

## Dynamic identifiability analysis of the transient storage model for solute transport in rivers

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### ABSTRACT

The use of dynamic mathematical models to simulate the behaviour of environmental systems is common practice. However, the output of these models remains uncertain, despite their widespread use and long history of application. This uncertainty arises, amongst other factors, from errors in the data, randomness in natural processes, incorrect assumptions in the model structure with respect to the processes taking place in the natural system, and the inability of calibration procedures to unambiguously identify an optimal parameter set to represent the system under investigation. The latter two problems may be caused by the inability of the calibration procedure to retrieve sufficient information from the model residuals. In this paper, a new approach called *Dynamic Identifiability Analysis* is presented in order to partly overcome this limitation. A case study shows how the proposed methodology can be applied to increase the identifiability of parameters of a river solute transport model.

**Key words** | environmental modelling, uncertainty, parameter identifiability, dynamic identifiability analysis, river solute transport, hyporheic

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### INTRODUCTION

River water quality modelling is a fundamental tool in water resource and environmental studies concerned with an effective application of river water quality management and control (e.g. Orlob 1981; Thomann & Mueller 1987; Chapra 1997). Accurate solute transport modelling underpins all river water quality models and therefore, over the last two decades, research has been concerned with the development of a more appropriate model structure to represent solute transport in natural channels. The distributed Transient Storage (TS) model structure (Bencala & Walters 1983; Jackman *et al.* 1984; Wörman 2000), which appeared as a modified version of the commonly used Advection Dispersion Equation (ADE) (Taylor 1954), can accurately represent solute transport processes in rivers subject to transient storage or dead-zone effects under steady flow conditions. Recently, the TS model structure has become more popular and widely used via the One-dimensional Transport with Inflow and Storage model structure (OTIS) (Runkel 1998).

However, it is currently not possible to estimate solute transport parameters reliably from hydraulic variables and channel characteristics, and therefore, successful application of the TS model requires the estimation of model parameters for each particular river stretch of interest, for example using data from tracer experiments. The dependence on tracer experiments presents complications as not all tracer experiments provide good excitations for system identification and parameter estimation purposes and the implementation of an appropriate experimental design is generally required (e.g. Wagner & Harvey 1997). In addition, problems of the lack of identifiability of model parameters estimated from tracer data, using currently available optimisation methods based on a single performance criterion, may be frequently encountered (e.g. Lees *et al.* 2000; Harvey & Wagner 2000; Camacho 2000).

In this paper a dynamic approach to the identification of reliable solute transport models, i.e. model structure and parameter set combinations, is investigated,

ultimately leading to an improved predictive ability of solute transport models. It is believed that a general modelling methodology for dynamic solute transport prediction in rivers needs a sound integrated modelling framework. This modelling framework should incorporate objective methods of system identification and parameter estimation, and elements of uncertainty analysis to quantify the prediction ability of the models.

It is important to stress that the identifiability procedure used here is not restricted to use with solute transport or water quality model structures. Wagener *et al.* (2001c) developed this approach as a generic tool applicable to any dynamic conceptual model structure in which at least some of the model parameters must be identified from measured system input and output data (Wheater *et al.* 1993).

## IDENTIFICATION OF DYNAMIC CONCEPTUAL MODELS

### Background

A general conceptual dynamic model can be written in mathematical form as

$$\hat{y}(t | \theta) = g(t | I, \theta) \quad (1)$$

where  $I$  is a matrix of system inputs,  $t$  is the time step,  $\theta$  is a parameter vector or parameter set,  $g(\cdot)$  is a collection of usually non-linear functions and  $\hat{y}$  is the simulated system output at time step  $t$  using parameter set  $\theta$ . The aim of the calibration procedure is to estimate the parameter set  $\theta$  that represents best the characteristics of the natural system investigated. The calibration procedure is often supported by an automatic search algorithm, which makes the task less time consuming and can, with an appropriate procedure, allow for the estimation of parameter uncertainty and interactions.

The prediction ability obtained with a specific parameter set is typically measured by analysing the model's residuals  $\varepsilon$ , i.e. the distance between simulated and observed time series, which can be calculated as follows:

$$\varepsilon(t | \theta) = y(t) - \hat{y}(t | \theta) \quad (2)$$

where  $y(t)$  is the observed system output. The residual vector is usually aggregated into a single value, i.e. an Objective Function (OF), if an automatic search algorithm is utilised. The algorithm's task is to make the 'size' of this value as small (or as large, depending on the definition) as possible by adjusting the parameter vector  $\theta$ . The parameter set can only be uniquely located within the parameter space, i.e. it is only globally identifiable, if it yields a unique response vector (Kleissen *et al.* 1990; Mous 1993). Such a unique vector is often given, but aggregating the model residuals into a single value has the disadvantage that it unavoidably leads to the loss of information.

A common OF in environmental modelling is the sum of squared errors, or its non-dimensional representation as the coefficient of efficiency ( $R^2$ , Nash & Sutcliffe 1970)

$$R^2 = 1 - \frac{\sigma_r^2}{\sigma_y^2} \quad (3)$$

where  $\sigma_r^2$  is the variance of the residuals and  $\sigma_y^2$  is the variance of the observed variable. However this OF emphasises the fitting of time series values of higher magnitude due to the use of squared residual values (Legates & McCabe 1999). Hence, information about parameters important for the model fit during periods containing data of low magnitudes is often lost. This loss can lead to identifiability problems with respect to parameters related to the model response in those periods (e.g. Wagener *et al.* 2001a). The problem can often be noticed by visual inspection of the output time series, whereby parameters yielding identical objective function values show obvious differences between the output time series (Gupta *et al.*, 1998; Wagener *et al.* 2001b), i.e. the selected objective function is not capable of distinguishing between visually different model behaviour.

The problem of information loss, associated with the use of a single OF, also restricts the analysis of model structural error. Boyle *et al.* (2000) show that using different objective functions to evaluate the model performance for different response modes can reveal deficiencies in the model structure. An appropriate

model structure should have a (single) consistent set of parameter values to represent all response modes.

A number of researchers have tried to avoid this problem of information loss by partitioning the continuous output time series, in order to specify different objective functions to measure the model performance during different response periods, thereby increasing the amount of information retrieved from the residuals. Some partitioning approaches are described here.

