

This discussion paper is/has been under review for the journal Hydrology and Earth System Sciences (HESS). Please refer to the corresponding final paper in HESS if available.

**Resolving structural  
model errors**

J. H. Spaaks and  
W. Bouten

# Resolving structural errors in a spatially distributed hydrologic model

J. H. Spaaks<sup>1,2</sup> and W. Bouten<sup>1</sup>

<sup>1</sup>Institute for Biodiversity and Ecosystem Dynamics, University of Amsterdam, Amsterdam, The Netherlands

<sup>2</sup>Netherlands eScience Center, Amsterdam, The Netherlands

Received: 12 January 2013 – Accepted: 15 January 2013 – Published: 7 February 2013

Correspondence to: J. H. Spaaks (jspaaks@uva.nl)

Published by Copernicus Publications on behalf of the European Geosciences Union.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Abstract

In hydrological modeling, model structures are developed in an iterative cycle as more and different types of measurements become available and our understanding of the hillslope or watershed improves. However, with increasing complexity of the model, it becomes more and more difficult to detect which parts of the model are deficient, or which processes should also be incorporated into the model during the next development step. In this study, we use two methods (SCEM-UA and SODA) to calibrate a purposely deficient 3-D hillslope-scale model to error-free, artificially generated observations. We use a multi-objective approach based on distributed pressure head at the soil-bedrock interface and hillslope-scale discharge and water balance. SODA's usefulness as a diagnostic methodology is demonstrated by its ability to identify the timing and location of processes that are missing in the model. We further show that SODA's state updates provide information that could readily be incorporated into an improved model structure, and that this type of information cannot be gained from parameter estimation methods such as SCEM-UA. We conclude that SODA can help guide the discussion between experimentalists and modelers by providing accurate and detailed information on how to improve spatially distributed hydrologic models.

## 1 Introduction

Our understanding of hillslope and watershed hydrology is typically summarized in numerical models. Ideally, such models are the result of an iterative process that involves modeling, experimental design, data collection, and analysis of the model-data mismatch (e.g. Box and Tiao, 1973, Sect. 1.1.1 "The role of statistical methods in scientific investigation" and Popper, 2009, Sect. 1.1.3 "Deductive testing of theories"). Especially when combined with laboratory experiments, this *iterative research cycle* (Fig. 1) has proven to be a useful method for theory development. Its usefulness stems from the fact that in laboratory experiments, the state of the system under study as well as

HESSD

10, 1819–1858, 2013

### Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



its parameters and the forcings/disturbances to which the system is subjected, can usually be measured more or less accurately. This allows the investigation to focus on the one remaining uncertain factor, namely the hypothesis/model structure. There is, however, a stark contrast between experiments carried out in the laboratory and those carried out in the field. As hydrologists, we are often dealing with open systems (e.g. von Bertalanffy, 1950), meaning that flows such as precipitation, groundwater recharge, and evapotranspiration cross the system's boundary. Unfortunately, we often lack the necessary technology to observe these flows (or how they affect the state of the system) at the scale triplet of interest, and manipulation experiments are generally impossible (e.g. Young, 1983). Furthermore, many hydrological models have parameters that cannot be measured directly, either because of practical considerations or because the parameters are conceptual. The uncertainty associated with the parameters, state, forcings, and output makes theory development at the scale of watersheds and hillslopes much more difficult than for small scale experiments in the laboratory.

So, it is certainly not straightforward to collect enough data of sufficient quality in field experiments. This is not the only challenge though: making sense of the data (i.e. analysis) has proven just as difficult. In the remainder of this paper, we will focus on the latter problem. When discussing the analysis stage of the iterative research cycle, it is useful to distinguish between two possible scenarios. In the first scenario, the modeling is performed because a prediction is needed (for instance in support of estimating the chance of a flood of a certain magnitude). In this context, a good predictive model is one that is capable of estimating the variable of interest with little bias and small uncertainty, which can be demonstrated by performing a traditional split-sample test (e.g. Klemeš, 1986). In this scenario, the mechanisms underpinning the model structure need not concern the modeler too much – the important thing is that the model gives the right answer, even when it does so for the wrong reasons (e.g. Kirchner, 2006).

Being right for the wrong reasons is not acceptable under the second scenario, in which the purpose of the modeling is to test and improve our understanding of how things work. Since it is axiomatic that for complex systems, the initial model structure

is at least partly incorrect, the challenge that we are facing in the analysis stage of the iterative research cycle is how to *diagnose* the current, incorrect model structure, such that we can make an informed decision on what needs to be changed for the next, hopefully more realistic model structure (e.g. Gupta et al., 2008).

5 A common way of diagnosing how a given model can be improved, is through an analysis of model-observation residuals. It is important to note, though, that such an analysis is only possible after the model has been parameterized. In case the model parameters cannot be measured directly, the parameter values need to be determined by means of parameter estimation methods. In recent years, various authors have discussed the pitfalls associated with parameter estimation, specifically when applied to cases in which data error and model structural error cannot be neglected (e.g. Kirchner, 2006; Ajami et al., 2007). For example, it has been demonstrated how model parameters can compensate for model structural errors by assuming unrealistic values during parameter estimation (e.g. Clark and Vrugt, 2006). Without the right parameter values, interpretation of the residual patterns – and therefore model improvement – becomes much more difficult. To overcome these difficulties, various lines of research have been proposed that attempt to increase the diagnostic power of the analysis by extending the traditional parameter estimation paradigm in various ways.

20 For example, one line of research has argued that a multi-objective approach can provide more insight into how a model structure may be deficient (Yapo et al., 1998; Gupta et al., 1998). In the multi-objective approach, the performance of each model run is evaluated using not just one, but multiple objectives. Individual objectives can vary in the function used (RMSE, HMLE, mean absolute error, Nash–Sutcliffe efficiency, etc.; e.g. Gupta et al., 1998), in the variable that the objective function operates on (streamflow, groundwater tables, isotope composition, major ion concentrations, etc.; e.g. Mroczkowski et al., 1997; Franks et al., 1998; Kuczera and Mroczkowski, 1998; Dunn, 1999; Seibert, 2000), or in the transformation, selection, or weighting that is used (e.g. Vrugt et al., 2003a; Tang et al., 2006). After a number of model runs have been executed, the population of model runs is divided into a “good” set and a “bad”

## HESSD

10, 1819–1858, 2013

### Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



set. The good set consists of points that are non-dominated, meaning that any point in this set represents in some way a best point. Together, the non-dominated points make up the Pareto front (Goldberg, 1989; Yapo et al., 1998). The multi-objective approach is useful for model improvement because it enables analyzing the trade-offs that occur between various objectives in the Pareto front. If the various objectives have been formulated such that individual objectives predominantly reflect specific aspects of the system under consideration, then inferences can be made about the appropriateness of those aspects (Gupta et al., 1998; Yapo et al., 1998; Boyle et al., 2000, 2001; Wagener et al., 2001). For a recent review of the multi-objective approach, see Efstratiadis and Koutsoyiannis (2010).

A second line of research abandons the idea of using just one model structure for describing system behavior but instead uses an ensemble of model structures. The ensemble may be composed of multiple existing model structures that are run using the same initial state and forcings (e.g. Georgakakos et al., 2004). Alternatively, the ensemble may be made up of model structures that are assembled from a limited set of model structure components using a combinatorial approach (e.g. Clark et al., 2008). The predictions generated by members of the ensemble may further be combined in order to maximize the predictive capabilities of the ensemble, for example by using Bayesian Model Averaging (e.g. Hoeting et al., 1999; Raftery et al., 2003, 2005; Neuman, 2003). Regardless of how the ensemble was constructed, differences between members of the ensemble can be exploited to make inferences about the appropriateness of specific model components.

The idea underpinning the third line of research originates with calibration attempts in which it was found that the optimal values of a given model's parameters tend to change depending on what part of the empirical record is used in calibration (see for example Fig. 2b in Gupta et al., 1998). This is generally taken as an indication that the model is structurally deficient, because it is unable to reproduce the entire empirical record with a single set of parameters (Gupta et al., 1998; Yapo et al., 1998; Wagener et al., 2001; Lin and Beck, 2007). Due to the deficiency, the model does not extract

## HESSD

10, 1819–1858, 2013

### Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



all of the information that is present in the observations, which in turn means that the residuals contain “information with nowhere to go” (Doherty and Welter, 2010). Over the last few decades, various mechanisms have been proposed with which such misplaced information can be accommodated. For example, the Time Varying Parameter (TVP) approach (Young, 1978) and the related State Dependent Parameter (SDP) approach (Young, 2001) relax the assumption that the model parameters are constant during the entire empirical record. Somewhat related to TVP is the DYNIA approach of Wagener et al. (2003). DYNIA attempts to isolate the effects of individual model parameters. To do so, it uses elements of the well-known Generalized Sensitivity Analysis (GSA) and Generalized Likelihood Uncertainty Estimation (GLUE) methods (Spear and Hornberger, 1980; Beven and Binley, 1992). DYNIA facilitates making inferences about model structure by analyzing how the probability distribution of the parameter values changes over simulated time, and by analyzing how the distribution is affected by certain response modes, such as periods of high discharge. Relaxing the time-constancy assumption is not the only mechanism with which misplaced information may be accommodated though; some authors have advocated the introduction of auxiliary parameters, whose primary purpose is to absorb the misplaced information, such that the actual model parameters can adopt physically meaningful values during parameter estimation (e.g. Kavetski et al., 2006a,b; Doherty and Welter, 2010; Schoups and Vrugt, 2010).

