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Is the groundwater reservoir linear? Learning from data in hydrological modelling

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Abstract

Although catchment behaviour during recession periods appears to be better identifiable than in other periods, the representation of hydrograph recession is often weak in hydrological simulations. Reason lies in the various sources of uncertainty that affect hydrological simulations, and in particular in the inherent uncertainty concerning model conceptualizations, when they are based on an a-priori representation of the natural system. When flawed conceptualizations combine with calibration strategies that favour an accurate representation of peak flows, model structural inadequacies manifest themselves in a biased representation of other aspects of the simulation, such as flow recession and low flows.

In this paper we try to reach good model performance in low flow simulation and make use of a flexible model structure that can adapt to match the observed discharge behaviour during recession periods. Moreover, we adopt a step-wise calibration procedure where we try to avoid that the simulation of low flows is neglected in favour of other hydrograph characteristics.

The model used is designed to reproduce specific hydrograph characteristics and is composed of four reservoirs: an interception reservoir, an unsaturated soil reservoir, a fast reacting reservoir, and a slow reacting reservoir. The slow reacting reservoir conceptualises the processes that lead to the generation of the slow hydrograph component, and is characterized by a storage-discharge relation that is not determined a-priori, but is derived from the observations following a “top-down” approach.

The procedure used to determine this relation starts by calculating a synthetic master recession curve that represents the long-term recession of the catchment. Next, a calibration procedure follows to force the outflow from the slow reacting reservoir to match the master recession curve.

Low flows and high flows related parameters are calibrated in separate stages because we consider them to be related to different processes, which can be identified separately. This way we avoid that the simulation of low discharges is neglected in

favour of a higher performance in simulating peak discharges. We have applied this analysis to several catchments in Luxembourg, and in each case we have determined which form (linear or non linear) of the storage-discharge relationship best describes the slow reacting reservoir. We conclude that in all catchments except one (where human interference is high) a linear relation applies.

1. Introduction

The common description of hydrological processes in a catchment (see e.g. Chorley, 1978) assumes a portion of the catchment to be saturated with water, residing in permeable formations that serve as conduits for transmission and storage. This zone is normally referred to as the "groundwater reservoir".

This or similar definitions of the groundwater reservoir are adopted in catchment conceptualisations of most hydrological models, in particular physically based models. The SHE model (Abbott et al., 1986a, b) and the REW model (Reggiani et al., 1998; Reggiani and Rientjes, 2005) are examples of such models. In their conceptualisations there is a "saturated zone" represented by the portion of the aquifer that is below the water table. The water movement in this zone is mainly controlled by soil properties such as porosity and hydraulic conductivity, and is usually described by a typical single-phase flow equation for porous media, such as Darcy's Law.

The correct description of groundwater movement in these models relies on knowledge of the properties and structure of the rock formations in the saturated zone. However, in many hydrological applications, where the main purpose of the model is to reproduce the rainfall-runoff relation of a catchment, often little is known about the structure of the catchment and in particular about the underground properties. Details about the sequence, lithology, thickness and structure of the rock formations that determine the occurrence, storage and movement of groundwater are usually lacking. Consequently little is known about the patterns and dynamics that water follows from its infiltration into the ground to its re-emergence at the earth's surface. Piezometric measurements or tracer analyses can be very useful to get some insight into groundwater behaviour (e.g. Uhlenbrook and Leibundgut, 2002), but those measurements are rarely available, and their interpretation is by no means a simple task.

When models using the above definition of a groundwater reservoir are applied to a catchment with an unknown geology, often gross simplifications are made to describe sub-surface properties and model parameters related to the representation of the groundwater behaviour are estimated through calibration against observed discharge. Normally this is done by adjusting subsurface parameters in such a way that the hydrograph obtained matches the amount of low flow and the flow recession. In this situation one may wonder whether it is reasonable to assume that the representation of the groundwater reservoir reflects its real behaviour, and if the conceptualisation of the model is still representative.