- (a) The partitioning can be based on experience with a specific model structure (Wheater *et al.* 1986; Harlin 1991). Only periods during which a parameter is of particular importance are selected for its calibration. However, this approach is subjective and requires experience with a specific model structure.
- (b) The periods can also be selected based on the hydrologist's understanding of the natural system. The partitioning then distinguishes between different system response modes and is therefore model independent (e.g. Dunne 1999; Boyle *et al.* 2000; Wagener *et al.* 2001a). The difficulty lies in the identification of all periods that are dominated by a particular hydrological process. The influence of some processes might, for example, only be present over a very short period of time.
- (c) A more objective approach to segmentation is the use of parameter sensitivity (e.g. Kleissen 1990; Beck *et al.* 1990; Wagner & Harvey 1997; Harvey & Wagner 2000). This approach is based on the assumption that informative data for parameter estimation are generally those for which the model response shows a high sensitivity to changes in the parameter values (Wagner & Harvey 1997). Kleissen (1990) developed an optimisation procedure that involves the calculation of the first-order sensitivity of each parameter (around a current best estimate) in time. Only data segments during periods where the parameter shows a high degree of sensitivity are included in the local optimisation scheme. This approach has the disadvantage that it only analyses the parameter sensitivity around a best estimate and uses a local optimisation scheme. The sensitivity can be different for different parameter sets. Harvey &

Wagner (2000) reduce this problem by starting with a uniform random sampling procedure and calculating the sensitivity around each parameter set so derived. However, this approach can result in a large number of model simulations.

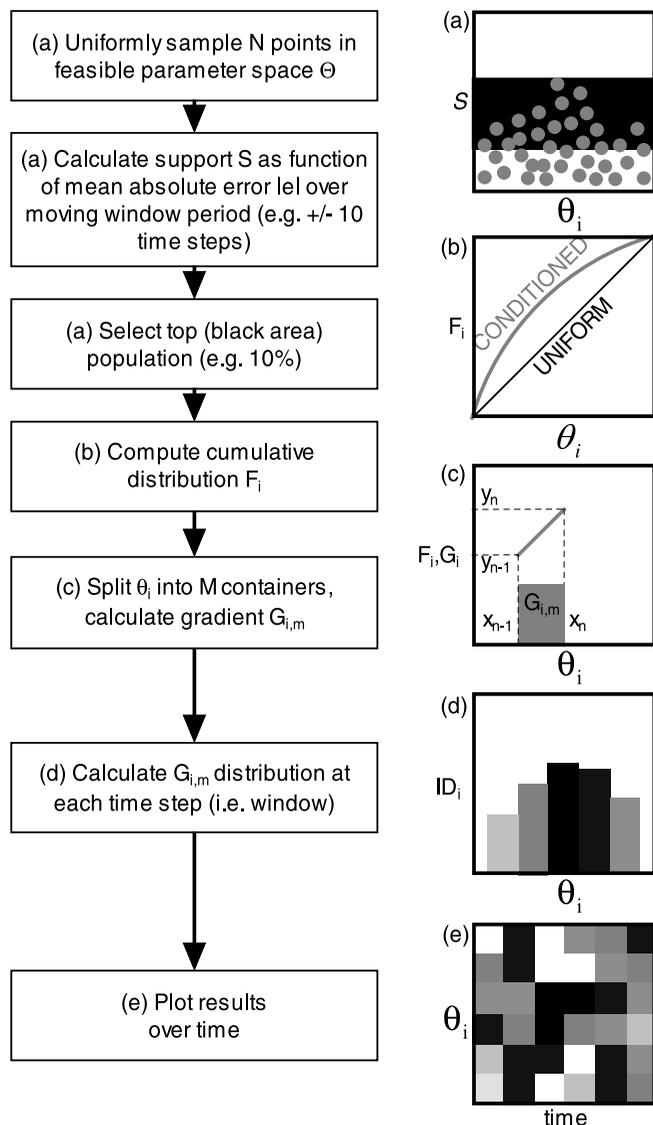
- (d) The observed system output can also be segmented purely based on similarities in the data using methods like cluster (Boogaard *et al.* 1998) or wavelet analysis. These approaches require an additional step to create a link between identified periods and model parameters.

The problem with all these approaches is that they are either subjective ((a) and (b)), difficult to use in a global optimisation procedure (c), or only solve part of the problem (d), i.e. no link to model components and therefore parameters. It is believed that an approach, which is independent of a specific model structure or time series, accounts for the problem of local minima and uses the strengths of the methods described above, could be highly advantageous. The objective is to develop a calibration and analysis methodology that maximises the use of the information available in the residuals.

### Dynamic identifiability analysis

A new method, introduced here, is an extension to the popular Regional Sensitivity Analysis (RSA) method of estimating the sensitivity of the model output to changes in the parameter values (Spear & Hornberger 1980; Hornberger & Spear 1980). The version used here is based on an investigation of the sensitivity of a parameter distribution when it is conditioned on a given measure of performance, i.e. OF, as introduced by Beven & Binley (1992). Deviations from an initially uniform distribution, and differences between those parts of the distribution performing well and poorly, indicate the sensitivity of the model response to changes in the parameter.

This approach is extended to measure the changing levels of parameter identifiability over time in a method called DYNamic Identifiability Analysis (DYNIA) (Wagener *et al.* 2001c), which consists of the steps shown in Figure 1. An objective function, e.g. the mean absolute error, is calculated, not over the whole calibration period



**Figure 1** | Flow chart of the DYNamic Identifiability Analysis (DYNNIA).

but as a running mean over a selected window size. The cumulative distribution of the best performing percentile (e.g. 10%) of the parameter distribution conditioned on this measure is calculated. The gradient of this cumulative distribution is an indicator of the identifiability of the parameter. A more identifiable parameter shows a locally higher gradient. For numerical approximation, the range of each parameter is split into 20 bins of equal width and the gradient is calculated in each. This binning is done

for every time step and the values of the gradients are indicated by grey shading. A higher degree of identifiability is indicated by a higher gradient and a darker shading. This process leads to a time-parameter diagram showing patches of different grey shadings (Figure 2).

