dominant transport mechanisms. The storage zone is defined as the portion of the stream that contributes to transient storage, i.e. stagnant pockets of water and porous areas of the streambed. Water in the storage zone is considered immobile relative to water in the stream channel. The exchange of solute mass between the stream channel and the storage zone is modelled as a first-order mass transfer process. Conservation of mass for the stream channel and storage zone yields (Bencala and Walters, 1983; Runkel and Broshears, 1991):

$$\frac{\partial C}{\partial t} = -\frac{Q \partial C}{A \partial x} + \frac{1}{A}\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial x}) + \alpha(C_S - C) + \frac{q_{LIN}}{A}(C_L - C) \tag{3.1}$$

$$\frac{dC_S}{dt} = \alpha \frac{A}{A_S}(C - C_S) \tag{3.2}$$

where: C - solute concentration in the stream [g/m^3], t – time [s], Q - flow discharge [m^3/s], A - the main channel cross-sectional area [m^2], x - distance downstream [m], D - the coefficient of longitudinal dispersion [m^2/s], C_S - the concentration in the storage zone [g/m^3], α - the exchange coefficient [1/s] and A_S - the storage zone cross-sectional area [m^2], q_{LIN} - lateral volumetric inflow rate (m^3/s-m), C_L - solute concentration in lateral inflow.

Since it is not possible to estimate solute transport parameters reliably from hydraulic variables and channel characteristics, application of the transient storage model (3.1-3.2) requires estimation of model parameters for each particular river reach, 2N-3N, 3N-5N, 5N-6N and 6N-7N (Figure 2.1), based on data from tracer experiment including measurements of lateral inflow and discharge. Estimation of model parameters, namely D, A, A_S and α, was performed by minimizing the residuals between the simulated and observed concentrations. A general least squares objective function and Nealder-Mead minimization algorithm were used in this study. The results of the estimation procedure are given in Table 3.1. They are analogous to that obtained by Rowiński et al. (2004) for a similar model but different numerical scheme.

Table 3.1:
Parameters of transient storage models

Parameters	**Sections**			
	2N-3N	**3N-5N**	**5N-6N**	**6N-7N**
D [m^2/s]	10,31	1,65	6,96	1,59
A [m^2]	9,71	34,70	11,29	25,02
A_s [m^2]	6,13	22,62	4,46	7,05
α [1/s]	4,82e-006	1,7863e-005	1,2913e-005	6,5701e-005

Note that values of the parameters differ between reaches. These big differences result from a high variability of geometric and hydraulic conditions between the reaches. A comparison of observed and simulated data is presented in figure 3.1.

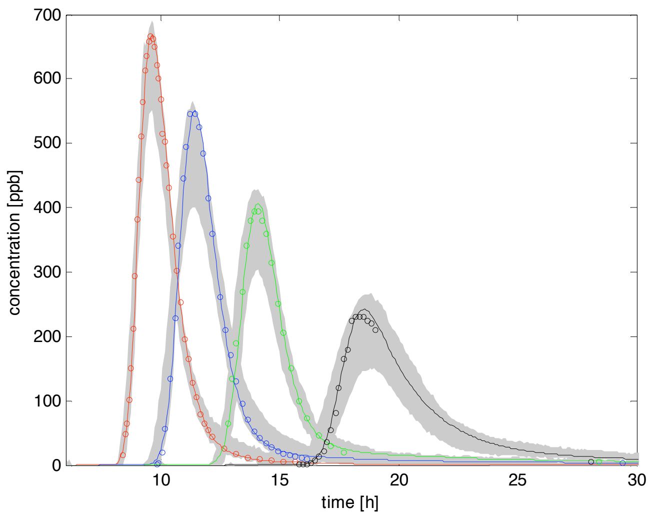

Figure 3.1: Comparison of observed (dots) and simulated (solid line) concentrations of Rhodamine WT at cross-section 3N, 5N, 6N and 7N with 95% confidence bounds

To asses the uncertainty related to model parameters, the Generalized Likelihood Uncertainty Estimation Technique (GLUE) of Beven and Binley (1992) was applied. In GLUE, model realisations are weighted using some assumed likelihood measure, via conditioning on observations, and weights are used to formulate a cumulative distribution of predictions. The weights have the form of exponent to the minus of the sum of square errors between simulated and observed concentrations, divided by one tenth of the mean error variance (Romanowicz and Beven, 2006).