In contrast to parameter-oriented methods described above, state-oriented methods let the misplaced information be absorbed into the model states. The most widespread of the state-oriented methods is the Kalman Filter (KF; Kalman, 1960) and its derivatives, notably the Extended KF (EKF; e.g. Jazwinski, 1970) and the Ensemble KF (EnKF; Evensen, 1994, 2003). The family of KFs has further been extended with that of Particle Filters (PFs), which have become popular due to their ability to cope with complex probability distributions. Both KFs and PFs use a sequential scheme to propagate the model states through simulated time, assimilating observations one-by-one as the simulation progresses. Assimilating observations sequentially, rather than *en bloc*,

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



allows for retaining information about when and where simulated behavior deviates from what was observed. This is a particularly attractive property when the objective is to evaluate and improve a given model. Nonetheless, filtering methods have hitherto been used mostly to improve the accuracy and precision of either the parameter values themselves or the predictions made with those parameters (Eigbe et al., 1998). That is, the focus has been on the a posteriori estimates. In contrast, we argue that an analysis of *how the a priori estimates are updated* may yield valuable information about the appropriateness of the model structure: if there are no apparent patterns in the updating, the model structure is as good as the data allow. On the other hand, if there are patterns present in the updating, an alternative model formulation exists that better captures the observed dynamics. Analysis of state updating patterns could thus provide a much needed diagnostic tool for improving model structures.

The aim of our study is to demonstrate that, when a model does not have the correct structure given the data,

1. parameter estimation may yield error patterns in which the origin of the error is obscured due to compensation effects;
2. combining parameter estimation with ensemble Kalman Filtering provides accurate and specific information that can readily be applied to improve the model structure.

By using error-free, artificially generated observations, we avoid any issues related to accuracy and precision of field measurements, as well as any issues related to incommensurability of field measurements and their model counterparts.

## 2 Methods

### 2.1 General setup of this study

This study consists of three parts: (1) generation of the artificial measurements; (2) calibration with a parameter estimation algorithm (SCEM-UA; Vrugt et al., 2003b); (3) calibration with a combined parameter and state estimation algorithm (SODA; Vrugt et al., 2005). In the first part, we generated the artificial measurements by simulating the hydrodynamics of a small, hypothetical hillslope with a relatively shallow soil, using the SWMS\_3D model for variably saturated flow (Šimůnek, 1994; Šimůnek et al., 1995). We then introduced a model structural error by making some small simplifications to the model structure. Hereafter, we use the terms “forward model” and “inverse model” to differentiate between these two model structures. Due to the simplifications, the inverse model is structurally deficient: it does not fully capture the complexity apparent in the artificial measurements. In the second and third part of this study, the inverse model was calibrated to the artificial measurements using SCEM-UA and SODA, respectively. We analyzed the model output associated with the optimal parameter combination(s) for both methods, and we evaluated how useful each result was for identifying the structural deficiency in the inverse model.

### 2.2 Generation of the artificial measurements

We used the SWMS\_3D model (Šimůnek, 1994; Šimůnek et al., 1995) to generate artificial measurements. SWMS\_3D implements the Richards equation for variably saturated flow through porous media (Richards, 1931):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial s} \left[ K(h) \frac{\partial (h+z)}{\partial s} \right] - B \quad (1)$$

in which  $\theta$  is the volumetric water content,  $t$  is time,  $s$  is distance over which the flow occurs,  $K$  is hydraulic conductivity,  $h$  is pressure head,  $z$  is gravitational head, and  $B$

HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





is a sink term. While  $B$  is normally used for simulating water extraction by roots, we instead used it to simulate downward vertical loss of water from the soil domain to the underlying bedrock. The SWMS\_3D model solves the Richards equation using the Mualem–van Genuchten functions (van Genuchten, 1980):

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{(1 + |\alpha h|^n)^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \quad (2)$$

$$K(h) = \begin{cases} K_s \cdot S_e^{\frac{1}{2}} \left[ 1 - \left( 1 - S_e^{\frac{1}{m}} \right)^m \right]^2 & h < 0 \\ K_s & h \geq 0 \end{cases} \quad (3)$$

with:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (4)$$

in which  $\theta_r$  is the residual volumetric water content,  $\theta_s$  is the saturated volumetric water content,  $\alpha$  is the air-entry value,  $n$  is the pore tortuosity,  $m = 1 - 1/n$ ,  $n > 1$ , and  $K_s$  is the saturated hydraulic conductivity.

The soil domain is represented by a grid of 15 rows, 7 columns and 5 layers of nodes. The soil depth is spatially variable, ranging from 0.16 to 1.47 m (Fig. 2). Horizontally, the nodes are regularly spaced at 3 m intervals. Vertically, the nodes are distributed uniformly over the local soil depth (Fig. 3). In what follows, we use a shorthand notation for the horizontal location of a node: e.g. X03Y12 refers to a location 3 m from the left of the hillslope and 12 m from the seepage face at the bottom. Unless specifically stated otherwise, this notation always refers to the lowest of 5 nodes at a given XY-location. The top of the domain represents the atmosphere-soil interface. It is a more or less planar surface with an incline of approximately  $13^\circ$ . The bottom of the domain represents the soil-bedrock interface. The model exclusively simulates the hydrodynamics of the soil domain: neither the atmosphere nor the bedrock is explicitly included in the model.

**Resolving structural model errors**

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Instead, the interface between atmosphere and soil is treated as a source of soil water, whereas the soil-bedrock interface is treated as a sink. In order to mimic typical field situations, the sink mechanism is set up as a spatially heterogeneous process. Using this configuration, we represent bedrock material that is somewhat permeable in most places, but that also has small areas where the bedrock material has disintegrated. In these areas, transient saturation infiltrates the underlying bedrock more quickly.

To simulate the vertical loss of water from the soil domain, we let the sink term  $B$  in Eq. (1) operate on all nodes at the soil-bedrock interface except those that were part of the seepage face (Fig. 3). We used a spatially heterogeneous pattern for the sink rate (Fig. 4). Nodes X00Y18, X06Y30, X09Y15, X15Y39 and X18Y09 were assigned a relatively high sink rate; hereafter, they are referred to as “hotspots”. The other nodes for which we enabled the sink term were assigned a relatively low value. The magnitude of the sink term is determined according to:

$$B = \begin{cases} 0 & h < 0 \\ r_{\text{sink}(\text{high})} \cdot h & h \geq 0 \text{ hotspots} \\ r_{\text{sink}(\text{low})} \cdot h & h \geq 0 \text{ not a hotspot} \end{cases} \quad (5)$$

in which  $r_{\text{sink}(\text{high})}$  and  $r_{\text{sink}(\text{low})}$  are sink efficiency parameters.  $r_{\text{sink}(\text{high})}$  was set to  $0.30 \text{ h}^{-1}$  while  $r_{\text{sink}(\text{low})}$  was set to  $0.01 \text{ h}^{-1}$ . Note that we do not mean to claim that this concept is necessarily realistic – its sole purpose here is to introduce a structural difference between the forward model and the inverse model (described below). Further details about the SWMS\_3D settings are listed in Table 1.

To determine the initial state, we set the pressure head to zero at the lower boundary of the domain and simulated how the pressure head pattern developed over the next 96 h (simulated time) using the forward model. No rain was applied during this warm-up phase. The final state of this simulation was used as initial state for all subsequent simulations, for both the forward model (during generation of the artificial measurements) and the inverse model (during optimization with SCEM-UA and SODA).

**Resolving structural model errors**J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



We used the following boundary conditions: all of the nodes located at  $y = 0$  were assigned a seepage face boundary condition (Fig. 3), meaning that they shed water only if the pressure head is positive. At the atmosphere-soil interface, nodes which were not part of the seepage face were assigned an atmospheric boundary condition, across which infiltration occurs. Precipitation was applied at a rate of  $6 \text{ mm h}^{-1}$  for a period of 6 h ( $t = 96\text{--}102$  h). Evaporation and transpiration were not included in this study. Nodes located on the outside of the domain that were not part of the seepage face, the atmosphere-soil interface, or the soil-bedrock interface were assigned a no-flow boundary condition.