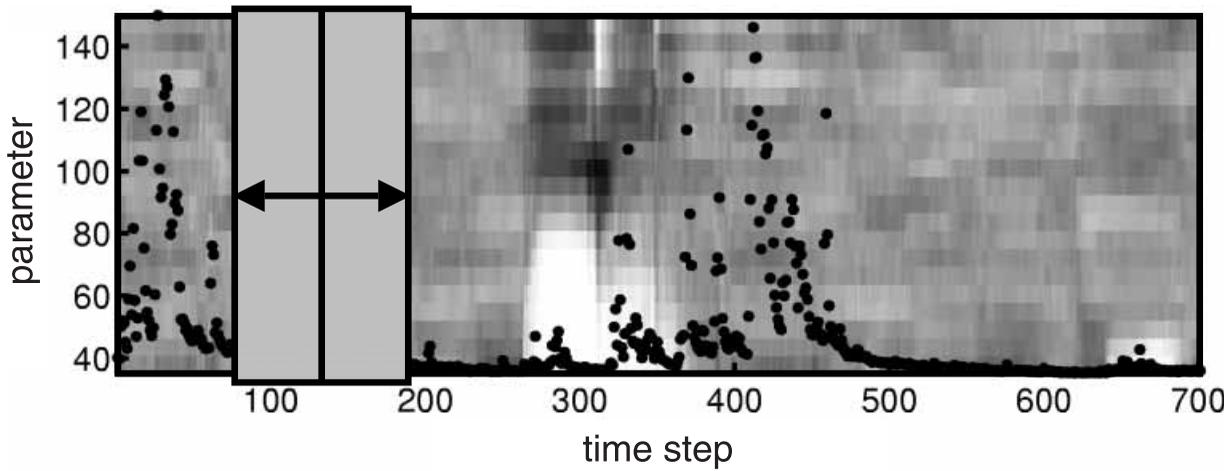
It should be noted that this approach only assesses the univariate marginal distribution and does not account for parameter dependence. Parameter dependence or interaction can be estimated by detailed investigation of the response surface or the variance-covariance matrix. Parameter interaction can, however, be indicated by the movement of identifiability regions of different parameters into similar or opposite directions during specific periods.

Additionally, the 90% confidence limits can be added to the DYNIA plot. These will be narrow in periods where the parameter is identifiable and wide otherwise. A measure of one minus the normalised distance between the confidence limits can be used to quantify these differences. A small value of this measure, resulting from narrow confidence limits, indicates that this data period contains information about the analysed parameter. These plots are therefore subsequently referred to as information content plots.

## THE TRANSIENT STORAGE MODEL

### Model structure

Comprehensive presentations of the TS model structure are given by Bencala & Walters (1983) and Runkel (1998). Discussion in this paper is limited to the variant of the general TS model structure appropriate for conservative solutes, steady uniform flow and a constant dispersion coefficient within a river reach (Figure 3). This TS model is governed by two equations, representing mass balances for solute in the stream and for solute in the storage zone. The mass balance in the stream includes transfer of solute mass due to advection, dispersion and first-order exchange due to transient storage. The mass balance in the storage zone includes transfer of mass due to first-order exchange with the main channel. The model equations are (Bencala & Walters 1983)



**Figure 2** | Example output of the DYNIA procedure. The black dots show an observed time series. The (moving) window (black rectangle) used to calculate the identifiability measure at each time step (centred vertical line) can be seen. The shading shows light grey colours where the response surface is flat, and black areas where peaks appear, i.e. the parameter becomes identifiable.

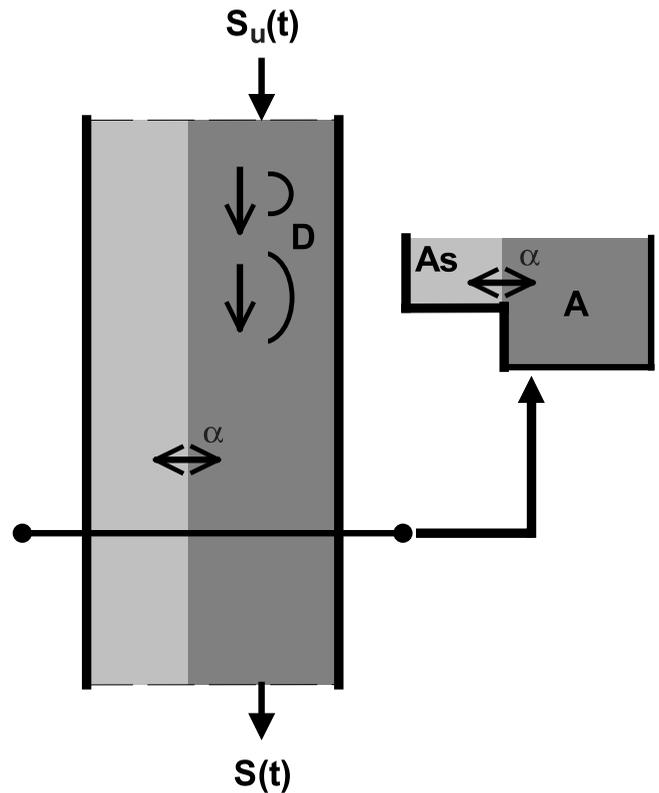
$$\frac{\partial c}{\partial t} + u_x \frac{\partial c}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left( AD \frac{\partial c}{\partial x} \right) + \alpha (c_s - c) \quad (4a)$$

$$\frac{dc_s}{dt} = -\alpha \frac{A}{A_s} (c_s - c) \quad (4b)$$

where  $c_s$  is the concentration in the storage zone [ $M L^{-3}$ ],  $c$  is the concentration in the main or active channel [ $M L^{-3}$ ],  $A$  is the main channel cross-sectional area normal to the flow [ $L^2$ ],  $A_s$  is the storage zone cross-sectional area normal to the flow [ $L^2$ ],  $\alpha$  is the exchange coefficient [ $T^{-1}$ ],  $u_x$  is the mean flow velocity in the main channel [ $L T^{-1}$ ] expressed in the original paper as  $u_x = Q/A$ ;  $Q$  is the flow discharge [ $L^3 T^{-1}$ ];  $t$  is time [ $T$ ],  $D$  is the coefficient of longitudinal dispersion in the main channel [ $L^2 T^{-1}$ ] and  $x$  is the longitudinal distance [ $L$ ].

Bencala & Walters (1983) conceptualise the transient storage mechanisms as occurring in adjacent zones to the main stream, representing

- relatively stagnant zones of water that are stationary relative to the faster moving water near the centre of the channel, and
- coarse gravel of the streambed and the porous areas within the stream bank through which flow may occur.



