Investigation of the behaviour of two karst spring discharge reservoir models with respect to the initialization bias

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Abstract This paper investigates the analytical properties of the sensitivity to the initial conditions on the calibration and simulation results of two karst spring discharge reservoir models, based on the perturbation approach. The emphasis is laid on the influence of model nonlinearity on the sensitivity of the model output to the initial conditions. It is shown that depending on model structure, nonlinearity may either speed up or delay the dissipation of the initialisation bias. The analytical results are confirmed by application examples on real-world simulations.

Key words initialisation bias; initial conditions; global model; perturbation approach; model sensitivity; calibration

INTRODUCTION

The specification of the initial state of a given model inevitably leads to an initialization bias in the model output. Two main approaches are classically adopted to address the initialization bias problem in conceptual hydrological modelling: (a) the calibration of the initial state estimate, and (b) the truncation of the model output. The sensitivity of the model output to the initial conditions is strongly linked to the choice of the calibration or that of the warm-up (truncated) period. Indeed, the calibration should be performed on periods when the model output is sensitive to the variable to be calibrated. Conversely, the warm-up period should stop as soon as the model output becomes insensitive to the initial state, since as little data as possible should be removed from the analysis.

This paper investigates the sensitivity of the simulation results of two reservoir models for karst spring discharge calculation to their initial conditions, based on the local perturbation approach. The issues addressed are: (a) what is the influence of model nonlinearities on the sensitivity behaviour, (b) what is the influence of the recharge conditions on the sensitivity behaviour, and (c) are some model structures associated with slower sensitivity decrease than others?

ANALYSIS OF THE FLEURY MODEL (FLEURY, 2005)

Model functioning and governing equations

The model functioning may be described as follows (see model structure in Fig. 1(a)):

(a) The reservoir H receives the incoming precipitations and it is affected by evapotranspiration until the water level reaches a minimum value $H_{\min}$.
(b) Part of the water contained in the reservoir H leaks to the lower reservoirs S and R, provided that the water level in H is larger than zero (discharge Q_H).
(c) The distribution of Q_H between the reservoirs S and R depends on the water level in the reservoir S. When the water level in S rises above a threshold value S_{sill}, the proportion of water routed to the reservoir R increases.
(d) The water in the lower reservoirs S and R leaks to the outlet of the catchment via classical, linear discharge laws.

The mass balance equations of the Fleury model are the following:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \begin{cases} P - ET - Q_H & \text{if } H_{\min} < H \le 0 \\ \max(P - ET, 0) & \text{if } H = H_{\min} \end{cases} \tag{1a}$$

$$\frac{\mathrm{d}S}{\mathrm{d}t} = XQ_H - Q_S \tag{1b}$$

$$\frac{\mathrm{d}R}{\mathrm{d}t} = (1-X)Q_H - Q_R \tag{1c}$$

H, R and S are the water levels in reservoirs H, R and S, respectively, P is the precipitation rate, ET is the evapotranspiration rate, $H_{\min}$ is the minimum water level in the reservoir H, Q_H is the discharge rate from the reservoir H towards the reservoirs S and R, Q_R and Q_S are the discharge rates from the reservoirs R and S respectively, X_W and X_D are the distribution coefficients for Q_H in high and low water level periods, respectively ($X_D > X_W$), X is defined as:

$$X = X_D \quad \text{if } S > S_{\text{sill}} \text{ and } X = X_W \quad \text{if } S > S_{\text{sill}} \tag{2}$$

and S_{sill} is the threshold level that triggers the switch in the distribution coefficient. The internal fluxes are assumed to obey the following laws:

$$Q_H = \varepsilon_H \max(P - ET, 0) \tag{3a}$$

$$Q_S = k_S S \tag{3b}$$

$$Q_R = k_R R \tag{3c}$$

where k_R and k_S are specific discharge coefficients and

$$\varepsilon_H = \begin{cases} 1 & \text{if } H = 0 \\ 0 & \text{if } H < 0 \end{cases} \tag{4}$$