With the settings described above, we ran the SWMS\_3D model. Before the onset of rain,  $188.0 \text{ m}^3$  of water was present in the soil. During the simulation, approximately  $26.3 \text{ m}^3$  of precipitation was applied. After the simulation ended, a total volume of about  $15.7 \text{ m}^3$  had been extracted vertically from the soil domain according to Eq. (5), while a total of about  $12.1 \text{ m}^3$  was removed from the domain as seepage from the seepage face. At the end of the simulation period at  $t = 216$  h,  $186.5 \text{ m}^3$  of water was present in the soil, slightly less than before precipitation started. Figure 5 shows how pressure head developed at the soil-bedrock interface for all nodes during the simulation period ( $t = 96$  through  $t = 216$  h). Transient saturation occurred in about 60 % of the nodes, but dissipated relatively quickly for most nodes once precipitation stopped.

Upon completion of the run, we saved 3 variables: (1) the total volume of soil water that had been extracted according to Eq. (5); (2) the time series of discharge from the seepage face at the bottom of the hillslope; (3) the space-time distributed pattern of pressure head at the soil-bedrock interface. These variables were then used as error-free artificial observations with which to calibrate the inverse model during the subsequent SCEM-UA and SODA runs.

## 2.3 Inverse model and calibrated parameters

The inverse model differs only slightly from the forward model, in that it assumes that the sink is spatially homogeneous. Equation (5) thus simplifies to:

$$B = \begin{cases} 0 & h < 0 \\ r_{\text{sink}} \cdot h & h \geq 0 \end{cases} \quad (6)$$

For field studies, it is common to make this assumption, even in cases where soft data suggests the presence of preferential-flow features such as cracks in the bedrock. Even though its validity may often be questionable, the modeler's hand is forced by the lack of direct observations.

Using SCEM-UA and SODA, we calibrated 2 parameters:  $K_s$ , the saturated hydraulic conductivity (Eq. 3), and  $r_{\text{sink}}$ , which controls the rate at which water is lost from the soil domain as it infiltrates the bedrock (Eq. 6).

## 2.4 SCEM-UA

The Shuffled Complex Evolution Metropolis (SCEM-UA) algorithm has been discussed in detail elsewhere (e.g. Vrugt et al., 2003b); only a summary is presented here.

SCEM-UA is a parameter estimation algorithm which was developed to better deal with uncertainty in parameter estimates, while improving the efficiency and effectiveness of searching the parameter space. The algorithm is based on the popular SCE parameter estimation algorithm (Duan et al., 1992), but where SCE uses a multidimensional simplex to generate offspring, SCEM-UA uses Markov chains combined with a Metropolis simulated-annealing scheme (Metropolis et al., 1953; Kuczera and Parent, 1998).

Following the classical approach to inverse modeling, SCEM-UA assumes that the hydrological model structure  $f(\cdot)$  is a perfect description of the processes as they occur in reality, and that data errors are negligible. The model output vector  $Y$  is calculated

**HESSD**

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



using the model forcings  $U$  by propagating the model initial state  $X_0$  using the model structure  $f(\cdot)$  and the model parameters  $\theta$ :

$$Y = f(X_0, U, \theta). \quad (7)$$

The model output is compared with observations  $Z$ , and the goodness-of-fit is expressed in an objective function  $g(\cdot)$ :

$$\text{OF} = g(Y, Z) \quad (8)$$

where OF represents the objective score. Points in the parameter space thus become associated with an objective score. Note that the single-objective approach described here can be extended to include multiple objectives using the concept of Pareto-optimality (Yapo et al., 1998; Gupta et al., 1998; Vrugt et al., 2003a).

The goal of parameter estimation is to find the parameter combinations(s)  $\theta$  whose associated output follows the observations as closely and consistently as possible (Vrugt et al., 2005). In order to find the part of the parameter space that yields the best parameter combinations, SCEM-UA proceeds as follows:

1. Initialize a population of points in the parameter space, divide them over multiple complexes as per Duan et al. (1992);
2. While convergence has not been achieved, do:
  - a. Sample new points from the feasible parameter space;
  - b. Determine the objective score OF for each point, by:
    - i. running the model
    - ii. running the objective function(s)
  - c. Accept or reject each new point according to the Metropolis rule;
  - d. Shuffle complexes;

**Resolving structural model errors**

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



e. Calculate Gelman-Rubin convergence statistic (Gelman and Rubin, 1992).

SCEM-UA reliably finds the part of the parameter space that yields the best possible objective scores. It has been used successfully to identify model parameters in a variety of disciplines including hydrology, soil chemistry, and ecology (e.g. Vrugt et al., 2003b, 2007; Nierop et al., 2002).

## Objective functions

We use the following 3 functions to evaluate the performance of individual parameter combinations:

$$OF_1 = |\epsilon_{\text{obs}} - \epsilon_{\text{sim}}| \quad (9)$$

in which  $\epsilon_{\text{obs}}$  and  $\epsilon_{\text{sim}}$  are the total observed and total simulated vertical water loss, respectively.  $\epsilon$  is calculated as:  $\epsilon = V_{\text{init}} + V_{\text{in}} - V_q - V_{\text{end}}$ , in which  $V_{\text{init}}$  is the total volume of water that is present in the soil at  $t = 96$  h,  $V_{\text{in}}$  is the total volume of infiltration,  $V_q$  is the total volume of discharge that is removed from the soil as seepage, and  $V_{\text{end}}$  is the total volume of water that is present in the soil at  $t = 216$  h;

$$OF_2 = \sqrt{\frac{1}{n_t} \sum_{t=1}^{n_t} (q_{\text{obs},t} - q_{\text{sim},t})^2} \quad (10)$$

in which  $n_t$  is the number of time steps, and  $q_{\text{obs},t}$  and  $q_{\text{sim},t}$  are the observed and simulated hillslope-scale discharge for the  $t$ -th time step, respectively;

$$OF_3 = \sqrt{\frac{1}{n_i} \sum_{i=1}^{n_i} (h_{\text{obs},i} - h_{\text{sim},i})^2} \quad (11)$$

in which  $n_i$  is the product of the number of rows and columns in the grid times the number of time steps;  $h_{\text{obs},i}$  and  $h_{\text{sim},i}$  are the observed and simulated pressure head

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



at the soil-bedrock interface for the  $i$ -th combination of row, column and time step, respectively.

The rationale behind this combination of objective functions is as follows. The inverse model simulates redistribution of the available water, i.e. initial storage and infiltration. The redistribution is subject to losses due to bedrock infiltration (vertically) and seepage (laterally). Successful calibration of the model requires that the volume of water that leaves the domain is accurate, which is achieved by minimizing the first two objectives (Eqs. 9 and 10). However, the first two objectives are not capable of extracting any spatial information. Using just the first two objectives could therefore lead to a proliferation of equally realistic solutions of pressure head patterns internal to the hillslope. To avoid that, the third objective (Eq. 11) attempts to use the spatial information in the pressure head data series, such that the solutions that were equally realistic based on just the first two objectives, can now be differentiated.

## 2.5 SODA

The Simultaneous parameter Optimization and Data Assimilation (SODA Vrugt et al., 2005) algorithm may be viewed as an extension of SCEM-UA. It combines SCEM-UA's parameter estimation procedure with an Ensemble Kalman Filter (EnKF; Evensen, 1994, 2003) such that uncertainty in the model states can be accommodated. SODA's general structure is therefore similar to the SCEM-UA structure outlined earlier, except that Step 2.b is different. Instead of running the model for all time steps at once, the EnKF generates an ensemble of model predictions, each of which having slightly different states. Each ensemble member is then propagated time step by time step, using the parameter combination suggested by the parameter estimation part of SODA. Step 2.b thus becomes:

2.b. Determine the objective score OF for each point, by:

- i. Generating an ensemble of model states based on the last a posteriori state (or the initial state);

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- ii. Propagating each ensemble member one time step, using the model structure, the model forcings, and the parameter combination. This results in an a priori state estimate for each ensemble member. Use the same parameter combination for all ensemble members and time steps;
- 5   iii. Determining the magnitude and direction of the state updates by calculating the weighted average of the a priori state estimates and the observations (the weights are related to the degree of uncertainty in each component);
- iv. Adding the state updates to the a priori state estimates to get the a posteriori state estimates.
- 10   v. Returning to (i) if the current time is less than the simulation end time;
- vi. Running the objective function(s).

The major advantage of this approach is that, when errors are introduced on the model states (either as a result of errors in the model initial state, errors in the model forcings, or by the use of an imperfect model structure), their propagation through time is limited by the EnKF's intermediate updating.

### Objective functions

For water balance and discharge, we let SODA use the same objective functions and observations that were used for SCEM-UA (Eqs. 9 and 10). The pressure head information, however, is used in a different way: rather than aggregating all errors using the objective function defined by Eq. (11), the pressure head observations are used to update the a priori model prediction in the EnKF. This is necessary in order to retain the timing and localization information pertaining to errors that may occur, and is therefore crucial for model improvement.