**Figure 3** | Conceptual representation of the TS model parametrisation. The parameters of the TS model are:  $D$ , the coefficient of longitudinal dispersion in the main channel;  $A$ , the main channel cross sectional area normal to the flow;  $A_s$ , the storage zone cross-sectional area normal to the flow; and  $\alpha$ , an exchange coefficient describing the interaction between storage and main channel zones. The model uses, amongst others, the (upstream) input solute concentration  $S_u$  at time step  $t$  to calculate the output concentration  $S$ .

The effect of transient storage mechanisms, affecting the spreading of the solute tracer distribution and causing an increase in solute residence time, is modelled as *an idealised exchange process* between the main or active channel and the adjacent storage zone. The exchange process is modelled as a first-order mass transfer, i.e. the exchange of solute between the main or active channel and the storage zone is proportional to the difference in concentration between the stream and the storage zone.

Although the conceptualisation of these TS mechanisms is highly idealised, the model is appealing to practitioners because it is a simple one-dimensional approach, able to reproduce accurately highly skewed observed solute tracer distributions.

Implementation of the TS model requires an estimate of the storage zone cross-sectional area  $A_s$  and an empirical exchange coefficient  $\alpha$ , in addition to the main channel area  $A$ , or velocity  $u_x$  for a known discharge, and the dispersion coefficient  $D$  in the stream itself (Figure 3). The four parameters ( $\alpha$ ,  $A$ ,  $A_s$ ,  $D$ ) are estimated using data from a tracer experiment.

### Current automatic calibration procedures

Conventionally, automatic calibration for the TS model is done using an extended version of the U.S. Geological Survey One-dimensional Transport with Inflow and Storage (OTIS) model (Runkel 1998). The extended version, OTIS-P (Runkel 1998), couples the solution of a more general form of Equation (4a,b), including additional terms to account for lateral inflow, first-order decay and sorption, with the non-linear regression package STARPAC (Donaldson & Tyron 1990). OTIS-P provides the means for objective parameter estimation in which the optimal set of parameter estimates is determined using Non-linear Least Squares (NLS) techniques (Wagner & Gorelick 1986; Donaldson & Tyron 1990; Runkel 1998). The goal of NLS is to determine the array of parameter estimates,  $\hat{\theta}$ , that minimises the weighted sum of squared differences between simulated and observed concentrations. The residual sum of squares  $RSS(\hat{\theta})$  objective function to be minimised is given by

$$RSS(\hat{\theta}) = \sum_{k=1}^N \{w_k [c_k - f(\zeta, \hat{\theta})_k]^2\} \quad (5)$$

where  $N$  is the number of observations,  $c_k$  is the observed main channel solute concentration [ $M L^{-3}$ ],  $f(\zeta, \hat{\theta})_k$  is a non-linear function that simulates the  $k$ th observed concentration, i.e. the solution of Equations (4a, b),  $\zeta$  is the independent variable, i.e.  $\zeta = t$  for time variable problems and  $w_k$  is a weighting factor assigned to the  $k$ th observation. The minimisation problem may be unweighted, where each error is given equal importance, i.e.  $w_k = 1$   $k = 1, N$ . Alternatively, weights may be assigned based on the magnitude of the solute concentration (Wagner & Gorelick 1986; Runkel 1998)

$$w_k = 1/f(\zeta, \hat{\theta})_k^2 \quad (6)$$

In the OTIS-P model an adaptive NLS technique that minimises  $RSS(\hat{\theta})$  using an iterative procedure (Dennis *et al.* 1981) is applied. The iterative procedure continues until either a criteria based on the relative change in the parameters or a criteria based on the change in the residual sum of squares is met (Runkel 1998).

The problem with this type of approach is its complete dependence on the chosen OF, in this case a sum of squared errors type function. The limitations of this method and the improved use of information through a dynamic approach become apparent in the application example.

## APPLICATION EXAMPLE

### River Mimram tracer experiment

Camacho (2000) describes the details of the River Mimram (UK) steady flow tracer experiment and includes the tracer data. Approximately 10 kg of sodium chloride was gulf-injected into the river upstream of the Panshanger flow-gauging flume's hydraulic jump, and the resulting tracer cloud was measured over time at three sampling stations A, B and C located 100 m, 140 m and 190 m downstream, respectively (Table 1).

**Table 1** | River Mimram channel discretisation and discharge

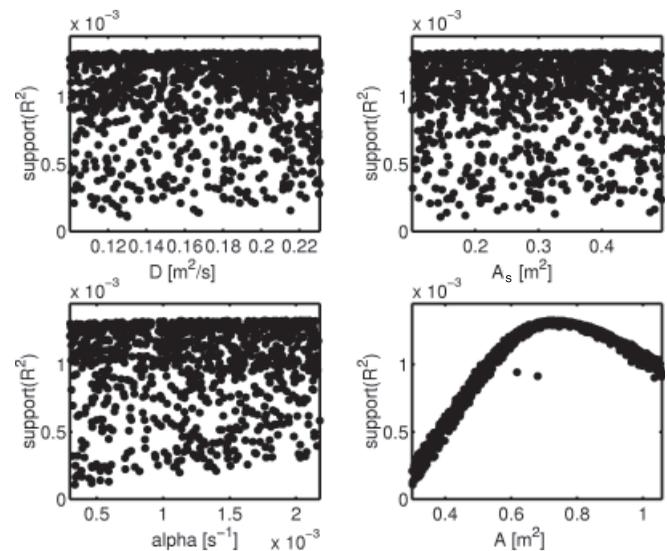
Reach	Sampling sites upstream-downstream	Length (m)	Discharge ( $\text{m}^3 \text{s}^{-1}$ )
A	Gulp injection–Site A	100	0.251
B	Site A–Site B	40	0.251
C	Site B–Site C	50	0.251

Measurements of conductivity were taken at irregular time intervals at the centre of each cross section in the main channel. The concentration of sodium chloride was computed using the conductivity meter calibration curves and interpolated over a uniform sampling interval of 10 seconds. At the flume's throat, the cross section is only about 50 cm wide and so lateral mixing is enhanced. In addition, the hydraulic jump provides adequate vertical mixing and the flume is located some 90 m upstream of the first sampling station. The data are considered relatively reliable, since discharge estimates obtained using standard dilution gauging procedures (Herschy 1995) are in close agreement (0.11–11%) with the measured flume discharge, which was constant at  $0.251 \text{ m}^3 \text{ s}^{-1}$  during the measurement (Camacho 2000).