4. Aggregated Dead Zone (ADZ) model

As an alternative to the transient storage model described by means of partial differential equations (3.1-3.2), a data-based mechanistic approach was introduced (Beer and Young, 1983; Beven and Young, 1998; Wallis, 1989; Young and Lees, 1993). In this approach a so-called aggregated dead zone (lumped) model is identified and the parameters are estimated from the observed time series data using system identification techniques (Young, 1984). In the ADZ model the change of solute concentration in a river reach is described as:

$$\begin{aligned} Cout_k &= \frac{B(z^{-1})}{A(z^{-1})} Cin_{k-\delta} \\ Cobs_k &= Cout_k + \xi_k \end{aligned} \tag{4.1}$$

where Cin_k is the concentration at the upstream end of the river reach at time k, the $Cout_k$ is the estimated concentration at the downstream end of the river reach, $Cobs_k$ is the measured concentration at the downstream end of the river reach, z^{-1} is the backshift operator, δ is advection time delay, A and B are polynomials of the backshift operator of the order 'm' and 'n' respectively, and ξ represents the combined effect of all stochastic inputs to the system, including measurements noise.

$$B(z^{-1}) = b_0 + b_1 z^{-1} + b_2 z^{-2} + \ldots + b_m z^{-m} \tag{4.2}$$

$$A(z^{-1}) = 1 + a_1 z^{-1} + a_2 z^{-2} + \ldots + a_n z^{-n} \tag{4.3}$$

The order of the ADZ model describing the transport of solute in river reach is described by triad [n m δ] and is determined in statistical time series analysis technique using the recursive-iterative simplified, refined instrumental variable (SRIV) method (Young, 1984) available in Captain Toolbox developed at the University of Lancaster. The optimum model is identified using three criteria. The coefficient of determination, R_T^2 shows how much of data variation is explained by the model output. The second measure is the Young Information Criterion (YIC), which is related to fit and error on parameters estimates and takes into account the over-parameterization problem. A low value of YIC indicates a well defined model. The third measure is the Akaike Information Criterion. AIC has a component related to the simulation fit but is penalized by the number of parameters in the model. A low value of AIC indicates a well defined model.

Identification of model structure and estimations of parameters of the transfer functions models were conducted independently for every river section using the SRIV method of recursive estimation in the Captain toolbox. The obtained values of R_T^2, for all analysed cross-sections, are given in Table 4.1. R_T^2 is defined as:

$$R_T^2 = 1 - \sigma_T^2 / \sigma_y^2 \tag{4.4}$$

where σ_T^2 and σ_y^2 denote the variances of prediction errors and observed concentrations, respectively.

Analysis shows that the second-order models are the most parametrically efficient model structures which accurately describe the observed solute transport in these reaches.

Table 4.1:
Results of identification of Aggregated Dead Zone model

	Sections			
	2N-3N	**3N-5N**	**5N-6N**	**6N-7N**
Model (n m δ)	2 2 29	2 2 19	2 2 30	2 2 50
R_T^2	0.9996	0.9994	0.9970	0.9934
Residence time [h] Slow pathway	3.36	172.02	166.88	19.29
Residence time [h] Fast pathway	1.34	3.53	3.39	0.72

Note, that for all river reaches the optimal transfer function is second order and can be decomposed into a parallel connection of two first order ADZ transfer functions in the following form:

$$Cout_k = \left(\frac{\beta_q}{1+\alpha_q z^{-1}} + \frac{\beta_s}{1+\alpha_s z^{-1}} \right) Cin_{k-\delta} \tag{4.5}$$

In practice, the residence times of two parallel connections are of quite different magnitudes and they are denoted as quick and slow processes in the above equation (subscript q and s respectively). The most plausible physical explanation is that the pure time delay allows for the flow-induced pure advection of the solute. The quick-flow parallel pathway then represents the 'main stream-flow' that is relatively unhindered by vegetation, while the slow-flow pathway represents the solute that is captured by heavy vegetation and so dispersed more widely and slowly before rejoining the main flow and eventually reaching the main channel.