The discharge at the outlet of the catchment Q is defined as the sum of the specific discharges Q_R and Q_S, multiplied by the total area A of the catchment:

$$Q = A(Q_S + Q_R) \tag{5}$$

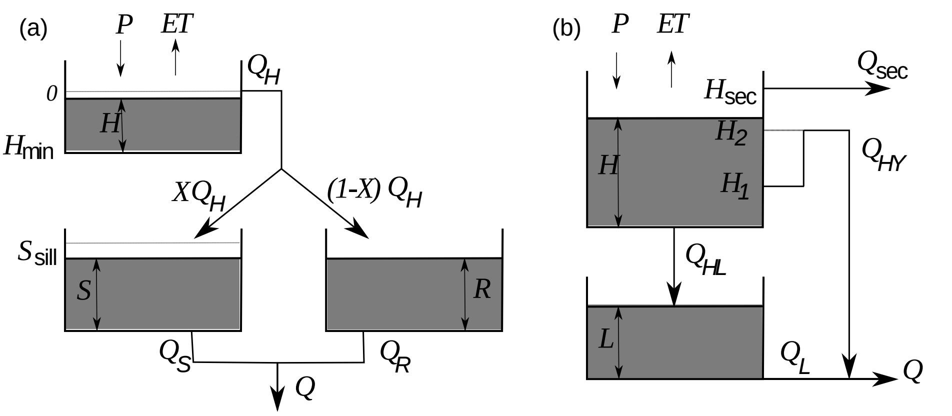

Fig. 1 Structure and notations for: (a) the hysteresis-based model, (b) the Fleury model.

Model sensitivity to the initialization bias: general properties of the sensitivity to R_0

The impact of the initial level R_0 in the reservoir R on the simulated spring discharge decreases exponentially with a time constant $T = 1/k_R$.

Model sensitivity to the initialization bias: general properties of the sensitivity to S_0

Let H_{S0}, S_{S0}, R_{S0} and Q_{S0} be the sensitivities of H, S, R and Q to the initial water level S_0 in the reservoir S. The fact that the value of the distribution coefficient X depends on the water level in the reservoir S means that that the sensitivity of the level R to the initial water level in S is non-zero. Assume that the threshold S_{sill} is not activated. Then the behaviour of the sensitivity to S_0 is similar to that of the sensitivity to R_0. The impact of the initial level S_0 on the simulated spring discharge decreases exponentially with a time constant $T = 1/k_S$.

The activation of the threshold S_{sill} triggers a decrease in S_{S0} and an increase in R_{S0} (see Fig. 2). The activation of the threshold S_{sill} thus hastens the disappearance of the influence of the initial condition S_0. However, the activation of S_{sill} results in a pulse for the sensitivity R_{S0} of the water level in reservoir R and therefore in a pulse for the sensitivity Q_{S0} of the spring discharge.

The de-activation of the threshold S_{sill} has no impact on the behaviour of the sensitivities to S_0 (see Fig. 2).

Model sensitivity to the initialization bias: General properties of the sensitivity to H_0

Let H_{H0}, S_{H0}, R_{H0} and Q_{H0} be the sensitivities of H, S, R and Q to the initial water level H_0 in the reservoir H. The reservoir H differs from the reservoirs S and R in that its response is all-or-nothing. The sensitivity H_{H0} is piecewise constant. It is equal to one at the beginning of the simulation and it cancels when the reservoir H overflows for the first time or when it dries out.

Consider the case where H has not dried out. Then the first activation of the overflow triggers a pulse in the sensitivities S_{H0} and R_{H0}. On the contrary, a complete emptying of the reservoir H before the first overflow completely stops the propagation of the sensitivity to H_0 towards the reservoirs S and R. Also note that a simulation that begins with a low water period with no complete emptying of the reservoir H only delays the propagation of the sensitivity to H_0 within the model. Last, a complete emptying of the reservoir H after the first overflow has no impact on the propagation of the sensitivity to H_0.