With respect to the TS model structure application in this paper, parameter estimation is carried out on a reach by reach basis applying Fischer's routing method (Fisher 1973) between sampling stations and starting from the upstream reach A, where the upstream observed tracer distribution is available following a gulp injection. Thus, effectively the upstream boundary condition to reaches B and C already incorporates the effects of the initial mixing that occurs from the injection site along reach A.

## Results and discussion

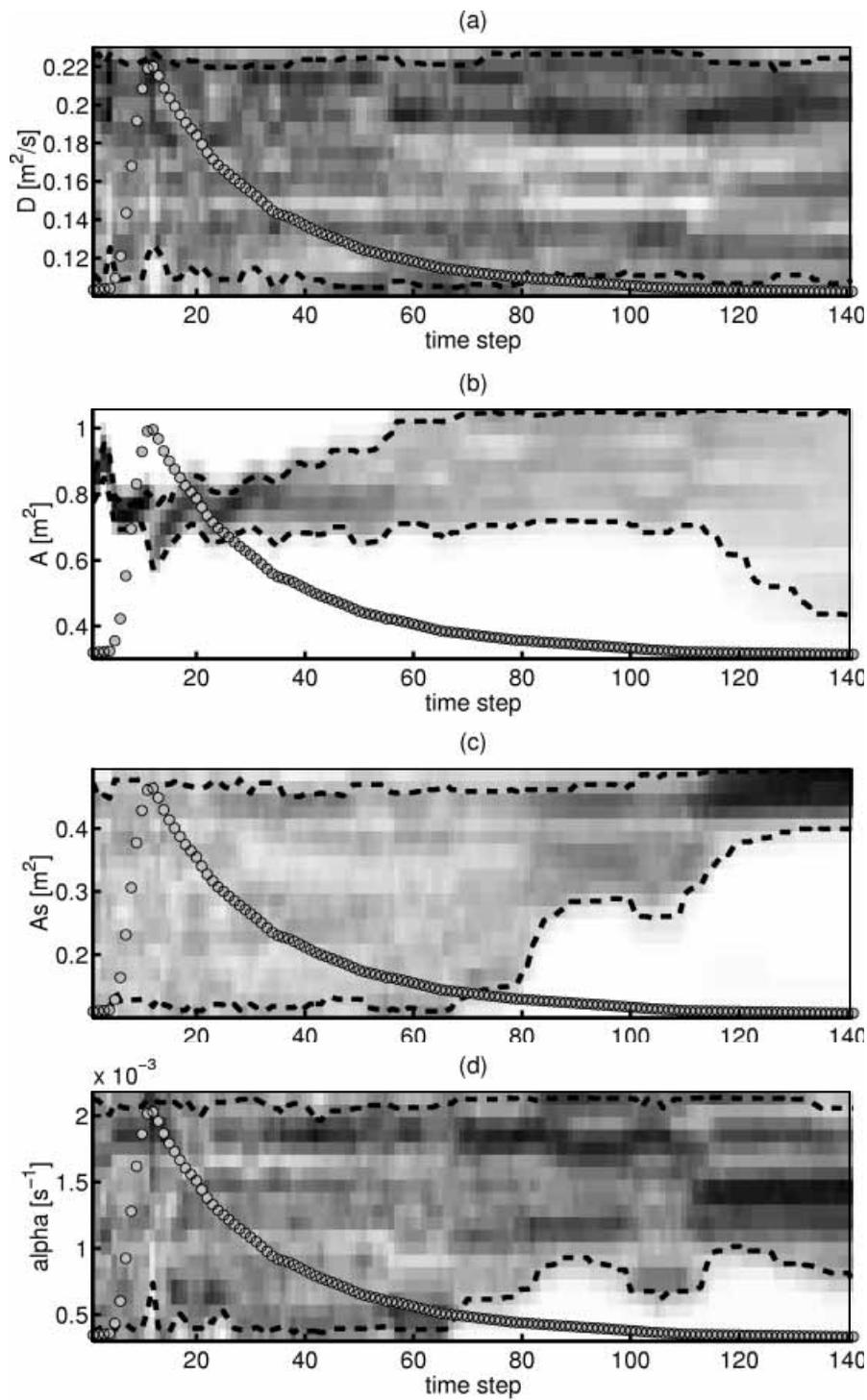
The analysis performed here is based on 1000 parameter sets, uniformly sampled from the feasible parameter space. The difficulty of identifying the correct parameter set for the transient storage model structure, i.e. those parameters which represent the characteristics of the natural system