Using calibrated transfer function models, a SIMULINK system describing the transport of solutes in the Upper Narew was built. A block diagram of a full semi-distributed system is presented in Figure 4.1. Every section is modelled as a second order transfer function model; the simulated output from a previous section becomes an input to the next section.

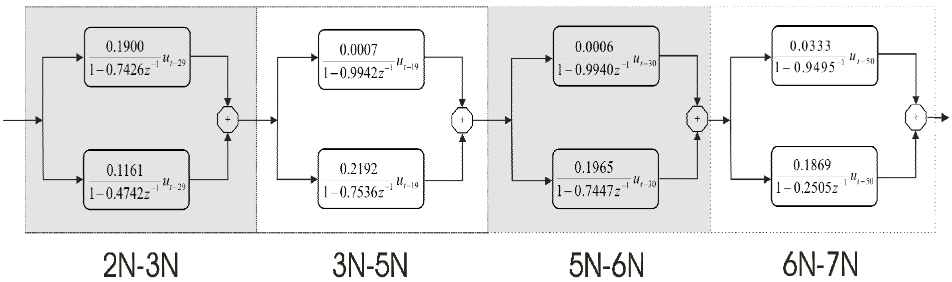

Figure 4.1: Transfer function block diagram of the whole analyzed river reach model

Figure 4.2 presents a comparison of measured concentrations of Rhodamine WT and those simulated using the ADZ model at four cross-sections. In the case of the cross-sections 3N, 5N and 6N, a very good fit is observed. The worst results are for the cross-section 7N, caused by a gap in measurements which makes the correct identification of model parameters impossible.

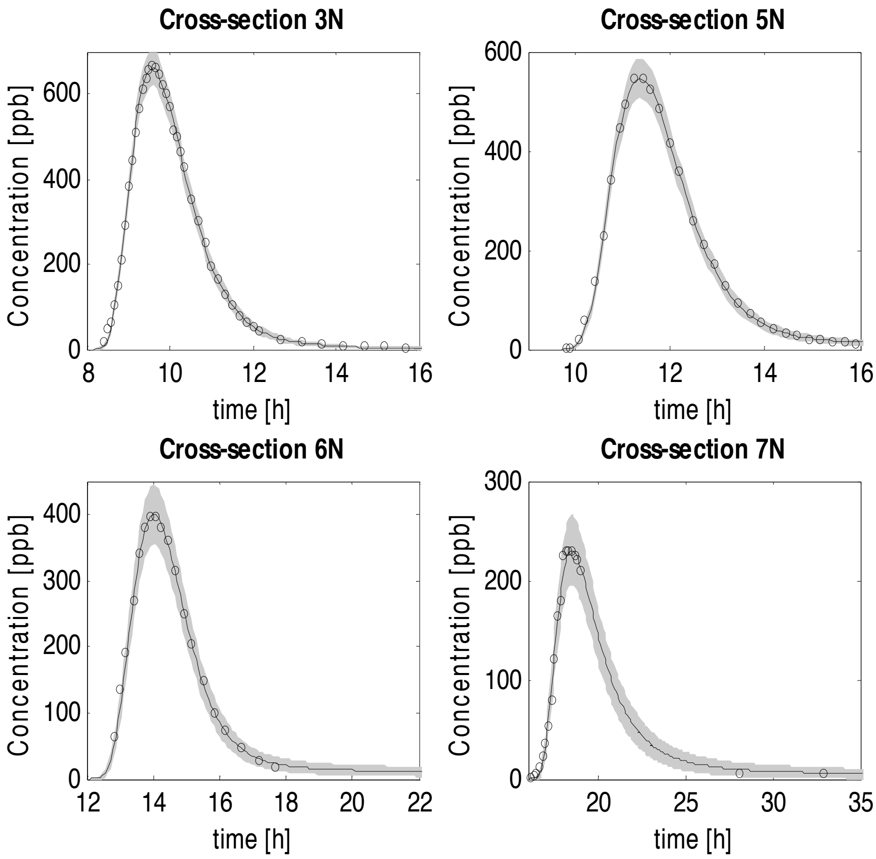

Figure 4.2: ADZ model results – application for the whole river reach, open circles represent measurements and shaded areas denote 95 % confidence bounds.