## 3 Results and discussion

### 3.1 Interpretation of the SCEM-UA results

Figure 6 shows the evolution of the parameter distribution during the SCEM-UA calibration. Once the distribution becomes stable after about 500 model evaluations,  $K_s$  is accurately and precisely identified, but the  $r_{\text{sink}}$  parameter has settled on a range of values that represents neither  $r_{\text{sink}(low)}$  nor  $r_{\text{sink}(high)}$ . Because the optimal parameters are unrealistic, the associated pressure head dynamics are also unrealistic. For example, Fig. 7 shows the difference between the simulated pressure head dynamics (generated using the Pareto-optimal parameter values  $\log_{10}(r_{\text{sink}}) \approx -1.30$  and  $\log_{10}(K_s) \approx -0.47$ ) and the artificial measurements. The error pattern is characterized by strong spatial auto-correlation, which implies that the simulated behavior does not represent the observed behavior well. Because of the structural deficiency, any value for  $r_{\text{sink}}$  will lead to errors somewhere in the hillslope. For  $r_{\text{sink}}$  values close to  $r_{\text{sink}(low)}$ , large errors would be introduced at the locations of the hotspots, because not enough water is extracted from the soil. Furthermore, the excess water would subsequently result in an overestimation of pressure head at the nodes that are located further downslope. In terms of the objective function, this means that  $r_{\text{sink}}$  values close to  $r_{\text{sink}(low)}$  perform relatively badly, even though assuming  $r_{\text{sink}} = r_{\text{sink}(low)}$  is a realistic assumption for 93 out of 98 nodes (see Fig. 4). In contrast, the errors that are introduced at the hotspots are not as large for  $\log_{10}(r_{\text{sink}})$  values from the 1.3–1.4 range, and less water flows past the hotspots, which in turn reduces the severity of the overestimation further downslope. While  $\log_{10}(r_{\text{sink}})$  values from the 1.3–1.4 range are unrealistic, their performance in terms of the objective functions is better. This example shows how the parameters can compensate for errors that are introduced on the model state as a result of deficient model structure. The compensation effect inherent to parameter estimation can be an advantage when the purpose of the modeling is to predict, but when the purpose is to scrutinize and improve one's understanding of a system, it is a disadvantage. Both points of view are explained below.

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



As a consequence of the compensation, the optimum of the parameter vector  $[r_{\text{sink}}, K_s]$  varies with the characteristics of the data used during calibration. This is corroborated by a number of experiments (results not reported) in which we repeated the experiment described in the Methods section using different precipitation intensities and durations. Comparing the results from those experiments suggests that calibrating the inverse model to smaller events tends to yield estimates of  $r_{\text{sink}}$  that are closer to  $r_{\text{sink(}low)}$ , depending on whether the hotspot locations become saturated during the calibration period (activation of response modes). When the purpose of the modeling is to predict certain variables (notably discharge), it is therefore important to have as long a calibration period as possible, since longer calibration periods are more likely to activate all behavioral modes. After calibration, not only do the optimal parameter values compensate for any structural deficiency in the model, but the compensation also reflects the frequency with which the deficiency manifested itself during the calibration period. Assuming that this frequency is stable, the optimal parameters will – on average – give the most reliable predictions, in spite of the deficient model structure and biased parameters.

So, on the one hand the compensation effect is desirable, since it reduces the average prediction error. On the other hand though, when the purpose of the modeling is to scrutinize and improve one's understanding of a system, the compensation effect inherent to parameter estimation is undesirable. This is largely due to two problems related to how errors on the model states are treated. Keeping in mind that all models are simplifications and are therefore structurally deficient to some degree, the first problem is that errors on the model state are propagated in time and in space (recall our description of how excess soil water that was not extracted at the hotspots gave rise to systematic overestimation further downslope). The first problem then leads to the second problem, viz. that of compensation: the overestimation that occurs downslope is less severe for unrealistic parameter values. Due to these two problems, residuals can not be interpreted as being “new and local”, and as a result, it is difficult to relate patterns in the residuals to physically meaningful processes.

## HESSD

10, 1819–1858, 2013

### Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



Considering the abundance and high quality of the data (no measurement error, no incommensurability), an experienced hydrologist would probably be able to make an educated guess based on Fig. 7 about what goes wrong in the inverse model and how it could be improved – perhaps by focusing on where errors are first introduced, and relating them to the value of various model variables at that time and place. In the next section, we show that the SODA methodology bears some resemblance to this approach, albeit that SODA is a more formalized and fully automated methodology.

### 3.2 Interpretation of the SODA results

Figure 8 shows the evolution of the parameters during the SODA calibration. The figure shows that, after about 600 model evaluations, SODA draws exclusively from the narrow range around  $\log_{10}(K_s) \approx -0.45$  and  $\log_{10}(r_{\text{sink}}) \approx \log_{10}(r_{\text{sink}(\text{low})}) = -2$ . The inverse model applies  $r_{\text{sink}}$  to all sink nodes at the soil-bedrock interface, leading to an overestimation of pressure heads at the hotspots. However, when this happens, the EnKF recognizes that the simulation is systematically deviating from the artificial measurements, and adjusts the model states accordingly. By adjusting the state downward, water is implicitly extracted from the soil. Pressure head in the hillslope is thus affected by two flows that are part of the model (i.e. net lateral subsurface flow and the sink term of Eq. 6), as well as by the implicit sink that is external to the model. The implicit sink represents any vertical losses that occur in excess of what Eq. (6) accounts for. Without the implicit extraction of water from the soil domain, the lower part of the hillslope would be much too wet, which would in turn lead to biased optimal parameters.

From a model evaluation perspective, the state updates are interesting because they essentially form a record of how model structural error affects the model states. Moreover, the information contained within the record is specific to both a location and a time, making it possible to relate the magnitude and direction of state updates to physically relevant processes. Figure 9 shows the state updating that was performed when SODA evaluated the inverse model using  $\log_{10}(r_{\text{sink}}) \approx -1.97$  and  $\log_{10}(K_s) \approx -0.46$ . Two types of responses can be distinguished in the figure: on the one hand, most of

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



the states do not need any updating. For those nodes, the inverse model provides an appropriate representation of the observations, at least when the model is run with parameter values from the optimal range. On the other hand, there are other nodes that need substantial updating (e.g. X00Y18, X06Y30, X09Y15, and X18Y09). These nodes coincide with hotspots (recall Fig. 4). The structural difference between the inverse model and the forward model leads to consistently deviating a priori estimates of pressure head in these areas.

Besides model evaluation, state adjustment patterns are also helpful in generating the inspiration and guidance for constructing new, improved hypotheses. Such guidance is necessary to avoid making ad hoc decisions with regard to model design. As an example of how SODA can help to formulate an improved model design, Fig. 10 shows the magnitude of the state updating as a function of pressure head for the nodes that have the strongest cumulative updates. The figure suggests that the inverse model structure could be improved by including an additional linear term at the locations for which the strongest cumulative updating was performed. Figure 10 further shows that no state updating was needed for node X06Y30 when the pressure head was below 0. This is consistent with the difference between Eqs. (5) and (6). We argue that relations such as those visualized in Figs. 9 and 10 greatly stimulate the discussion between modeler and experimentalist about what process could explain the state updating patterns. At the same time, these relations also guide model improvement by setting constraints on the functional form of the relation.

### 3.2.1 Implications for experimental design

In this study, we are using artificial measurements which are error-free. As a result, the EnKF places much more confidence on the observations than it does on the a priori estimate of the model state: the a posteriori model state is effectively determined by “resetting” the a priori model state to the value of the observation. When the confidence balance is strongly in favor of the observations, any errors that may have been introduced since the last observation time are canceled almost completely after the

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



states are updated at the time of the next observation. However, if a lot of time passes in between observation times (relative to the dynamics of the modeled process) the error can still significantly affect other model states. For example, we used 60-min observation intervals, but the SWMS\_3D model used integration time steps of 1–20 min (Table 1). Small overestimation errors introduced at the hotspots could thus spread to neighboring nodes, where the a priori estimate of model state was subsequently reset to (a value close to) the observed state during state updating. This explains the small state updates that the EnKF performed at the nodes adjacent to the hotspots at X00Y18, X06Y30, X09Y15, and X18Y09 (Fig. 9). Because the spreading of errors is stronger when the measurements are taken at larger intervals, it is important that the observation frequency is balanced with the time scale of the modeled process. Similarly, when individual measurements are associated with realistic measurement noise (as opposed to being error-free), the EnKF will not place as much confidence on the measurements. Consequentially, errors are not corrected as quickly, and the state updating pattern will be more difficult to interpret. This problem can be alleviated by measuring at smaller intervals, or by installing a more precise measurement device. When setting up future field experiments, it may thus be worthwhile to increase the measuring frequency, even at the cost of the experiment's duration.

In terms of experimental design, it also remains important that the measurements contain all relevant behavioral modes, i.e. information content is more important than sheer data volume (e.g. Sorooshian et al., 1983; Gupta and Sorooshian, 1985); even powerful methods of analysis cannot extract information that is not present. For example, the forward model includes 5 hotspots, but only 4 of these can be identified from the SODA analysis (compare Figs. 4 and 9). The reason for this is that the difference between the forward model and the inverse model only becomes apparent when saturated conditions occur at the location of one of the hotspots. If saturated conditions do not occur, the inverse model's behavior cannot be distinguished from the forward model's behavior: the sink term  $B$  is equal to zero for both models (Eqs. 5 and 6). Since saturated conditions did indeed not occur at X15Y39 (see Fig. 5), node X15Y39

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



can not be identified as a hotspot from these measurements, regardless of the method used.