An alternative definition of a groundwater reservoir that may be closer to what is represented by the model could stem from the following observation. Looking at an observed hydrograph, it is normally possible to distinguish a “fast response” component, representing the discharge associated to a rainfall event, and a “slow response”, that sustains stream flow in periods of no rainfall (e.g. Rutledge, 1993; Nathan and McMahon, 1990). According to this observation, the groundwater reservoir may be defined as the portion of a catchment storing the water that is responsible for the generation of the “slow response” hydrograph component. At this stage it is avoided to identify different hydrograph components through terms like “baseflow” or “rainfall-excess”, to emphasize that the interpretation of the natural processes underlying a certain response is here a possible objective rather than a starting point. Following this approach, the groundwater reservoir is primarily conceptual, but it is possible (even if non necessary) to give it a physical interpretation.

Implicitly, this definition is adopted in the conceptualisation of many rainfall-runoff models where specific components aim at reproducing particular characteristics of system response rather than representing realistically the internal physical processes involved. We can however extend this definition to all situations where a model, conceptual or physically based, is calibrated on rainfall and discharge data only, while little is known about catchment properties and behaviour below the surface. In these cases, in fact, the representation of the groundwater behaviour is orientated towards an optimal simulation of system response, rather than a realistic representation of the groundwater processes within the system, that are in general very complex, and mostly unknown.

Following Klemeš (1983) and Sivapalan et al. (2003), the first definition can be interpreted as "bottom-up", because it is based on the (often assumed) knowledge, understanding and description of the true properties, true state and true dynamics of the system, while the second definition can be regarded as "top-down", because it originates from an interpretation of system response.

The "top-down" approach is used as a guideline in the course of this work. In the present case, in fact, we try to identify and isolate dominant processes of the system, analysing its overall response. In particular we concentrate on determining the catchment discharge behaviour during periods of flow recession and low flows. During these periods, catchment response is more regular and better identifiable than in other periods. Consequently it should in principle be more easily predictable. Notwithstanding this, low flow representation is often a weak point of hydrological simulations. This may be due to a combination of several reasons. Among them we identify the following: 1) the conceptualization of the hydrological processes present in the catchment may not be appropriate for a certain situation; 2) the objective functions used for model calibration often stress the simulation of peak flows rather than low flows. Ideally, if a model was able to reproduce perfectly the response of a natural system, it would be theoretically possible to calibrate it to perform this task. In practice hydrological models involve structural errors that affect their capability of reproducing simultaneously all aspects of the system response. The calibration procedure, and in particular the choice of a specific objective function, might favour or penalize model performances in reproducing certain features of the system behaviour (e.g. Gupta et al., 1998). When a calibration strategy puts a strong constraint on the simulation of high flows, other characteristics of the system response may result to be improperly represented.

In this paper we try to reach good model performance in low flow simulation and propose a methodology to overcome these limitations. The first problem is tackled by trying to infer from the discharge data an appropriate conceptualization that allows a good representation of low flows. The second problem is tackled by separating the calibration of the parameters that are mostly related to the simulation of high flows from the parameters related to the low flows representation. This should assure that trying to give a good representation of peak flows does not penalize the representation of low flows.

The groundwater reservoir is conceptualized as a lumped store, and we try to infer from the data an appropriate storage-discharge (S-D) relation that characterizes its behaviour. Obviously in the “top-down” approach followed, the conceptualisation sought aims at providing an appropriate representation of system response, rather than a realistic description of the groundwater processes involved. The S-D relation is obtained without making prior assumptions on its shape, and is derived analysing the observed discharge data. The procedure followed starts by calculating a Master Recession Curve (MRC) (e.g. Lamb and Beven, 1997), which is obtained by matching several hydrograph recession segments to form one single curve. The MRC combines the slow components of each recession, therefore it is a synthetic curve representing the long-term recession of the catchment and the depletion over time of the groundwater reservoir. Subsequently, a calibration procedure is followed to assure that the response of the groundwater components of the model matches the MRC.

The procedure has been applied to eight catchments in Luxembourg, and the S-D relationships obtained for each catchment have been analysed. As a result we observe that in all undisturbed catchments a linear relationship is appropriate to describe the observed groundwater behaviour.

2. The representation of the groundwater reservoir in hydrological models

Conceptualisation of the groundwater reservoir requires formalizing this compartment and the interaction with other compartments of the catchment in mathematical terms. Different models in general use different conceptualisations and different mathematical representations of the groundwater reservoir.