Consider the case where the first activation of the overflow happens before H dries out. If the threshold S_{sill} is not activated, then for $t > t_H$ the sensitivities S_{H0} and R_{H0} decrease exponentially. The activation of the threshold S_{sill} results in a decrease in S_{H0} and in an increase in R_{H0}.

ANALYSIS OF THE HYSTERESIS-BASED MODEL (TRITZ *et al.*, 2011)

Model functioning and governing equations

The mass balance equations of the hysteresis-based model are the following:

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \begin{cases} P - ET - Q_{HL} - Q_{HY} - Q_{sec} & \text{if } H > 0 \\ \max(P - ET, 0) & \text{if } H = 0 \end{cases} \tag{6a}$$

$$\frac{\mathrm{d}L}{\mathrm{d}t} = Q_{HL} - Q_L \tag{6b}$$

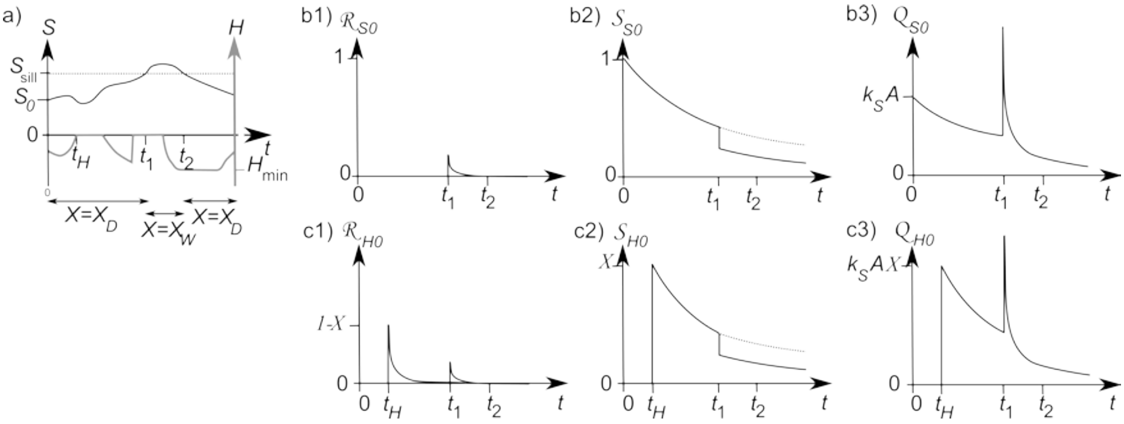

Fig. 2 Fleury model. Typical behaviour of the sensitivities to H_0 and S_0 contingent on the reservoir H overflow and on the activation of the threshold S_{sill}. The reservoir H overflows for the first time at time t_H. The threshold S_{sill} is activated at time t_1 and de-activated at time t_2. Graph (a): water level in the reservoirs S (dark line) and H (bold, grey line), Graphs (b): sensitivity of R (graph b1), S (graph b2) and Q (graph b3) to S_0, Graphs (c): sensitivity of R (graph c1), S (graph c2) and Q (graph c3) to H_0.