### 3.2.2 Next steps

We consider SODA a step towards making better use of information in observations. We have shown that despite some issues, it is possible to identify model structural deficiency – in this case, the location of sink hotspots. Furthermore, we have shown that it is possible to build relations between the state updates and other variables in the model. While it may not be automatically clear what process (processes) they represent, such relations help to guide model improvement and experimental design. However, we are aware of the simplifications that were made in the setup of this study, in particular with regard to measurement noise, sparsity of data, incommensurability of observed variables with their model counterparts, and with regard to the possibility of having more than one source of model structural error. These issues require more investigation.

Also, the development of inverse modeling algorithms is ongoing; of particular interest within the context of this study is particle-DREAM (Vrugt et al., 2013), which is conceptually similar to SODA in that it combines a parameter estimation algorithm (DREAM) with state estimation (particle filtering). This procedure combines DREAM's efficient sampling of the parameter space with the particle filtering's flexibility in handling the probability distribution of the model states. It should be possible to exploit the state updates of the particle filter in a similar fashion as described here for SODA, but more research on this topic is needed.

## 4 Conclusions

As models get more complex, there is a growing need for better tools with which to evaluate them (e.g. Beck, 1987; Gupta et al., 1998; Kirchner, 2006). It has been argued in

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



the literature that model evaluation should not be limited to ranking model runs (differentiating between the good and the bad representations of the real world), but should also provide some guidance on how to improve a given model structure (Beck, 1987; Lin and Beck, 2007; Gupta et al., 2008). In this study, we purposely used a deficient model structure, which we calibrated by both a parameter estimation approach (SCEM-UA), and by a combined parameter and state estimation approach (SODA). We then assessed how suitable each method was for providing aforementioned guidance.

Three main conclusions that can be drawn from this work are:

1. State adjustment patterns generated by SODA are helpful in evaluating when and where model structural errors occur;
2. Relations can be constructed between SODA's state adjustments and the model states themselves. Such relations can readily be adopted in an improved version of the model. Perhaps most importantly, they stimulate the discussion between modeler and experimentalist about what process could explain them, while at the same time guiding the discussion by setting constraints on the functional form of the relation.
3. SCEM-UA cannot provide information that is as informative as that provided by SODA. Parameter estimation methods such as SCEM-UA lack a strategy with which the propagation of errors is reduced. Due to compensation effects, tuning the parameters of a structurally deficient model may therefore result in optimal parameter values without any physical relevance. This inhibits a straightforward interpretation of the model-observation residuals with regard to model improvement.

By using error-free, artificially generated observations, we were able to focus strictly on the usefulness of the algorithms, while avoiding any issues relating to the quality of observations. Future work into this topic should further increase the dissimilarity between the forward and the inverse model. We hope that sharing this work with the

## HESSD

10, 1819–1858, 2013

### Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



hydrological community will inspire many new avenues of research, both on the side of model diagnostics and on the side of experimental design.

*Acknowledgements.* The authors wish to express their gratitude to J. A. Vrugt, for kindly providing the algorithms, and for his many useful comments on an earlier version of this manuscript.

5 This work is part of the programme of BiG Grid, the Dutch e-Science Grid, which is financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Netherlands Organisation for Scientific Research, NWO). Further funding was provided by the Netherlands eScience Center (<http://esciencecenter.com>) which is supported by SURF and NWO. N. S. Anders, M. U. Kemp, J. D. McLaren, L. E. Veen, I. Soenario and W. Vansteelant are thanked for  
10 the continued criticism during the writing of this manuscript.

## References

- Ajami, N. K., Duan, Q., and Sorooshian, S.: An integrated hydrologic Bayesian multimodel combination framework: confronting input, parameter, and model structural uncertainty in hydrologic prediction, *Water Resour. Res.*, 43, W01403, doi:10.1029/2005WR004745, 2007. 1822
- 15 Beck, M. B.: Water quality modeling: a review of the analysis of uncertainty, *Water Resour. Res.*, 23, 1393–1442, doi:10.1029/WR023i008p01393, 1987. 1840, 1841
- Beven, K. and Binley, A.: The future of distributed models: model calibration and uncertainty prediction, *Hydrol. Process.*, 6, 279–298, 1992. 1824
- 20 Box, G. E. P. and Tiao, G. C.: *Bayesian Inference in Statistical Analysis*, Addison-Wesley-Longman, Reading, Massachusetts, 1973. 1820
- Boyle, D. P., Gupta, H. V., and Sorooshian, S.: Toward improved calibration of hydrologic models: combining the strengths of manual and automatic methods, *Water Resour. Res.*, 36, 3663–3674, 2000. 1823
- 25 Boyle, D. P., Gupta, H. V., Sorooshian, S., Koren, V., Zhang, Z., and Smith, M.: Toward improved streamflow forecasts: value of semidistributed modeling, *Water Resour. Res.*, 37, 2749–2759, doi:10.1029/2000WR000207, 2001. 1823
- Clark, M. P. and Vrugt, J. A.: Unraveling uncertainties in hydrologic model calibration: addressing the problem of compensatory parameters, *Geophys. Res. Lett.*, 33, L06406, doi:10.1029/2005GL025604, 2006. 1822
- 30

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





Resolving structural  
model errorsJ. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- Clark, M. P., Slater, A. G., Rupp, D. E., Woods, R. A., Vrugt, J. A., Gupta, H. V., Wagener, T., and Hay, L. E.: Framework for Understanding Structural Errors (FUSE): a modular framework to diagnose differences between hydrological models, *Water Resour. Res.*, 44, W00B02, doi:10.1029/2007WR006735, 2008. 1823
- 5 Doherty, J. and Welter, D.: A short exploration of structural noise, *Water Resour. Res.*, 46, W05525, doi:10.1029/2009WR008377, 2010. 1824
- Duan, Q., Gupta, V. K., and Sorooshian, S.: Effective and efficient global optimization for conceptual rainfall-runoff models, *Water Resour. Res.*, 28, 1015–1031, 1992. 1830, 1831
- 10 Dunn, S. M.: Imposing constraints on parameter values of a conceptual hydrological model using baseflow response, *Hydrol. Earth Syst. Sci.*, 3, 271–284, doi:10.5194/hess-3-271-1999, 1999. 1822
- Efstratiadis, A. and Koutsoyiannis, D.: One decade of multi-objective calibration approaches in hydrological modelling: a review, *Hydrolog. Sci. J.*, 55, 58–78, doi:10.1080/02626660903526292, 2010. 1823
- 15 Eigbe, U., Beck, M. B., Wheeler, H. S., and Hirano, F.: Kalman filtering in ground-water flow modelling: problems and prospects, *Stoch. Hydrol. Hydraul.*, 12, 15–32, doi:10.1007/s004770050007, 1998. 1825
- Evensen, G.: Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics, *J. Geophys. Res.*, 99, 10143–10162, 1994. 1824, 1833
- 20 Evensen, G.: The Ensemble Kalman Filter: theoretical formulation and practical implementation, *Ocean Dynam.*, 53, 343–367, doi:10.1007/s10236-003-0036-9, 2003. 1824, 1833
- Franks, S. W., Gineste, P., Beven, K. J., and Merot, P.: On constraining the predictions of a distributed model: the incorporation of fuzzy estimates of saturated areas into the calibration process, *Water Resour. Res.*, 34, 787–797, doi:10.1029/97WR03041, 1998. 1822
- 25 Gelman, A. and Rubin, D. B.: Inference from Iterative Simulation Using Multiple Sequences, available at: <http://www.jstor.org/stable/pdfplus/2246093.pdf>, *Stat. Sci.*, 7, 457–472, 1992. 1832
- Georgakakos, K. P., Seo, D., Gupta, H., Schaake, J., and Butts, M. B.: Towards the characterization of streamflow simulation uncertainty through multimodel ensembles, *J. Hydrol.*, 298, 222–241, doi:10.1016/j.jhydrol.2004.03.037, 2004. 1823
- 30 Goldberg, D. E.: *Genetic Algorithms in Search, Optimization, and Machine Learning*, Addison-Wesley, Boston, Massachusetts, 1989. 1823

Resolving structural  
model errorsJ. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