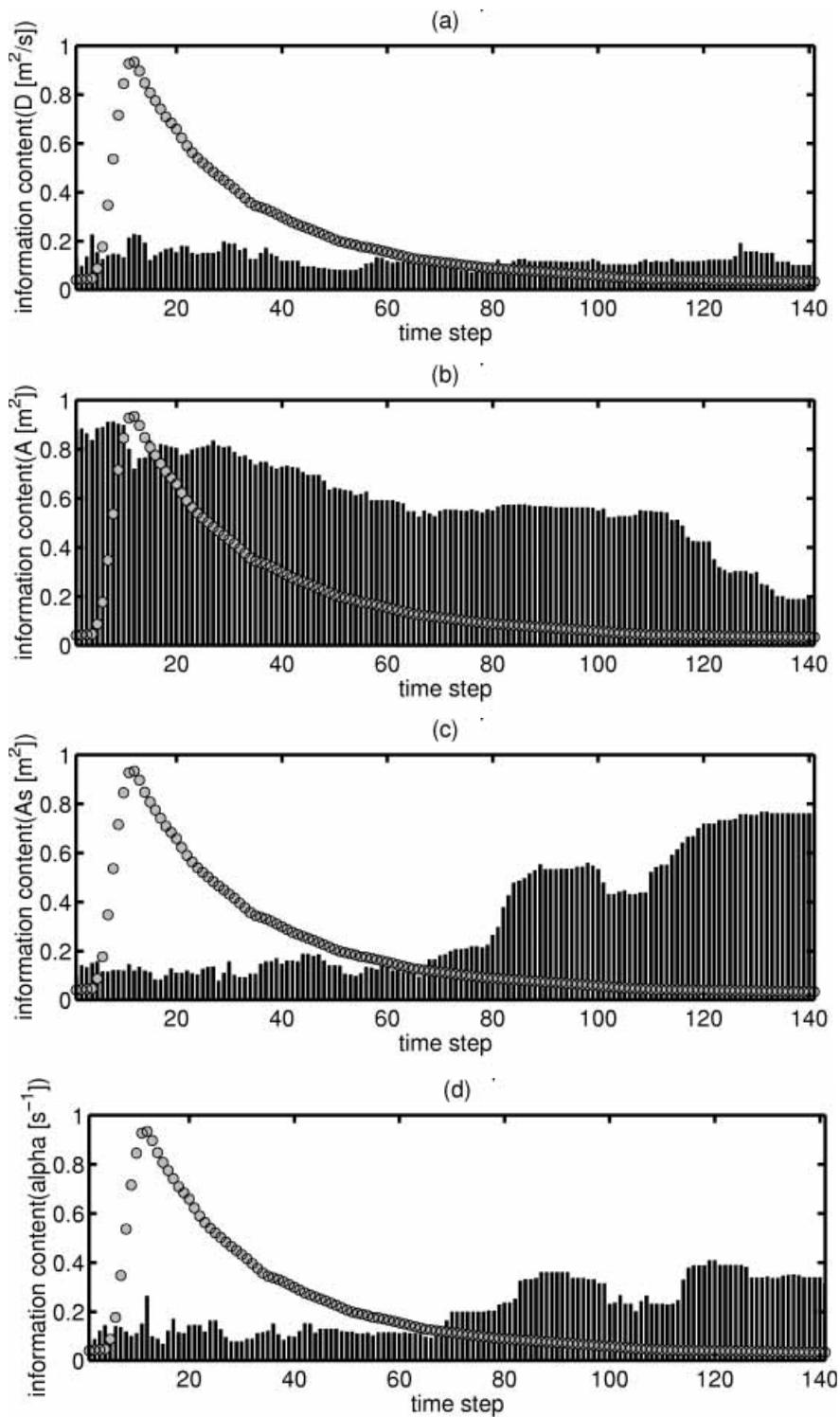
**Figure 4** | Dotted plot showing the projection of the response surface, i.e. the support values (normalised and transformed coefficient of efficiency  $R^2$  values, with higher values indicating better models), into the individual parameter dimensions: the dispersion coefficient  $D$ ; the main channel area  $A$ ; the storage zone area  $A_s$ ; and the exchange coefficient  $\alpha$ . The plot is based on a uniform random search sampling 1000 sets from the feasible parameter space.

under investigation, is demonstrated by the scatter plots in Figure 4. These plots represent individual Monte Carlo simulations based on a uniform random search, sampling 1000 points from the feasible parameter space. The parameters  $D$ ,  $A_s$  and  $A$  show flat distribution surfaces when plotting their support against the individual parameter values. The support measure is the transformed OF, i.e. the coefficient of efficiency. It can be seen that very different combinations of those parameters yield identical performances in terms of the selected OF. From this analysis, only the  $A$  parameter seems identifiable, i.e. shows a clear peak. However, it has to be considered that this is a univariate analysis and that some structure of the response surface may be lost by the projection into a single parameter dimension (Beven 1998).

The same 1000 parameter sets were input into the DYNIA procedure. A window size of three time steps is selected in this case because *the concentration history is sensitive to the parameters over relatively narrow time spans that are associated with specific segments of the concentration history* (Wagner & Harvey 1997). The results of this analysis are shown in Figures 5 and 6.



**Figure 5** | The results of the DYNIA procedure for the different parameters of the TS model structure using gulp injection. The dashed black lines indicate the 90% confidence limits, while the grey dots indicate the observed solute concentrations. The parameters are: (a) the dispersion coefficient  $D$ ; (b) the main channel area  $A$ ; (c) the storage zone area  $A_s$ ; and (d) the exchange coefficient  $\alpha$ .



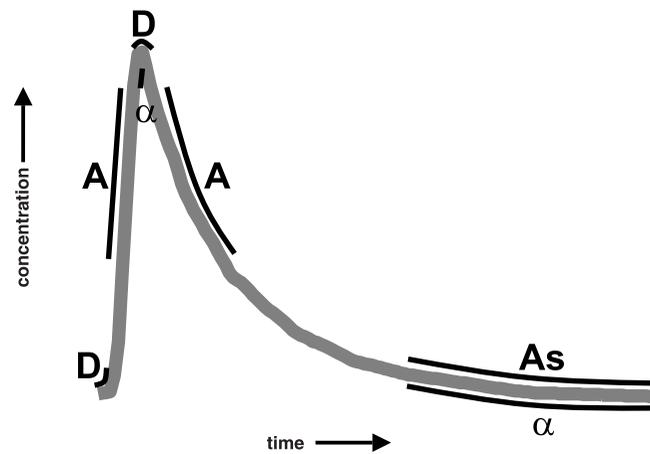
**Figure 6** | Graphs showing the information content (black bars) of the tracer data with respect to the TS parameters during the different time steps to identify individual parameters. The observed solute concentration is shown as grey dots. The parameters are: (a) the dispersion coefficient  $D$ ; (b) the main channel area  $A$ ; (c) the storage zone area  $A_s$ , and (d) the exchange coefficient  $\alpha$ .

Figure 5(a) shows that those values for the dispersion coefficient  $D$  associated with good performance are widely distributed over the whole parameter space, indicated by the scatter of light and dark grey shades. This result suggests a clear identifiability problem with respect to this parameter using the available data. This conclusion is also emphasised by the wide 90% confidence limits (dashed lines). They indicate the probability that the correct parameter value is lying within that range and reflect the amount of information available in a certain period of the tracer data to identify a specific parameter. Figure 6 shows the values of one minus the width of the confidence limits at each time step, normalised with respect to the feasible parameter range. It can be seen that the information content of the tracer data with respect to the dispersion coefficient  $D$  is very low. High values of the information content (Figure 6(a)) during the tracer concentration distribution peak, however, suggest that a constant injection strategy might have been advantageous for a better estimation of this parameter.

The channel area  $A$  in Figure 5(b) shows a dense area of well identified values during the rising limb of the tracer distribution (the first five or so time steps with zero concentration have to be ignored). For the remaining time, the parameter values are widely distributed over the parameter range, indicated by light grey shading and wide confidence limits.