Looking at the exchange between the groundwater reservoir and the river, a range of solutions of various complexities is adopted by various models. In its most general form, this exchange can be represented as a function of several variables (e.g. storage, distribution of storage in the catchment, shape of the water table, hydraulic gradient), parameters (e.g. hydraulic conductivity, porosity), and boundary conditions. This description is often adopted in models that try to describe runoff processes at a high spatial and temporal resolution. An emblematic example of such models is SHE described by Abbott et al. (1986a, b). The storage-discharge relationship characterising the exchange between the groundwater reservoir and the river reach in such models, generally accounts for non-linear responses, and, being dependent on more variables than just the storage, also takes account of possible hysteretic behaviour.

Often the description of hydrological processes is simplified, resulting in conceptualisations that focus on runoff generation processes at catchment scale. In such a case the integrated response of the groundwater reservoir is normally modelled in a lumped fashion, where parameters describe catchment scale characteristics and the reservoir storage is usually assumed as the only variable influencing discharge. An example of such an approach is the semi-distributed Topmodel (Beven et al., 1995). In the original version of the model, the S-D relation is expressed as an exponential function of the reservoir storage, dependent on one recession parameter. The physically-based semi-distributed REW model, through an averaging procedure resulting in macroscopic mass and momentum conservation equations applied at the catchment scale, uses a linear relation to describe the exchange between the groundwater reservoir and the river. Both these models all apply a "bottom-up" definition to characterize the groundwater reservoir.

Simpler conceptual models representing the catchment as a combination of interconnected stocks and fluxes, often describe the groundwater reservoir as a single linear reservoir, implying that the outflow through the outlet is linearly proportional to the storage in the reservoir, characterized by a storage constant (the average residence time). An example of such models is the HBV-96 model described by Lindström et al. (1997). In some cases baseflow is considered to be generated by a reservoir with multiple outlets or by a series of two or more stocks. In such a case overall behaviour may result in a non-linear relation between storage and discharge. The Sacramento Soil Moisture Accounting model (Burnash et al., 1973) and the Tank model (Sugawara, 1995) are examples of such representations. As explained earlier, the models in this category implicitly are “top-down” models in view of their characterisation of the groundwater reservoir.

This brief overview, which doesn’t claim to be exhaustive and complete, has the purpose of showing that both conceptual and physically based models can (implicitly) assume very simple or more complex conceptualisations of the groundwater reservoir. In particular the simplest concept of the linear groundwater reservoir can be the result of either straightforward thinking (following from the logarithmic depletion curve) or the result of averaging the mass balance and momentum laws in a physically based fashion, like in the REW approach.

In this paper we use a simple conceptual model that represents the groundwater reservoir as a lumped store. The behaviour of this store is characterised by a S-D relation inferred from discharge data. The procedure will be described on the basis of an example.

3. Study area

The study area comprises eight catchments in Luxembourg. In the central and southern part of Luxembourg, the geology mostly consists of an alternation of marls, sandstone and limestone. This alternation strongly influences the relief of the area, which is mostly characterised by cuestas. The soil profile is dominated by large flat areas of marls that alternate with deep valleys cut into sandstone or limestone formations, where the stream channels are deeply incised and the lower portions of the slope profiles are strongly convex. On the northern part of Luxembourg, the geology is mainly represented by a compact geological formation of Schists belonging to the Ardennes massif.

Marls formations can be considered to be impervious and highly responsive to rainfall. The response of Schist formations is highly dependent on the water content of the basin. During dry periods they tend to retain rainfall water, as the wet season starts they saturate quickly and their response to rainfall becomes more pronounced. Areas of outcropping sandstone and limestone normally represent zones of infiltration of rainfall water.

The sub-basins chosen represent the variability of basin sizes, geological conditions, physiographical properties, as well as the availability and quality of streamflow data. The main physiographical characteristics of the sub-basins and the major geologic units are summarized in Table 1. The locations of the catchments are shown in Fig. 1. Some of the catchments are nested, in particular the Attert-Useldange catchment includes the Schwebich-Useldange catchment, and the Alzette-Pfaffenthal catchment includes the Alzette-Hesperange and the Petrusse-Luxembourg catchments.

The rainfall observation network in the study areas has an average density of one instrument per 30 km^2, with automatic rain gauges functioning since the mid-1990s measuring rainfall at a 15-min interval.