- Gupta, H. V., Sorooshian, S., and Yapo, P. O.: Toward improved calibration of hydrologic models: multiple and noncommensurable measures of information, *Water Resour. Res.*, 34, 751–763, 1998. 1822, 1823, 1831, 1840
- Gupta, H. V., Wagener, T., and Liu, Y.: Reconciling theory with observations: elements of a diagnostic approach to model evaluation, *Hydrol. Process.*, 22, 3802–3813, doi:10.1002/hyp.6989, 2008. 1822, 1841
- Gupta, V. K. and Sorooshian, S.: The relationship between data and the precision of parameter estimates of hydrologic models, *J. Hydrol.*, 81, 57–77, 1985. 1839
- Hoeting, J. A., Madigan, D., Raftery, A. E., and Volinsky, C. T.: Bayesian model averaging: a tutorial, *Stat. Sci.*, 14, 382–401, 1999. 1823
- Jazwinski, A. H.: *Stochastic Processes and Filtering Theory*, Academic Press, New York, 1970. 1824
- Kalman, R. E.: A new approach to linear filtering and prediction problems, available at: <http://www.cs.unc.edu/~welch/kalman/media/pdf/Kalman1960.pdf>, *T. ASME J. Basic Eng.*, 82, 35–45, 1960. 1824
- Kavetski, D., Kuczera, G., and Franks, S. W.: Bayesian analysis of input uncertainty in hydrological modeling: 1. Theory, *Water Resour. Res.*, 42, W03407, doi:10.1029/2005WR004368, 2006a. 1824
- Kavetski, D., Kuczera, G., and Franks, S. W.: Bayesian analysis of input uncertainty in hydrological modeling: 2. Application, *Water Resour. Res.*, 42, W03408, doi:10.1029/2005WR004376, 2006b. 1824
- Kirchner, J. W.: Getting the right answers for the right reasons: linking measurements, analyses, and models to advance the science of hydrology, *Water Resour. Res.*, 42, W03S04, doi:10.1029/2005WR004362, 2006. 1821, 1822, 1840
- Klemeš, V.: Operational testing of hydrological simulation models, *Hydrolog. Sci. J.*, 31, 13–24, 1986. 1821
- Kuczera, G. and Mroczkowski, M.: Assessment of hydrologic parameter uncertainty and the worth of multiresponse data, *Water Resour. Res.*, 34, 1481–1489, doi:10.1029/98WR00496, 1998. 1822
- Kuczera, G. and Parent, E.: Monte Carlo assessment of parameter uncertainty in conceptual catchment models: the Metropolis algorithm, *J. Hydrol.*, 211, 69–85, 1998. 1830

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- Lin, Z. and Beck, M. B.: On the identification of model structure in hydrological and environmental systems, *Water Resour. Res.*, 43, W02402, doi:10.1029/2005WR004796, 2007. 1823, 1841
- Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E.: Equations of state calculations by fast computing machines, *J. Chem. Phys.*, 21, 1087–1091, 1953. 1830
- Mroczkowski, M., Raper, G. P., and Kuczera, G.: The quest for more powerful validation of conceptual catchment models, *Water Resour. Res.*, 33, 2325–2335, 1997. 1822
- Neuman, S. P.: Maximum likelihood Bayesian averaging of uncertain model predictions, *Stoch. Env. Res. Risk A.*, 17, 291–305, doi:10.1007/s00477-003-0151-7, 2003. 1823
- Nierop, K. G. J., Jansen, B., Vrugt, J. A., and Verstraten, J. M.: Copper complexation by dissolved organic matter and uncertainty assessment of their stability constants, *Chemosphere*, 49, 1191–1200, 2002. 1832
- Popper, K.: *The Logic of Scientific Discovery*, Routledge, first published as *Logik der Forschung*, 1935 by Verlag von Julius Springer, Vienna, Austria, 2009. 1820
- Raftery, A. E., Balabdaoui, F., Gneiting, T., and Polakowski, M.: Using Bayesian Model averaging to calibrate forecast ensembles, Tech. rep., Department of Statistics, University of Washington, Seattle, Washington, 2003. 1823
- Raftery, A. E., Gneiting, T., Balabdaoui, F., and Polakowski, M.: Using Bayesian Model averaging to calibrate forecast ensembles, *Mon. Weather Rev.*, 133, 1155–1174, 2005. 1823
- Richards, L. A.: Capillary conduction of liquids through porous mediums, *Physics*, 1, 318–333, 1931. 1826
- Schoups, G. and Vrugt, J. A.: A formal likelihood function for parameter and predictive inference of hydrologic models with correlated, heteroscedastic, and non-Gaussian errors, *Water Resour. Res.*, 46, W10531, doi:10.1029/2009WR008933, 2010. 1824
- Seibert, J.: Multi-criteria calibration of a conceptual runoff model using a genetic algorithm, *Hydrol. Earth Syst. Sci.*, 4, 215–224, doi:10.5194/hess-4-215-2000, 2000. 1822
- Šimůnek, J.: SWMS\_3D – numerical model of three-dimensional flow and solute transport in a variably saturated porous medium, software, available at: [http://www.pc-progress.com/Downloads/Programs\\_UCR/SWMS\\_3D.zip](http://www.pc-progress.com/Downloads/Programs_UCR/SWMS_3D.zip) (last access: 2 February 2013), 1994. 1826
- Šimůnek, J., Huang, K., and van Genuchten, M. T.: *The SWMS\_3D Code for Simulating Water Flow and Solute Transport in Three-Dimensional Variably-Saturated Media*, US Salinity Laboratory, Agricultural Research Service, Research Report No. 139, US Department of Agriculture, Riverside, California, 1995. 1826

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- Sorooshian, S., Gupta, V. K., and Fulton, J. L.: Evaluation of maximum likelihood parameter estimation techniques for conceptual rainfall-runoff models: influence of calibration data variability and length on model credibility, *Water Resour. Res.*, 19, 251–259, doi:10.1029/WR019i001p00251, 1983. 1839
- 5 Spear, R. C. and Hornberger, G. M.: Eutrophication in peel inlet – II. Identification of critical uncertainties via generalized sensitivity analysis, *Water Res.*, 14, 43–49, doi:10.1016/0043-1354(80)90040-8, 1980. 1824
- Tang, Y., Reed, P., and Wagener, T.: How effective and efficient are multiobjective evolutionary algorithms at hydrologic model calibration?, *Hydrol. Earth Syst. Sci.*, 10, 289–307, doi:10.5194/hess-10-289-2006, 2006. 1822
- 10 van Genuchten, M. T.: A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, 44, 892–898, 1980. 1827
- von Bertalanffy, L.: The theory of open systems in physics and biology, *Science*, 111, 23–29, 1950. 1821
- 15 Vrugt, J. A., Gupta, H. V., Bastidas, L. A., Bouten, W., and Sorooshian, S.: Effective and efficient algorithm for multi-objective optimization of hydrologic models, *Water Resour. Res.*, 39, 1214, doi:10.1029/2002WR001746, 2003a. 1822, 1831
- Vrugt, J. A., Gupta, H. V., Bouten, W., and Sorooshian, S.: A shuffled complex evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters, *Water Resour. Res.*, 39, 1201, doi:10.1029/2002WR001642, 2003b. 1826, 1830, 1832
- 20 Vrugt, J. A., Diks, C. G. H., Gupta, H. V., Bouten, W., and Verstraten, J. M.: Improved treatment of uncertainty in hydrologic modeling: combining the strengths of global optimization and data assimilation, *Water Resour. Res.*, 41, W01017, doi:10.1029/2004WR003059, 2005. 1826, 1831, 1833
- 25 Vrugt, J. A., van Belle, J., and Bouten, W.: Pareto front analysis of flight time and energy use in long-distance bird migration, *J. Avian Biol.*, 38, 432–442, doi:10.1111/j.0908-8857.2007.03909.x, 2007. 1832
- Vrugt, J. A., ter Braak, C. J. F., Diks, C. G. H., and Schoups, G.: Hydrologic data assimilation using particle Markov chain Monte Carlo simulation: theory, concepts and applications, *Adv. Water Resour.*, doi:10.1016/j.advwatres.2012.04.002, 2013. 1840
- 30

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion



- Wagener, T., Boyle, D. P., Lees, M. J., Wheater, H. S., Gupta, H. V., and Sorooshian, S.: A framework for development and application of hydrological models, *Hydrol. Earth Syst. Sci.*, 5, 13–26, doi:10.5194/hess-5-13-2001, 2001. 1823
- 5 Wagener, T., McIntyre, N., Lees, M. J., Wheater, H. S., and Gupta, H. V.: Towards reduced uncertainty in conceptual rainfall-runoff modelling: dynamic identifiability analysis, *Hydrol. Process.*, 17, 455–476, doi:10.1002/hyp.1135, 2003. 1824
- Yapo, P. O., Gupta, H. V., and Sorooshian, S.: Multi-objective global optimization for hydrological models, *J. Hydrol.*, 204, 83–97, 1998. 1822, 1823, 1831
- 10 Young, P.: A general theory of modeling for badly defined dynamic systems, in: *Modeling, Identification and Control in Environmental Systems – Proceedings of the IFIP Working Conference on Modeling and Simulation of Land, Air, and Water Resources Systems*, edited by: Vansteenkiste, G. C., 103–135, North-Holland Pub. Co., Amsterdam, 1978. 1824
- Young, P.: Uncertainty and forecasting of water quality, in: *The Validity and Credibility of Models for Badly Defined Systems*, Springer Verlag, 69–98, 1983. 1821
- 15 Young, P.: The identification and estimation of nonlinear stochastic systems, in: *Nonlinear Dynamics and Statistics*, Birkhäuser, Boston, 127–166, 2001. 1824

