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Can we predict solute concentrations in rivers and streams?

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Introduction

Solute transport models are important tools for the prediction of solute (tracer / nutrient / pollutant) concentrations in a variety of practical applications, ranging from nutrient modelling over pollution alarm systems to the identification of contaminant sources. Making use of such models, naturally, requires knowledge of the transport parameters involved. Whereas in recent years considerable progress has been made with respect to the physical meaning of the parameters governing longitudinal solute transport in open channel flows (Wörman et al., 2002, Salehin et al., 2003; Weitbrecht, 2004; Zaramella et al., 2006), the actual parameter values in real world applications typically have to be estimated from stream tracer experiments, and this state of the art is not likely to change radically for some time to come.

A stream tracer experiment used in parameter estimation, typically, does not take place at the same time as the intended application, but rather in a situation almost invariably characterized by a different flow rate. Of course, it would desirable to cover the range of expected flows by an adequate number of tracer experiments, but this is rarely feasible within the financial and time constraints frequently encountered in practice. Thus, the computation of pollutant concentrations (and their biogeochemical implications) due to a spill will often tacitly rest on the transfer of transport parameters from one flow rate to another, a procedure typically associated with errors of unknown magnitude. In the research reported here, nine tracer experiments repeated on the same reach of a small Austrian stream have been used to quantify that error. Results are hoped to indicate an answer, however preliminary, to the question posed in the title of this contribution.

Field study and Parameter Estimation

From 2000 to 2005 a series of stream tracer experiments was performed on the Mödling Brook, a small stream south of the Austrian Capital Vienna. The study reach was not subject to any notable changes during that time. To focus on the parameter estimation issue, a conservative tracer (chloride) was used, with instantaneous slug releases carried out at the same location on the stream each time. Breakthrough curves were measured 200.5 m downstream of the injection site, at time intervals of 1 min mostly (in some of the experiments the interval was shortened to 30s). All experiments were characterized by a steady flow regime, with flow rates mostly below mean flow of some 0.24 m^3/s. The steady-state condition was checked by means of a nearby stream gauge read before and after the passage of the tracer 'cloud'. All of the experiments remained within the favourable 'window of experimentation' defined by Schmid (2004) with respect to potential non-uniqueness problems.

Transport, mixing and exchange processes were modelled by the so-called transient storage equations (the 'dead zone model'), which, for conditions without lateral inflow, sorption and decay, can be written as follows (Schmid, 1995):

$$\frac{\partial C}{\partial t} + u \cdot \frac{\partial C}{\partial x} = K \cdot \frac{\partial^2 C}{\partial x^2} + \varepsilon \cdot T^{-1} \cdot (C_S - C) \tag{1}$$

$$\frac{\partial C_S}{\partial t} = T^{-1} \cdot (C - C_S) \tag{2}$$

with C denoting the cross-sectional average of concentration in the main stream, C_s concentration in the storage zone, u the average flow velocity, K the coefficient of longitudinal dispersion, x the space coordinate in flow direction and t time. The size of the dead zones is reflected by ε , the ratio of storage zone to main stream volume per unit length, and T is an exchange parameter related to dead zone residence time. These 'dead zones' may take the form of pockets at the bank or the bottom, the interstitial water in hyporheic zones or the near-stagnant zone between groins, if any.

The U.S.G.S. model 'OTIS-P' (Runkel, 1998) was used to estimate the four transport parameters u, K, ε and T. OTIS-P solves the transient storage equations numerically, using a Finite Difference scheme which combines a Crank-Nicolson type discretization of the 'parabolic part' (shear flow dispersion term) with a central difference representation of the advection term. The resulting difference equations are decoupled and a tridiagonal system of linear equations is derived, which, in turn, can be solved efficiently by the Thomas algorithm (Runkel and Chapra, 1993). Parameter estimation is performed by a non-linear least squares algorithm.

OTIS-P identified the presence of dead zones in each case ($\varepsilon > 0$), with storage zone

residence times (T) amounting to roughly between one and five minutes. The flow rates covered a range of approximately 1:7.