Figures 6(b) and 6(c) show the interaction between  $A$  and  $A_s$ . A large main channel area  $A$  is important to fit the rising limb of the tracer distribution, i.e. large amounts of the tracer arriving early, while large storage zones (high  $A_s$ ) values help to maintain the long tail. It can also be noticed in Figure 6(c) that the coefficient of efficiency  $R^2$  is putting more emphasis on fitting the high values of the distribution and that information in other parts is lost during the aggregation process. The region containing information has no influence on the shape of the dotted plot surface shown in Figure 4 for the entire period of record.

The parameter  $\alpha$  describing the exchange rate between the main channel and storage zone only shows specific areas of well identified values at the end of the concentration distribution tail (Figure 5(d)). Here, a small exchange rate leads to sufficient solute being available to maintain this part of the distribution. The inter-



**Figure 7** | Qualitative plot of periods of identifiability for the different TS model parameters using a gulp injection. The observed solute concentration is shown as a grey line, while the black lines indicate periods of identifiability for the different parameters. The parameters are: (a) the dispersion coefficient  $D$ ; (b) the main channel area  $A$ ; (c) the storage zone area  $A_s$ ; and (d) the exchange coefficient  $\alpha$ .

dependence between  $\alpha$  and the storage zone area can also be seen. Both parameters diverge in opposite directions, showing that they produce similar effects with respect to fitting the same periods. Figure 6(d) shows slightly higher values of the information content during the distribution peak, similar to Figure 6(a), suggesting again that a constant injection strategy, causing a plateau at the peak value, could have produced more information to identify this parameter.

This analysis of this tracer experiment thus shows that much more information (and insight) is derived using the dynamic approach in comparison to a simple Monte Carlo analysis as shown in Figure 4. An overall OF such as  $R^2$  is unable to identify parameters related to the tracer concentration tail, such as  $A_s$  and  $\alpha$ . DYNIA, on the other hand, reveals at which part of the concentration individual parameters are particularly identifiable. This knowledge is important for experimental design; for example, sampling efforts can be concentrated at those periods.

## CONCLUSIONS

The estimation of parameters of dynamic, conceptual environmental or hydrological models is a difficult

task. Manual calibration can yield good results, but the procedure is time consuming, requires experience and it is difficult to consider parameter interactions. Traditional, single-objective automatic calibration procedures, on the other hand, often lead to a large number of parameter sets performing similarly with respect to the selected measure. DYNIA attempts to overcome these problems by calculating parameter identifiability as a running mean. Possible applications of this method, next to the task of *model calibration or identification*, are:

- (a) the *analysis of model structures*. Model structural inadequacies will make themselves visible in cases where a parameter distribution shows distinct peaks, i.e. dark patches (Figure 4), which change value in time. The model has to adjust the parameter in order to predict the output correctly. A suitable model structure should show consistent parameter values, even for different system response modes.
- (b) The algorithm also relates *model parameters and response modes* of the natural system. The proper working of the model components can therefore be analysed.
- (c) The method can also be used to *design tracer experiments*, improving parameter identification by choosing the design which provides the highest information content for parameter estimation (e.g. Wagner & Harvey 1997).

A limitation of this method is its dependency on Monte Carlo simulations, which restricts the analysis of high-dimensional parameter spaces. Future research will focus, amongst other things, on the analysis of the potential of different types of tracer experiments to identify solute transport model parameters.

The analysis of the TS model structure showed the difficulty of identifying the model's parameters using conventional, single-objective, approaches. The dynamic approach allowed more of the information contained in the data to be used and a better picture of the more preferable parameter values for a particular case is obtained.

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## NOMENCLATURE

$\alpha$	exchange coefficient ( $T^{-1}$ )
$\varepsilon$	model residual
$\theta$	parameter vector
$\sigma_r^2$	variance of residuals
$\sigma_y^2$	variance of observed variable
$\zeta$	independent variable (e.g. time)
$\hat{\theta}$	parameter estimate
$A$	main channel cross-sectional area normal to flow ( $L^2$ )
$A_s$	storage zone cross-sectional area normal to flow ( $L^2$ )
$c$	concentration in main or active channel ( $M L^{-3}$ )
$c_s$	concentration in storage zone ( $M L^{-3}$ )
$D$	coefficient of longitudinal dispersion in main channel ( $L^2 T^{-1}$ )
$F$	cumulative distribution
$f(\cdot)$	non-linear function
$G$	gradient
$g(\cdot)$	collection of non-linear functions
$I$	matrix of system inputs
ID	identifiability measure
$i$	index
$k$	index
$m$	index
$N$	number of observations
$n$	index
$Q$	flow discharge ( $L^3 T^{-1}$ )
$R^2$	coefficient of efficiency
RSS	residual sum of squares
$S$	support
$t$	time step (T)
$u_x$	mean flow velocity in main channel ( $L T^{-1}$ )
$w$	weighting factor
$x$	longitudinal distance (L)
$y$	observed system output
$\hat{y}$	simulated system output