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten**Table 1.** Overview of the most relevant parameters in the SWMS\_3D model.

parameter description	SWMS_3D parameter name	value	units
geometry			
total number of nodes	NumNP	525	–
total number of boundary nodes	NumBP	133	–
total number of elements	NumEl	2016	–
soil hydraulic parameters			
residual water content	$\theta_r$	0.28	–
saturated water content	$\theta_s$	0.475	–
air entry value	$\alpha$	4.00	$\text{m}^{-1}$
pore tortuosity	$n$	2.0	–
saturated conductivity	$K_s$	0.35	$\text{m h}^{-1}$
numerical integration settings			
maximum number of iterations	MaxIt	31	–
tolerance on theta	TolTh	$1 \times 10^{-6}$	–
tolerance on head	Tolh	$1 \times 10^{-6}$	m
initial integration time step	dt	6	min
minimum integration time step	dtMin	1	min
maximum integration time step	dtMax	20	min
time step decrease factor	DMul	0.7	–
time step increase factor	DMul2	1.2	–

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

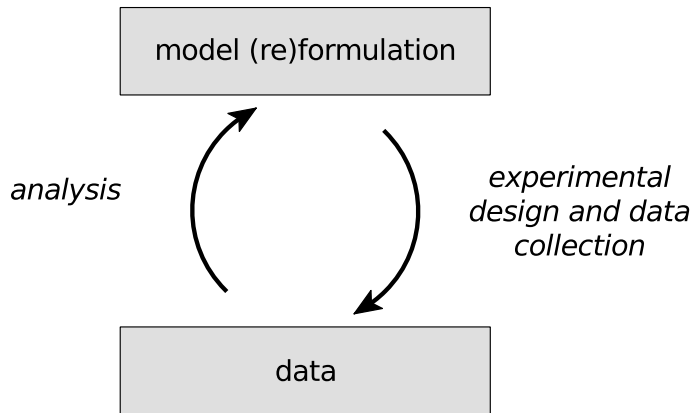
Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





**Fig. 1.** Iterative research cycle.

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

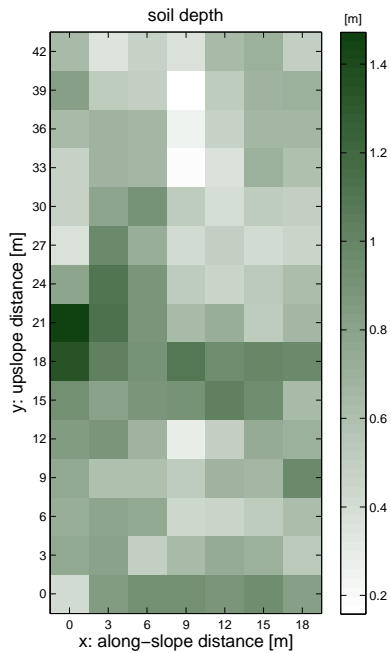
Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





**Fig. 2.** Soil depth distribution.

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

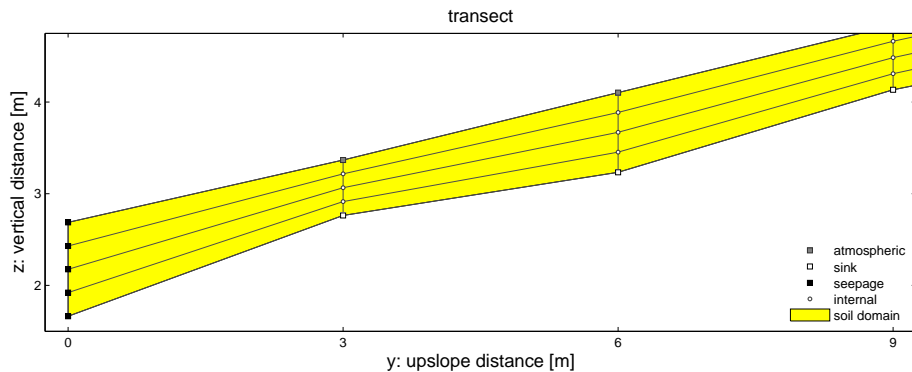
Full Screen / Esc

Printer-friendly Version

Interactive Discussion







**Fig. 3.** Transect of lower section of the domain with boundary node types shown. Infiltration enters the domain at the atmospheric boundary nodes. Excess water is removed from the domain either vertically at the sink nodes, or laterally as seepage.

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

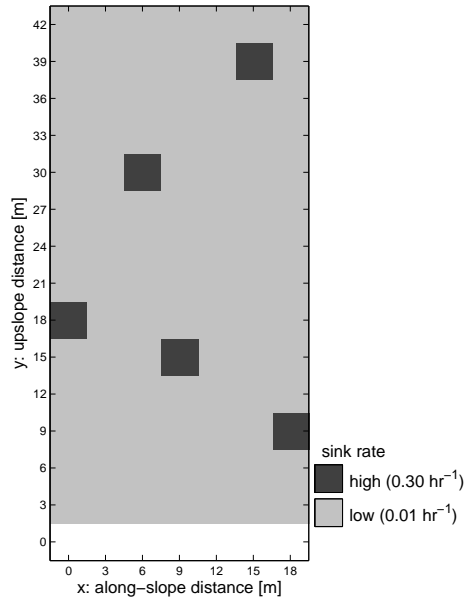
Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion





**Fig. 4.** Spatial distribution of the sink parameter as used in the forward model.

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

⏪

⏩

◀

▶

Back

Close

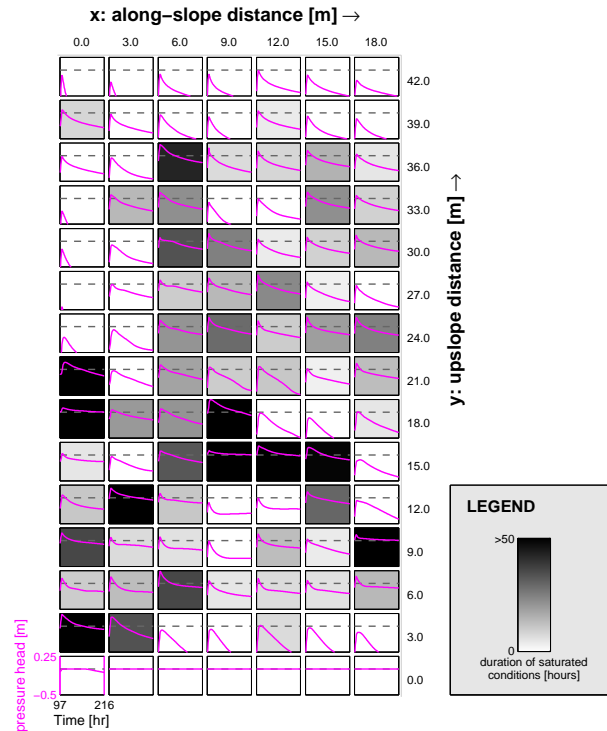
Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

**Fig. 5.** Artificial measurements: simulated traces of pressure head in space and time. For each node at the soil-bedrock interface, the figure contains a subplot showing a time series of the pressure head (magenta line) for  $t = 97\text{--}216$  h. Horizontal dashed lines represent zero pressure head. Each subplot's axes have been clipped vertically to  $[-0.5, 0.25]$  in order to better show the pressure head dynamics during relatively wet conditions. To further ease interpretation, each subplot was assigned a background color depending on how long saturated conditions lasted at a given location.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

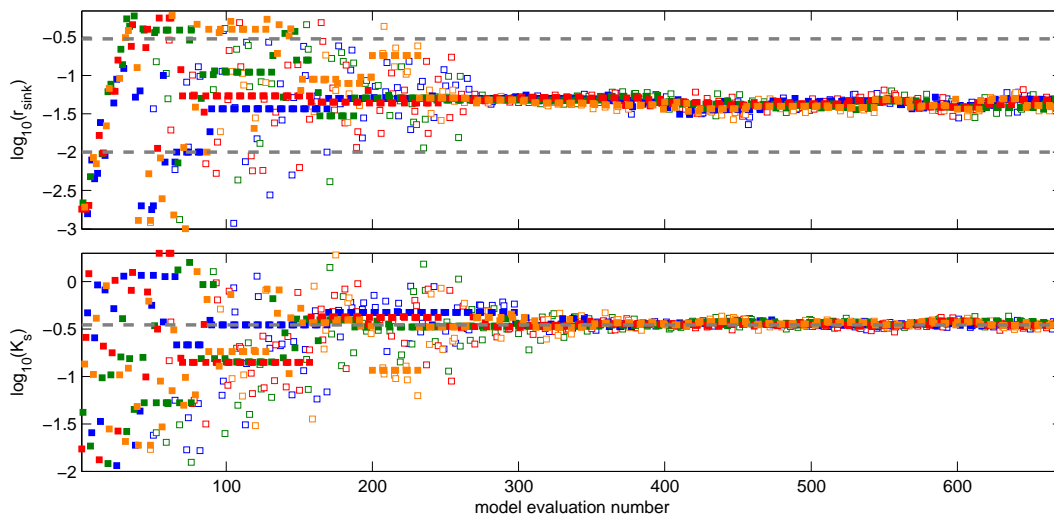
Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

