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On the design of tracer experiments for parameter estimation in longitudinal solute transport modelling: a case of non-uniqueness

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Introduction

Tracer experiments are an important tool in hydrologic and hydraulic studies on rivers and streams. As these experiments are typically associated with quite considerable effort and expense, thorough preparation and planning are required, in the course of which issues of experimental design aimed at a reduction in parameter uncertainty should be addressed. In this context, non-uniqueness of the inverse problem may pose a particular challenge to the researcher, as breakthrough curves obtained in certain experimental settings have been shown to agree well with more than one solution of the governing transport equations, with the (nearly matching) solutions based on quite different parameter sets. A particularly unsatisfactory situation arises, when the set of tracer data obtained in the experiment does not even permit the mere presence or absence of transient storage or dead zones to be diagnosed reliably.

The concept most widely used in longitudinal solute transport modelling is the transient storage (TS) model, see e.g. Nordin and Troutman (1980), Bencala and Walters (1983) and Schmid (1995, 2003). For completeness, it shall be added in this context that more sophisticated models exist, which address a particular solute exchange mechanism, i.e. the one between the main stream and hyporheic zones, in a more process-based manner (e.g. Wörman et al., 2002; Salehin et al., 2003). Estimation of TS model parameters (average flow velocity u, dispersion coefficient K, dead zone ratio ε and dead zone residence time T) tends to become non-unique whenever the passage of the tracer cloud through the stream reach under study is either too quick or too slow. In the former case the tracer has too little time to interact with the storage zones, which, in turn, do not leave much imprint on the breakthrough curve observed at the downstream end of the reach (Harvey and Wagner, 1997). In the latter situation, if downstream transport takes too long in relation to dead zone residence time, an equilibrium stage will be reached and the effect of the storage zones, again, cannot be extracted reliably from measured breakthrough curves, as it will increasingly resemble that of other velocity variations in the stream.

In this contribution, the case of non-uniqueness is treated where breakthrough curves resulting from an instantaneous slug release of a conservative tracer can be explained both by the transient storage model and its counterpart without dead zones, i.e. the advection-dispersion equation (AD model), a simplified subset of the TS equations. Criteria are given which help identify (and, subsequently, avoid) particularly unfavorable conditions for stream tracer experiments of the instantaneous injection type performed for parameter identification purposes. The criteria depend on the reach length between the injection and measuring sites, resp., a control which the experimenter is free to choose within reasonable limits. That choice is, consequently, proposed to be made in accordance with the criteria given here, so that domains in parameter space characterized by definite non-uniqueness of the inverse problem can be avoided and the reliability of a subsequent parameter estimation may be improved.

Method and results

The approach chosen can be outlined as follows: the (full) Transient Storage equations were solved for 216 sets of the transport parameters u, K, ε and T:

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

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

with x the space coordinate in main flow direction, t time, C the solute concentration in the main stream and C_S that in the storage zones. The solute of mass M_0 was assumed to be released instantaneously at time t = 0 at x = 0 into a stream of zero solute concentration prior to the injection. At the lower boundary a zero concentration gradient was assumed to be approached infinitely far from the injection site. The solution of this initial boundary value problem was performed partly by means of the method given by Hart (1995) and partly by a Laplace-transform based solution (Tritthart, 2002). Transport parameter values were selected within a broad, physically realistic range: u = 0.10 m/s, 0.50 m/s and 3.0 m/s, K = 0.10 m^2/s and 10.0 m^2/s, $\varepsilon g = 5$%, 10%, 20% and 200%, T = 100s, 2000 s and 20000 s and, finally, reach length L = 100 m, 1 km and 10 km. These ranges are believed to cover many of the conditions encountered in the field, with an emphasis on streams of small to medium size (dispersion coefficient K $\leq$ 10 m^2/s). By combination of these parameter values 216 TS input data sets were generated, resulting in 216 synthetic breakthrough curves, as computed by solution of the initial boundary value problem described before. Subsequently, each of the 216 breakthrough curves from the TS model was approximated by the AD model as closely as possible. This was done by variation of u and K and repeated evaluation of the well-known analytic solution to the one-dimensional advection-dispersion equation for instantaneous slug releases (e.g. Rutherford, 1994):

$$C\left(x,t\right)=\frac{M_0}{A\cdot\sqrt{4\cdot\pi\cdot K\cdot t}}\cdot\exp\left[-\frac{\left(x-u\cdot t\right)^2}{4\cdot K\cdot t}\right]. \tag{3}$$

with M_0 the injected mass and A the cross-sectional area of the main stream (without loss of generality both are set to unity here). A least squares criterion was adopted and a nested grid search performed within the ranges of 0.01 m/s $\leq$ u $\leq$ 5.00 m/s and 0.01 $m^2/s \leq$ K $\leq$ 100 m^2/s. After identification of the best performing pair (u, K) the corresponding AD-model breakthrough curve was plotted together with its TS model counterpart. The quality of the fit between TS and AD breakthrough curves was measured by the relative differences in peak concentration and time to peak, resp. In addition, all 216 plots of corresponding TS and AD model outputs were checked visually.

Analysis of the data set described above showed the percentage of close matches between TS and AD breakthrough curves to be high. Thus, it is not at all improbable that a tracer experiment of the instantaneous slug release type will produce a breakthrough curve which can be explained by both models, and from which, therefore, no unique set of transport parameters can be inferred. As it is highly desirable to recognize conditions associated with non-uniqueness at the stage of experimental design already, several predictors of a close match between TS and AD breakthrough curves were tested against this data set: Damköhler Index DaI, dead zone ratio ε, Peclet number Pe, a product of Peclet and Damköhler numbers and the coefficients of skewness (G_t) and kurtosis (k_u) of the normalized breakthrough curves. Damköhler indices and skewness as well as kurtosis coefficients proved to be the relatively best indicators of a close match between TS and AD based curves. Good agreement (less than 5% peak deviation) between the two models was found for:

$$DaI=\frac{L\cdot(1+\varepsilon)}{u\cdot T}\leq 0.6 \tag{4}$$

$$DaI \;\geq\; 60 \tag{5}$$

$$G_t \;\leq\; 1.05 \tag{6}$$

$$G_t \geq 5.5 \tag{7}$$

and

$$k_u \geq 40. \tag{8}$$

Each of the above criteria is sufficient by itself. This means that, if conditions in a tracer experiment are such that one of the above conditions is met (irrespective of the others), the type of non-uniqueness treated here must be expected to occur.

Conclusion

The study outlined here showed that quite stringent conditions must be observed, if problems of non-uniqueness are to be avoided in stream tracer experiments of the instantaneous slug release type. A set of criteria was given to aid researchers in their task of experimental design.

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