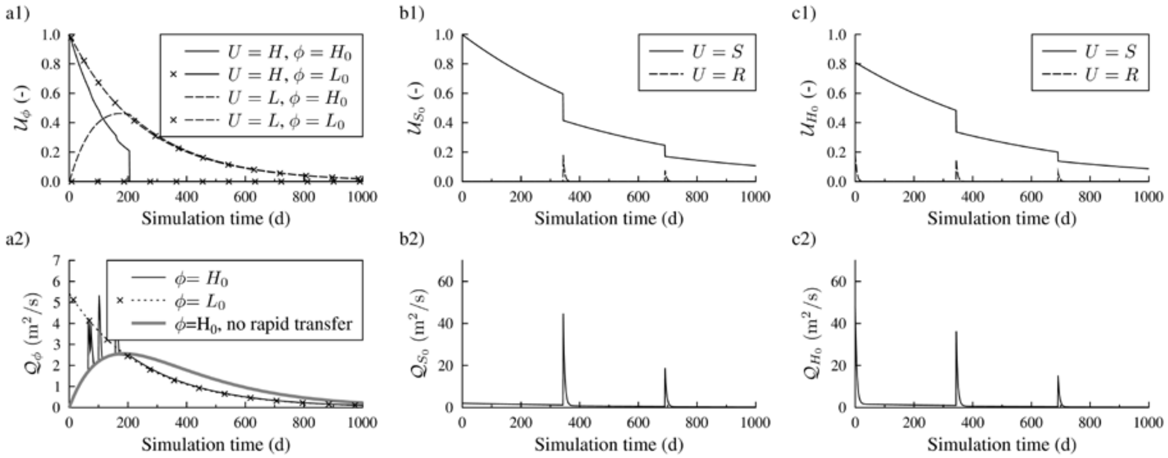

Fig. 3 Computational example. Graphs (a): hysteresis-based model. Sensitivity of the simulated water levels (graph 1) and of the simulated discharge (graph 2) to H_0 and L_0. Graphs (b): Fleury model. Sensitivity of the simulated water levels (graph 1) and of the simulated discharge (graph 2) to S_0. Graphs (c): Fleury model. Sensitivity of the simulated water levels (graph 1) and of the simulated discharge (graph 2) to H_0.

where H and L are the water levels in the reservoirs H and L respectively, P is the precipitation rate, ET is the evapotranspiration rate, Q_{sec} is the secondary springs discharge, Q_{HY} is the fast flow component through the epikarst zone to the outlet of the catchment, Q_{HL} is the infiltration rate to the lower reservoir and Q_L is the baseflow discharge from the lower reservoir L to the outlet of the catchment.

The internal fluxes are assumed to obey the following laws:

$$Q_{HY} = \varepsilon_{HY} k_{HY} \left(\frac{H - H_1}{H - H_2} \right)^{\alpha} \tag{7a}$$

$$Q_{HL} = k_{HL} H \tag{7b}$$

$$Q_{\mathrm{sec}} = \varepsilon_{\mathrm{sec}} k_{\mathrm{sec}} (H - H_{\mathrm{sec}}) \tag{7c}$$

$$Q_L = k_L L \tag{7d}$$

where k_{sec}, k_{HY}, k_{HL} and k_L are specific discharge coefficients, α is a positive exponent, H_{sec} is the threshold level in reservoir H above which the secondary springs are activated, H_1 and H_2 are the lower and upper threshold levels for the hysteretic discharge function respectively. $\varepsilon_{\mathrm{sec}}$ is the indicators of the secondary springs activation:

$$\varepsilon_{\mathrm{sec}} = \begin{cases} 1 & \text{if } H \geq H_{\mathrm{sec}} \\ 0 & \text{if } H < H_{\mathrm{sec}} \end{cases} \tag{8}$$

ε_{HY} is the indicator of the karst system connectivity. It is switched to 1 if H rises above H_2 and it is switched to 0 if H falls below H_1. The actual evapotranspiration rate is assumed to be equal to the potential evapotranspiration rate as long as the soil-epikarst reservoir H is not empty. The discharge at the outlet of the catchment Q is defined as the sum of the epikarstic and baseflow discharges, multiplied by the total area of the catchment A:

$$Q = A(Q_{HY} + Q_L) \tag{9}$$

Model sensitivity to the initialization bias: General properties of the sensitivity to L_0

The impact of the initial level L_0 on the simulated spring discharge decreases exponentially with a time constant $T = 1/k_R$. Note that neither the activation of the hysteretic transfer nor the activation of the secondary springs nor the drying of the reservoir H has an impact on the sensitivities to the initial level L_0.