**Fig. 6.** SCEM-UA: evolution of the parameters. Dashed lines represent value of  $r_{\text{sink}(\text{low})}$  and  $r_{\text{sink}(\text{high})}$  (upper plot) and  $K_s$  (lower plot). Markov chains are color-coded; open symbols are samples that have been rejected by the Metropolis scheme, solid colors have been accepted. Note that the vertical axes are logarithmic.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

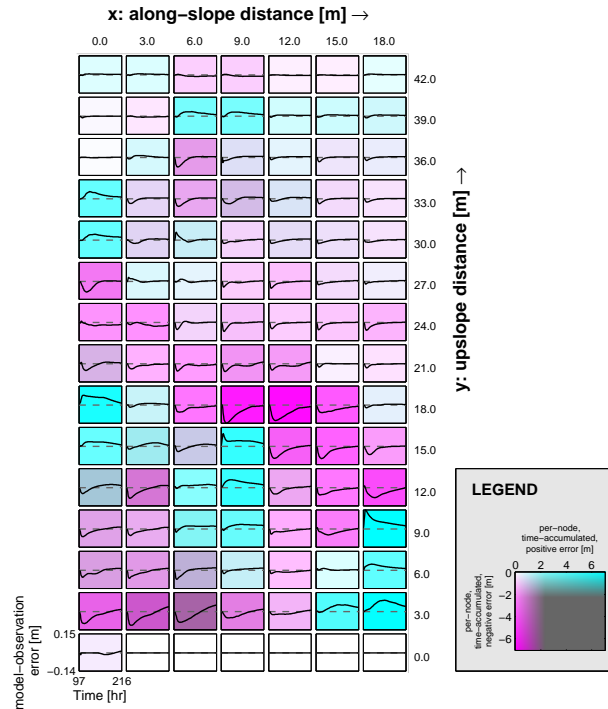
Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

**Fig. 7.** SCEM-UA: pressure head error in space and time, as associated with the Pareto-optimal parameter combination  $\log_{10}(r_{\text{sink}}) \approx -1.30$ ;  $\log_{10}(K_s) \approx -0.47$ . For each node at the soil-bedrock interface, the figure contains a subplot showing a time series of model-observation error (black line) for  $t = 97\text{--}216$  h. Horizontal dashed lines represent zero-error. To ease interpretation of the error pattern, each subplot was assigned a background color depending on the cumulative positive and cumulative negative error: magenta colors represent under-estimation of artificial measurements (simulated value is too dry) while cyan means over-estimation (too wet). Note the spatial auto-correlation and error propagation.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

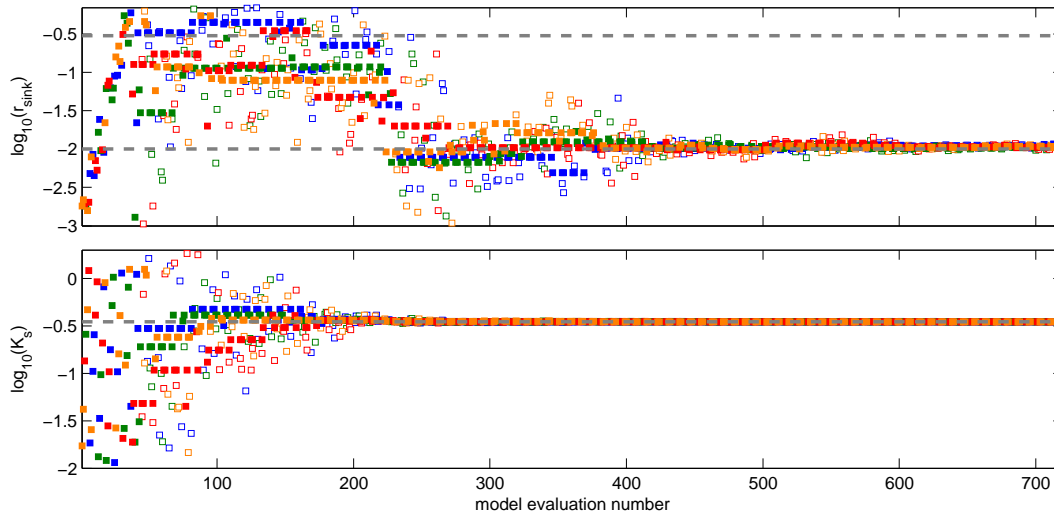
Interactive Discussion

# HESSD

10, 1819–1858, 2013

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten



**Fig. 8.** SODA: evolution of the parameters. Dashed lines represent value of  $r_{\text{sink}(\text{low})}$  and  $r_{\text{sink}(\text{high})}$  (upper plot) and  $K_s$  (lower plot). Markov chains are color-coded; open symbols are samples that have been rejected by the Metropolis scheme, solid colors have been accepted. Note that the vertical axes are logarithmic.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

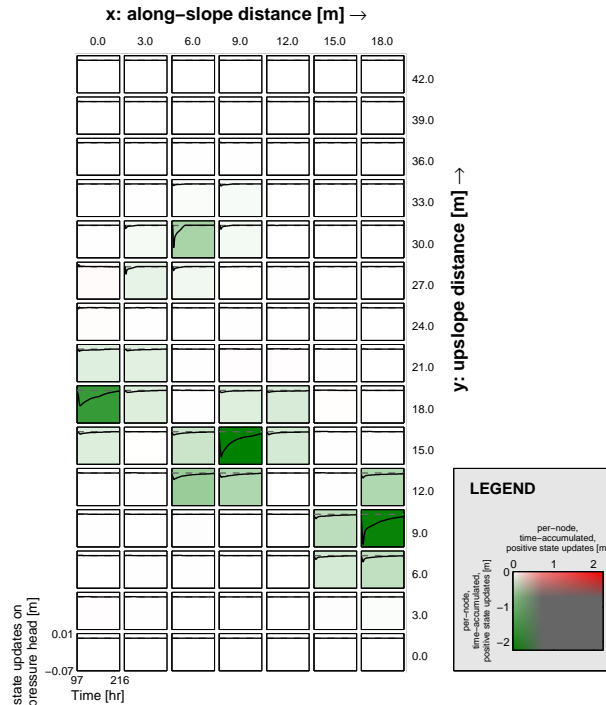
Full Screen / Esc

Printer-friendly Version

Interactive Discussion



## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

**Fig. 9.** SODA: pressure head state updates in space and time, as associated with the Pareto-optimal parameter combination  $\log_{10}(r_{\text{sink}}) \approx -1.97$ ;  $\log_{10}(K_s) \approx -0.46$ . For each node at the soil-bedrock interface, the figure contains a subplot showing a time series of state updates (black line) for  $t = 97\text{--}216$  h. Horizontal dashed lines represent zero-updates (no adjustment). To ease interpretation of the updating pattern, each subplot was assigned a background color depending on the cumulative positive and cumulative negative state update: red colors represent under-estimation of artificial measurements (a priori value is too dry) while green means over-estimation (a priori value is too wet). This figure uses a color scheme that is different from that of Fig. 7 to emphasize the difference in interpretation between errors and state updates.

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

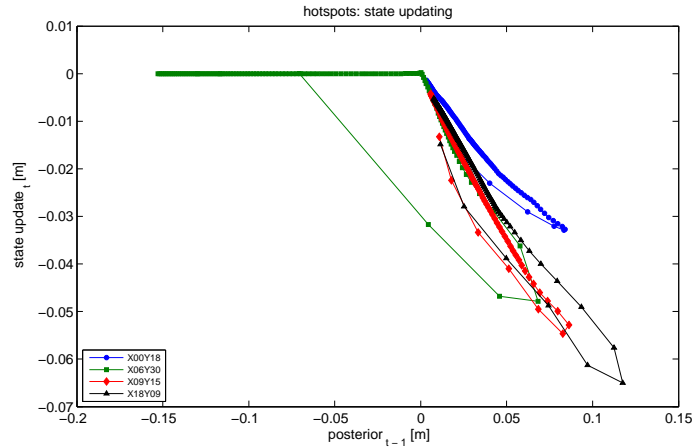
Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

## Resolving structural model errors

J. H. Spaaks and  
W. Bouten

**Fig. 10.** State updating as a function of state value for 4 hotspot nodes. The data for this figure originate from SODA's evaluation of  $\log_{10}(r_{\text{sink}}) \approx -1.97$  and  $\log_{10}(K_s) \approx -0.46$ .

Title Page

Abstract

Introduction

Conclusions

References

Tables

Figures

◀

▶

◀

▶

Back

Close

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