For the present study, hourly data of rainfall, potential evaporation and discharge have been used, provided by the hydro-climatological database of the CRP-GL. The hourly rainfall for each sub-basin was determined using the Thiessen polygons interpolation method. Daily estimates of potential evaporation and transpiration were calculated using the Penman-Monteith approach as a function of the following meteorological variables: temperature, wind speed, humidity and net radiation. The necessary data were measured at the meteorological station located at Luxembourg airport. Hourly estimates where then calculated distributing the total daily amounts through a sinus function. For model calibration a 3 years period was selected, starting from 1 September 2001 until 31 August 2004.

4. Model description

4.1. FLEX model structure

The FLEX (Flux Exchange) hydrological model is a lumped conceptual model that represents the relevant hydrological processes occurring in the catchments.

The model is composed of four reservoirs: an interception reservoir (*IR*), which takes into account the interception process, an unsaturated soil reservoir (*UR*), which represents the storage capacity of the soil, a fast reacting reservoir (*FR*) accounting for the formation of fast runoff components and a slow reacting reservoir (*SR*), representing the slow runoff components (Fig. 2).

4.1.1. Interception module

Rainfall reaches *IR*, which can be filled up to a specified threshold, represented by $I_{\max}$. Evaporation from intercepted water E_i can occur as long as water is available in the reservoir, and it is assumed to be linearly related to the potential evaporation E_p through the coefficient I_c:

$$E_i = I_c \cdot E_p \,. \tag{1}$$

4.1.2. Unsaturated soil module

Effective rainfall R_e leaves *IR* when the threshold $I_{\max}$ is exceeded. This amount is then partitioned into various components based on the value of an effective (i.e. after subtraction of interception, see: Savenije, 2004) runoff coefficient C_r (Eq. 2), expressed as an S-shaped function dependent on the ratio between the storage of the unsaturated soil reservoir S_u and its maximum storage S_{fc} (Fig. 2). Part of R_e infiltrates into *UR*, excess water from *UR* is then partitioned through the coefficient D into R_s, which flows to the slow reacting reservoir, and R_f, which enters the fast reacting reservoir (Eqs. 3, 4, 5).

$$C_r = \frac{1}{1 + \exp\left(\frac{-S_u/S_{fc}+1/2}{\beta}\right)} \tag{2}$$

$$R_u = (1 - C_r) \cdot R_e \, . \tag{3}$$

Percolation P_s from the unsaturated soil reservoir to the slow reacting reservoir is calculated as a linear function of S_u:

$$P_s = P_{\max}\left(S_u/S_{fc}\right) \, . \tag{4}$$

The specified input potential transpiration is converted into actual transpiration according to the following formula:

$$T_a = T_p \cdot \min\left(1, \frac{S_u}{S_{fc}} \cdot \frac{1}{L_p}\right) \, , \tag{5}$$

Where L_p is the ratio of S_{fc} below which T_p is constrained by S_u.

4.1.3. Transfer routine

As shown in Fig. 1, the transfer routine of the model consists of two lag functions and two reservoirs. The two lag functions are characterized by a triangular distribution of linearly increasing weights and are defined by the parameters N_{lagf} and N_{lags} that determine the number of time steps in the transformation routine. Those functions are used to offset the fluxes P_s and R_s that enter *SR* and the flux R_f that enters *FR* and mainly control the lag-time of the system and the simulation of the rising limbs of the hydrograph.

The fast reacting reservoir is a linear reservoir defined by the recession coefficient K_f , and the slow reacting reservoir is characterized by a storage-discharge relation to be determined. The drainage equations for the two recession components can be expressed as:

$$Q_f = K_f \cdot S_f \tag{6}$$

$$Q_s = f\left(S_s\right) , \tag{7}$$

where Q_f and Q_s are the fast and slow discharges and S_f and S_s are the storages of the fast and slow reservoirs, respectively. These reservoirs mainly control the simulation of the recession limbs of the hydrograph.

The model has a total of 10 parameters that are summarized in Table 2 together with their corresponding units, and an unknown functional relationship.

5. Calibration of low flows

The calibration procedure of the model is separated into two different stages. In a first stage all model parameters and the unknown functional relation are calibrated to fit hydrograph recessions and low flows. In a second stage parameters that mostly influence high flows are recalibrated to give a better fit to the high portions of the hydrograph.

The first calibration stage is composed of four steps that are hereafter described. The methodology followed is shown by means of an application to the Wark catchment, calculations in other catchments follow the same procedure.