Model sensitivity to the initialization bias: general properties of the sensitivity to H_0

Denote by H_{H0}, L_{H0} and Q_{H0} the sensitivities of H, L and Q to the initial water level H_0 in the reservoir H. Assume that neither the hysteretic transfer nor the secondary springs are activated. Also assume that the reservoir H does not dry out ($H > 0$). Then the governing equations for the sensitivity of H, L and Q to the initial water level H_0 in the reservoir H may be solved analytically, leading to:

$$Q_{H0} = A\frac{k_{HL}k_L}{k_L - k_{HL}}\left[\exp(-k_{HL}t) - \exp(-k_L t)\right] \tag{10a}$$

$$L_{H0} = \frac{k_{HL}}{k_L - k_{HL}}\left[\exp(-k_{HL}t) - \exp(-k_L t)\right] \tag{10b}$$

$$H_{H0} = \exp(-k_{HL}t) \tag{10c}$$

The sensitivity of the spring discharge to H_0 reaches its maximum at time $t_{\max}= \ln(k_L/k_{HL})/(k_L-k_{HL})$. The activation of the rapid transfer functions (hysteretic transfer or of the secondary springs) result in a faster decrease of H_{H0}. It is also associated with an increase of the sensitivity Q_{H0}.

Heavy rainfall events therefore help to erase the influence of the initial water level H_0. In other words, heavy rainfall events make the minimal length of the warm-up period shorter. However, since the influence of H_0 on the spring discharge Q is increased during these rainfall events, care should be taken not to include these events within the calibration period.

The drying of the reservoir H results in the cancellation of H_{H0}. After the emptying of the reservoir H, the sensitivities L_{H0} and Q_{H0} decrease exponentially.

Also note that subsequent filling of the reservoir H and the possible activation of the rapid transfer function will have no impact on the discharge sensitivity Q_{H0}.

A complete emptying of the reservoir H therefore prevents the simulated discharge from subsequent artefacts due to a burst in H_{H0} during the activation of the hysteretic transfer function.

COMPUTATIONAL EXAMPLE

The analysis of the sensitivity behaviour undertaken in Sections 2 and 3 is valid regardless of the particular values assigned to the parameters. The following computational example aims at illustrating some features of the sensitivity behaviour as a function of model structure.

Application site and data

The Durzon system is a Vauclusian karst system developed in a 400-m thick formation of middle to upper Jurassic limestones and dolomites (Bruxelles, 2001) in the Grands Causses area (France). The main outlet of the catchment is the Durzon spring. A recharge area of 116.8 km^2 is assumed in the present study (Fleury, 2005). Over the 2001/2008 period the spring discharges ranges from 0.5 to 18 m^3/s, with an average 1.4 m^3/s. The average annual rainfall is 1069 mm. The average daily temperatures range between –8 and +28°C and the average annual temperature is 10°C.
The daily potential evapotranspiration is estimated from the monthly potential evapotranspiration computed using Thornthwaite's formula (Thornthwaite, 1948) using a sine function-based interpolation as proposed by Tritz *et al.* (2011):

$$PET(t) = \overline{PET}\left[1 - a\cos\left(\frac{t - t_{\min}}{T}\right)\right] \tag{11}$$

where t is the time where the PET is to be interpolated, $\overline{PET}$ is the average value of the PET series computed from Thornthwaite's formula, T is the period of the PET signal, $t_{\min}$ is the time at which the PET is minimal and a is the dimensionless amplitude of the signal (see values in Table 1).

Table 1 Parameter set used for the computational example.