## REFERENCES

- Beck, M. B., Kleissen, F. M. & Wheeler, H. S. 1990 Identifying flow paths in models of surface water acidification. *Rev. Geophys.* **28**(2): 207–230.
- Bencala, K. E. & Walters R. A. 1983 Simulation of solute transport in a mountain pool-and-riffle stream: a transient storage model. *Wat. Res. Res.* **19**(3): 718–724.
- Beven, K. J. 1998 *Generalized Likelihood Uncertainty Estimation—User Manual*. University of Lancaster, unpublished.
- Beven, K. J. & Binley, A. M. 1992 The future of distributed models: model calibration and uncertainty in prediction. *Hydrol. Process.* **6**, 279–298.
- Boogaard, H. F. P. van den, Ali, Md. S. & Mynett, A. E. 1998 Self organising feature maps for the analysis of hydrological and ecological data sets. In: *Hydroinformatics '98* (ed. V. Babovic & L. C. Larsen). Balkema, Rotterdam, pp. 733–740.
- Boyle, D. P., Gupta, H. V. & Sorooshian, S. 2000 Towards improved calibration of hydrologic models: combining the strengths of manual and automatic methods. *Wat. Res. Res.* **36**, 3663–3674.
- Camacho, L. A. 2000 Development of a hierarchical modelling framework for solute transport under unsteady flow conditions in rivers. *PhD thesis*, Imperial College of Science, Technology and Medicine, London, UK.
- Chapra, S. C. 1997 *Surface Water-Quality Modelling*. McGraw-Hill, New York.
- Dennis, J. E. Jr., Gay, D. M. & Welsh, R. E. 1981 An adaptive nonlinear least-squares algorithm: Association for computing machinery. *Trans. Math. Software* **7**, 348–368.
- Donaldson, J. R. & Tyron, P. V. 1990 *User's Guide to STARPAC. The Standards Time Series and Regression Package*. Internal Rep. NBSIR 86-3448, National Institute of Standards and Technology, Gaithersburg, MD, USA.
- Dunne, S. M. 1999 Imposing constraints on parameter values of a conceptual hydrological using baseflow response. *Hydrol. Earth Syst. Sci.* **3**, 271–284.
- Fischer, H. B. 1973 Longitudinal dispersion and turbulent mixing in open channel flow. *Ann. Rev. Fluid Mech.* **5**, 59–78.
- Gutpa, H. V., Sorooshian, S. & Yapo, P. O. 1998 Toward improved calibration of hydrologic models: multiple and noncommensurable measures of information. *Wat. Res. Res.* **34**(4), 751–763.
- Harlin, J. 1991 Development of a process oriented calibration scheme for the HBV hydrological model. *Nordic Hydrol.* **22**, 15–36.
- Harvey, J. W. & Wagner, B. J. 2000. Quantifying hydrologic interactions between streams and their subsurface hyporheic zones. In: *Streams and Ground Waters* (ed. J. A. Jones, & P. J. Mulholland). Academic Press, San Diego, pp. 3–44.
- Hersch, R. W. 1995 *Streamflow Measurement*. 2nd Edition. E. & F. N. Spon, London, UK.
- Hornberger, G. M. & Spear, R. C. 1980 Eutrophication in Peel Inlet I, The problem: defining behaviour and a mathematical model for the phosphorous scenario. *Wat. Res.* **14**, 29–42.
- Jackman, A. P., Walters, R. A. & Kennedy, V. C. 1984 Transport and concentration controls for chloride, strontium, potassium and lead in Uvas Creek, a small cobble-bed stream in Santa Clara County, California, USA. 1. Conceptual model. *J. Hydrol.* **75**, 67–110.
- Kleissen, F. M. 1990 *Uncertainty and identifiability in conceptual models of surface water acidification*. PhD thesis, Imperial College of Science, Technology and Medicine, London, UK.
- Kleissen, F. M., Beck, M. B. & Wheeler, H. S. 1990 The identifiability of conceptual hydrochemical models. *Wat. Res. Res.* **26**(12), 2979–2992.
- Lees, M. J., Camacho, L. A. & Chapra, S. C. 2000 On the relationship of transient-storage and aggregated dead zone models of longitudinal solute transport in streams. *Wat. Res. Res.* **36**(1), 213–224.
- Legates, D. R. & McCabe, G. J. Jr. 1999 Evaluating the use of “goodness-of-fit” measures in hydrologic and hydroclimatic model validation. *Wat. Res. Res.* **35**(1), 233–241.
- Mous, S. L. J. 1993 Identification of the movement of water in unsaturated soils: the problem of identifiability of the model. *J. Hydrol.* **143**, 153–167.
- Nash, J. E. & Sutcliffe, J. V. 1970 River flow forecasting through conceptual models I, A discussion of principles. *J. Hydrol.* **10**, 282–290.
- Orlob, G. T. 1981 *Mathematical Modelling Of Water Quality: Streams, Lakes, And Reservoirs*. Int. Inst. for Appl. Syst. Analysis (IIASA), John Wiley & Sons, Chichester.
- Runkel, R. L. 1998 *One-dimensional transport with inflow and storage (OTIS): a solute transport model for streams and rivers*, U.S.G.S. Water Resources Investigations Report 4018, Denver, CO.
- Spear, R. C. & Hornberger, G. M. 1980 Eutrophication in Peel Inlet II, Identification of critical uncertainties via Generalised Sensitivity Analysis. *Wat. Res.* **14**: 43–49.
- Taylor, G. I. 1954 The dispersion of matter in turbulent flow through a pipe. *Proc. R. Soc. Ser. A* **223**, 446–468.
- Thomann, R. V. & Mueller, J. A., 1987 *Principles of Surface Water Quality Modelling and Control*. Harper & Row, New York.
- Wagener, T., Lees, M. J. & Wheeler, H. S. 2000 Incorporating predictive uncertainty into a rainfall-runoff modelling system. *Proceedings of the Hydroinformatics 2000 Conference, Iowa, USA*. Compact disk. University of Iowa, Iowa, USA.
- Wagener, T., Boyle, D. P., Lees, M. J., Wheeler, H. S., Gupta, H. V. & Sorooshian, S. 2001a A framework for the development and application of hydrological models. *Hydrol. Earth Syst. Sci.* **5**(1), 13–26.
- Wagener, T., Lees, M. J. & Wheeler, H. S. 2001b A toolkit for the development and application of parsimonious hydrological models. In: *Mathematical Models of Large Watershed Hydrology*, vol. 1 (ed. V. P. Singh & D. Frevert). Water Resources Publishers, Littleton, Colorado, USA, pp. 91–140.
- Wagener, T., McIntyre, N., Lees, M. J., Wheeler, H. S. & Gupta, H. V. 2001c Towards reduced uncertainty in conceptual

- rainfall-runoff modelling: dynamic identifiability analysis. *Hydrol. Process.* in press.
- Wagner, B. J. & Gorelick, S. M. 1986 A statistical methodology for estimating transport parameters: theory and applications to one-dimensional advective-dispersive systems. *Wat. Res. Res.* **33**(7), 1731–1741.
- Wagner, B. J. & Harvey, J. W. 1997 Experimental design for estimating parameters of rate-limited mass transfer: analysis of stream tracer studies. *Wat. Res. Res.* **33**(7), 1731–1741.
- Wheater, H. S., Bishop, K. H. & Beck, M. B. 1986 The identification of conceptual hydrological models for surface water acidification. *Hydrol. Process.* **1**, 89–109.
- Wheater, H. S., Jakeman, A. J. & Beven, K. J. 1993 Progress and directions in rainfall-runoff modeling. In: *Modeling Change In Environmental Systems* (ed. A. J. Jakeman, M. B. Beck & M. J. McAleer). John Wiley & Sons, Chichester, pp. 101–132.
- Wörman, A. 2000 Comparison of models for transient storage of solutes in small streams. *Wat. Res. Res.* **36**(10), 455–468.