5.1. Step 1: Calculation of a Master Recession Curve

The first step aims at determining the flow recession curve. The flow recession curve is determined using the method described by Lamb and Beven (1997) that combines recession periods to synthesize a Master Recession Curve (MRC). The procedure uses all recession periods that are longer than a specified threshold and combines them into one synthetic recession curve (Fig. 4).

The individual recession segments are sorted in ascending order based on the tail-end discharge values. The curve with the lowest tail-end discharge value is shifted over time until it overlaps with the next curve. The concatenation proceeds until the recession curve with the highest tail-end value is encountered. The purpose of this particular concatenation procedure is to exclude storm flow effects from the MRC. The MRC is therefore a synthetic curve that captures the long-term recession of the catchment over a wide range of flows, and can be held to represent the discharge produced by the depletion of the groundwater reservoir.

5.2. Step 2: Initial estimate of the Storage-Discharge relation

According to the adopted definition for the groundwater reservoir, the objective of the calibration procedure becomes that the slow reacting reservoir *SR* of the model empties in such a way that it matches the MRC. The MRC should therefore represent the discharge produced by the depletion of *SR*. To obtain a S-D relation for *SR* that generates a recession matching the MRC, we use the initial hypothesis that during recession periods no flux enters the *SR*. The MRC is extrapolated until zero discharge and we assume that at that point the reservoir is empty (storage is zero).

Subsequently, the MRC is integrated and a curve representing the storage-discharge relation is constructed (Fig. 5). This curve represents the initial estimate of the storage-discharge relation characterising the behaviour of *SR*.

The curve is then approximated with an appropriate trend line (in this case a second order polynomial function), and its equation is assumed to represent the unknown S-

D relation of Eq. (7). An emptying reservoir that is characterized by the S-D relation hence generates an outflow that closely matches the MRC.

5.3. Step 3: Calibration of other model parameters

Once the drainage equation in Eq. (7) has been fixed, other model parameters can be calibrated. Parameter values are estimated through a single objective calibration procedure, choosing an objective function that emphasises the simulation of low flows:

$$N_{LF} = \frac{1}{n}\left(\sum_{i=1}^{n}\left(\ln Q_{s,i} - \ln Q_{o,i}\right)^2\right) . \tag{8}$$

Due to the use of the logarithmic function, this equation gives additional weight to the error in simulating low flow. Calibrating model parameters to minimize N_{LF} therefore constrains the simulation of the lower portions of the hydrograph.

As a search method to identify the global optimum in the parameter space we have selected the Adaptive Cluster Covering (ACCO) strategy with local search developed by Solomatine (1995, 1999), which proves to be effective and efficient in global optimization problems. This algorithm is implemented in the global optimization tool GLOBE (Solomatine, 1999), which has been configured to calibrate the parameters of the FLEX model.

5.4. Step 4: Recalculation of the Storage-Discharge relation

In step 2 the S-D relation for *SR* has been calculated under the assumption that no flux enters *SR* during recession periods (i.e. there is no recharge, but also no capillary rise). This hypothesis is most often not satisfied, because in a wet climate there can still be percolation from *SM* to *SR* (similarly, in dry climates, there can be capillary rise or withdrawal by deep-rooting trees) that has to be simulated through the model. As a result, a recharge to *SR* may occur even during recession periods. If such a flux is present during flow recession and the storage-discharge relation calculated in Step 2 is used, *SR* will not empty according to the MRC. For this reason a recalculation of the S-D relation is necessary.

This situation is explained in Fig. 6. P_{tot} represents the total recharge to SR calculated by the model. This time series is determined considering the modelled flux entering SR in the time periods corresponding to the recession segments constituting the MRC.

Figure 6 also shows the recessions of an emptying reservoir characterized by a S-D relation as calculated in Step 2 in the two cases of no recharge and recharge represented by P_{tot}. It is possible to observe that the first curve matches well the MRC, while the second curve, that is representative of the recession simulated by the model, differs sensibly from the MRC.

The new estimate of the S-D relation is determined by forcing the outflow to the MRC and the inflow to P_{tot}. As a result the S-D relation is updated. This procedure is the same as in step 2, with the difference that in the calculation of the storage the flux entering *SR* is now taken into account.