Symbol	Value	Symbol	Value	Symbol	Value	Symbol	Value	Symbol	Value
H_{sec}	145 mm	H_1	100 mm	H_{min}	190 mm	k_R	1.8 10^{-1}/d	a	0.8
k_{sec}	2.9 10^{-2}/d	H_2	119 mm	X_D	0.81	H_0		t_{min}	15 January
k_{HY}	2 10^{-2}/d	k_L	4 10^{-3}/d	X_W	0.24	S_0		T	365d
α	2.4	H_0		S_{sill}	600 mm	R_0		$\overline{PET}$	1.95 mm/d
k_{HL}	7 10^{-3}/d	L_0		k_S	1.5 10^{-3}/d				

Computational example

Consider the hysteresis-based model. Figure 3(a) shows the sensitivities to the initial water levels in the reservoirs H and L. The sensitivities L_{L0} and Q_{L0} decrease exponentially. The activation of the hysteretic transfer on days 70, 110 and 160 results in a decrease of H_{H0} and in an increase of Q_{H0}. Note that the magnitude of both the decrease in H_{H0} and the increase in Q_{H0} remains limited, which must be related to the fact that the rainfall remains low. The drying of reservoir H at day 205 results in a sudden drop of H_{H0} and in a change in the derivatives of L_{H0} and Q_{H0}.

Consider the Fleury model. Figure 3(b) shows the sensitivities to the initial water level in the reservoir S. Up to day 375, the sensitivity of the water level in R to S_0 is equal to zero and the sensitivity of the water level in S to S_0 decreases exponentially. The activation of the switch in the distribution coefficient (activation of the threshold S_{sill} at day 375 and day 700) results in a sudden decrease in S_{S0}, and in a sudden increase in R_{S0}. The increase in R_{S0} triggers an increase in the discharge sensitivity Q_{S0}. Note that the de-activation of the threshold S_{sill} at day 550 has no impact on the sensitivities behaviour. Figure 2(c) shows the sensitivities to the initial water level in the reservoir H. Reservoir H is overflowing at the beginning of the simulation ($t_H = t_0$). The sensitivities S_{H0} and R_{H0} decrease exponentially until the threshold S_{sill} is activated. The activation of S_{sill} results in a decrease in S_{H0} and in an increase in R_{H0} and $Q_{H0.}$

For both models, the maximum discharge sensitivity values are reached during the activation of the threshold transfer functions. As for the hysteresis-based model, the drying of the reservoir H during the warm-up year prevents the simulated discharge from any subsequent sensitivity burst. In contrast, discharge sensitivity bursts for the Fleury model are triggered by any activation of the S_{sill} threshold. Also note that the maximum discharge sensitivity values for the Fleury model are approximately one order of magnitude higher than those of the hysteresis-based model.

CONCLUSION

As a general rule, the dissipation of the sensitivity is favoured by either very low or very high water periods. Indeed: (a) the drying of the upper reservoir stops the propagation of the sensitivity to the initial water level in that reservoir, (b) the activation of the rapid transfer functions in a given reservoir speeds up the propagation of the sensitivity to the initial water level in that reservoir. Conversely, situations unfavourable to the sensitivity dissipation are: (a) if the upper reservoir is disconnected from the lower reservoirs during the low water period, and the simulation begins with a low water period that does not result in a complete emptying of the upper reservoir. Then the propagation of the sensitivity is delayed until the first activation of the transfer functions towards the lower reservoirs, (b) if a threshold transfer function is associated to the water level in a reservoir with slow dynamics. Then sensitivity bursts associated with the activation of the threshold transfer function may occur years after the simulation starts.

Recent studies have emphasized the need to account for the influence of the karst flowpath network connectivity on the system response dynamics (Jazayeri 2009; Tritz *et al.,* 2011). The change in connectivity may be accounted for in the model structure by a threshold function, the activation of which depends on the water level in a given reservoir. As for the Fleury model, the threshold function triggers the switch in the distribution coefficient based on the water level in the lower, slow discharge reservoir. As regards the hysteresis-based model, the threshold function triggers the activation of the hysteretic transfer, based on the water level in the upper reservoir. The above developments show that the activation of the threshold function based on the water level in a slow dynamics reservoir is associated with far-reaching sensitivity bursts of the initialization bias.

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