Results and Discussion

Each of the parameter sets identified from the individual tracer experiments was used to compute all 9 breakthrough curves at x = 200.5 m, one to check successful model calibration and the other 8 to evaluate the errors due to the parameter transfer. The only parameter not transferred in the simulations was the flow velocity (u), which is directly related to the flow rate (Q) and, thus, cannot be transferred from one of the experiments to another. Instead, velocity was taken from the parameter set of the experiment to be simulated, as an analysis of potential methods to estimate u from Q was beyond the scope of the study reported here. In any case, an error in estimated flow velocity typically influences the timing, but not (or only marginally) the magnitude of the peak of the breakthrough curve.

The simulated maximum concentrations were compared to the observed peak values, with the associated error defined by

$$\Delta C\ [\%] = 100 \cdot (C_{sim} - C_{obs})\,/C_{obs} \tag{3}$$

where C_{sim}denotes the simulated and C_{obs} the observed maximum concentration.

Deviations between observed and computed breakthrough curves were found to be mostly around or below 1% in the course of model calibration, thus reflecting a successful choice of 'optimal' parameters by the non-linear least squares algorithm implemented in OTIS-P. The errors in peak concentrations were finally related to the ratios of respective flow rates ('runoff ratios'), i.e. the flow rate during the experiment to be simulated and the flow rate during the experiment from which the parameters were derived. The runoff ratio used here was defined as the larger of the above-mentioned flow rates divided by the smaller, thus reflecting the magnitude of the size step associated with the parameter transfer, irrespective of the direction of the change. By definition, this metric must necessarily be larger than or equal to one.

Individual peak errors reached 150%, but those associated with runoff ratios not exceeding 2.0 kept below 40%. Based on the data available for analysis in this study, this ratio of 1:2 between respective flow rates seems to be indicated as the limit of parameter transfer still associated with reasonable error bounds.

Conclusions

Modelling of longitudinal solute transport in fluvial systems requires knowledge of the transport parameters involved. At best, these parameters have been estimated from stream tracer experiments, usually conducted, however, at flow rates different from

those characterizing the intended application. Thus, the mathematical simulation of breakthrough curves invariably rests on a transfer of parameters, resulting in errors of an a priori unknown magnitude.

Nine tracer experiments conducted on the same reach of a small Austrian stream over a period of 6 years were analyzed to characterize the errors associated with the transfer of solute transport parameters across a range of flow rates. The results obtained suggest that parameter transfer across a range of flow rates not exceeding a ratio of 1:2 may be associated with errors below 40%, which is a mark typically considered acceptable in this type of modelling exercise.

References

Runkel R. L. (1998). "One-dimensional transport with inflow and storage (OTIS): a solute transport model for streams and rivers". Water Resour. Investigations Rep. 98-4018, U.S. Geological Survey, Denver, Co., 73 pp.

Runkel R. L. and Chapra S C. (1993). "An efficient numerical solution of the transient storage equations for solute transport in small streams". Water Resour. Res. 29 (1): 211-215.

Salehin, M., Packman, A.I. and Wörman, A. (2003). "Comparison of ransient storage in vegetated and unvegetated reaches of a small agricultural stream in Sweden: seasonal variation and anthropogenic manipulation". Adv. in Water Resources 26 (9), 951-964.

Schmid, B. H. (1995). "On the transient storage equations for longitudinal solute transport in open channels: temporal moments accounting for the effects of first-order decay". J. Hydr. Res. 33(5): 595-610.

Schmid, B.H. (2004). "Simplification in longitudinal transport modeling - case of instantaneous slug releases". J. of Hydrologic Engineering 9(4), 319-324.

Weitbrecht, V. (2004). "Influence of dead-water zones on the dispersive mass transport in rivers". PhD thesis, University of Karlsruhe, Universitätsverlag Karlsruhe, 129 pp.

Wörman, A., Packman A.I., Johansson, H. and Jonsson, K. (2002). "Effect of flow-induced exchange in hyporheic zones on longitudinal transport of solutes in streams and rivers". Water Resour. Res. 38 (1), 2-1 bis 2-15.

Zaramella, M, Marion, A. und Packman, A.I. (2006): Applicability of the transient storage model to the hyporheic exchange of metals. J. of Contaminant Hydrology 84 (1-2), 21-35.