5. Comparison of STF and mechanistic modelling (virtual reality)

To validate the ADZ model for the whole river reach, another tracer experiment is required. Unfortunately there was just one tracer test in this part of the river, so we used the mechanistic OTIS model to simulate *virtual reality describing solute transport* in the Upper Narew for a different input than that used in the calibration. The results were then compared with those obtained by means of the previously calibrated ADZ model. They are depicted in figure 5.1.

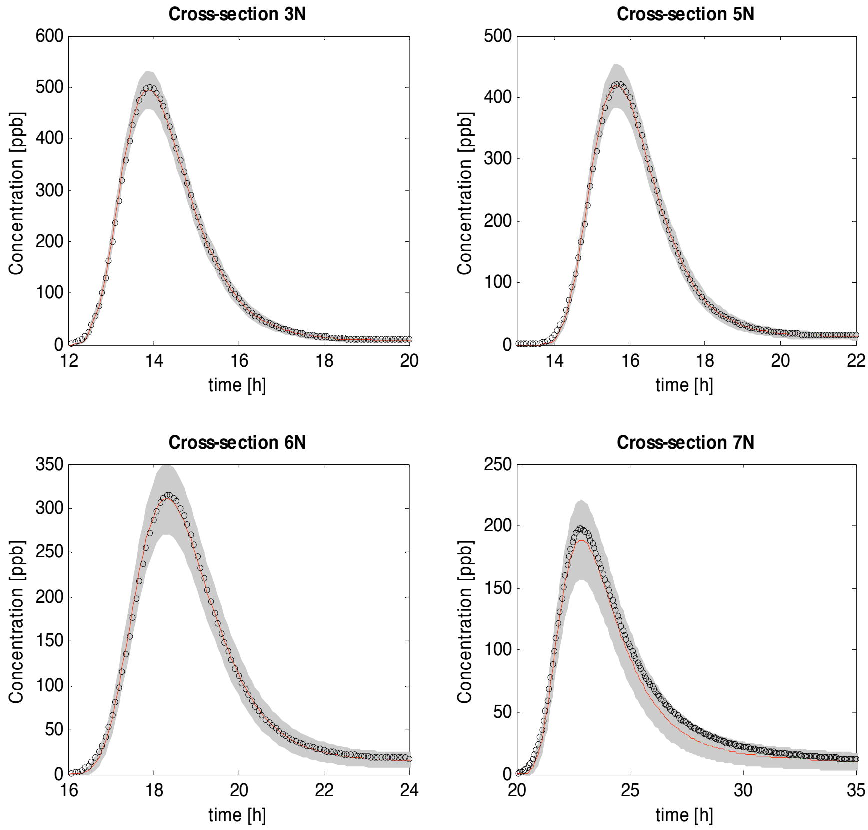

Figure 5.1: Validation of active mixing volume model. Open circles represent virtual reality simulated by mechanistic model, red solid line – ADZ model; shaded areas show 95% confidence bounds obtained from the ADZ model.

The results show a good similarity, with R_T^2 equal to 0.9995, 0.9994, 0.9991 and 0.9938 for cross-sections 3, 5, 6, and 7 respectively.

6. Conclusions

We have presented the application of a deterministic, mechanistic model (OTIS) and a stochastic ADZ model to dispersion processes in wetlands, based on the tracer experiment data from the reach of the River Narew situated within the Narew National Park. The GLUE procedure was applied to estimating the uncertainty of the OTIS model predictions related to the parameter and observational uncertainty. The stochastic ADZ model was used as an alternative to the mechanistic model. Due to its stochastic nature, the uncertainty of the model predictions is included in the model output. The dynamics of the dispersion process identified by the ADZ model have a second order, indicating the existence of slow and fast dispersion components in the studied River Narew reach. Due to the lack of a validation data set, we applied the mechanistic OTIS model output for a time period different from that used in the calibration stage, as a virtual reality, in order to validate the ADZ model. The obtained results show a comparison, good resemblance with 99% of the variation of the OTIS model output explained.

Acknowledgements

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