The recalculated S-D relation is shown in Fig. 7 (iteration 1). We see that the recalculated curve is steeper than the initial one, meaning that, in order to match the MRC, *SR* has to empty faster than estimated initially, as a result of the percolation flux entering the reservoir. As in step 2, the recalculated S-D relation is then approximated with an appropriate trend line, and applied to represent Eq. (7).

The internal results of the model are also used to check which part of the S-D relation calculated with the MRC is actually generated by the slow reacting reservoir of the model. The MRC represents the recession of the catchment over a wide range of flows, and the slow reacting reservoir of the model simulates only the lower parts of this recession. Therefore, only the lower portion of the MRC represented in Fig. 4 will be relevant in determining the S-D relation represented in Fig. 5. Figures 5 to 10 reporting the S-D relation and the MRC only refer to the lower portion of those curves that is significant to the operation of *SR*.

After a new S-D relation is calculated, step 3 and 4 are iterated until convergence in the determination of the S-D relation is achieved. Convergence is considered to be reached when the total amount of flux entering the *SR* in the current iteration does not differ more than 10% from the previous iteration. The value of 10% may seem high, but it serves the purpose, taking into account that different calibration runs may give slightly different parameter estimates due to parameter equifinality.

In this example, as shown in Fig. 7, only three iterations were necessary to reach convergence. We can see that the S-D relations for the 2 and 3 iterations are already very close. Also in the other catchments, three to five iterations were sufficient.

The recession curves corresponding to the recalculated S-D relation is shown in Fig. 8. Like in Fig. 6 the cases of an emptying reservoir with no recharge and with recharge represented by P_{tot} are shown. Also from this figure it is possible to observe that in order to have an overall result that matches the MRC the SR reservoir has to empty faster than estimated initially.

In Fig. 9 the initial and final estimates of the S-D relation are shown, together with the respective trend lines. From the figure it is evident that the two curves are different, meaning that it is necessary to go through the iterative procedure for the S-D estimate to become representative for groundwater reservoir depletion. We can also see clearly that the relation tends to become linear. This also appeared to be the case in the other catchments.

Some conceptual hydrological models do not consider continuous percolation from the soil moisture compartment to the groundwater compartment (e.g. the HBV model). In the FLEX model this could be realized by setting the flux P_s to zero. In this situation only the flux R_s would remain to feed the *SR* reservoir. This flux is mostly related to rainfall events, and can be therefore be considered to occur in time periods associated with the rising limbs of the hydrograph. When this is the case, during recession periods there would be no recharge to SR, and there is therefore no need to modify the S-D relation calculated in step 2 through the iterative procedure shown in this section. This is a possibility that would allow some simplifications in the calibration phase and consents to apply the S-D relation extracted from the data directly in the structure of the model. However in this case we have observed that this simplification, while allowing a fairly good representation of flow recessions, diminishes the overall performance of the model.

6. Results from the 8 catchments in Luxembourg

The same procedure was applied to the other selected catchments. In all cases a convergence could be reached in the determination of the S-D relation. The linearity of this relation can be determined by calculating the coefficient of determination R^2 with a linear trend line. Table 3 summarizes the results obtained on the eight catchments. The R^2 has been calculated both for the initial estimate determined in calibration step 2 and for the final estimate of the S-D curve. It can be seen that in general there is an increase in linearity of this relation, which shows that the apparent overall non-linear behaviour percolation into an otherwise linear reservoir.

In more arid climates it may be necessary to represent an upward flux that takes account of capillary rise or water uptake by deeply rooted vegetation. In the model this exchange can be represented by a flux from *SR* to *UR*. The calibration procedure would be analogous, the only difference being that an equation for the upward flux needs to be employed. In the present application the representation of this exchange was found not to be necessary. When an upward flux was considered, it was made negligible in the calibration procedure. This is a consequence of the dominant wet climate of the catchment, resulting in a predominantly downward flux.

From Table 3 we conclude that the final values of R^2 are quite high for almost all catchments, showing that in most cases a linear reservoir is quite suitable to simulate the groundwater response. The only exception is in the Petrusse catchment, whose initial and final S-D relations are represented in Fig. 10. The reason why this catchment behaves differently from the others lies in the fact that, unlike the other catchments, it is not a natural catchment anymore. The Petrusse catchment is highly urbanized (Table 1) with artificial drainage and sewerage. The sewer system (draining a continuous stream of household waste water) strongly influences the base flow, and alters the natural discharge especially during periods of low flows. But even in this catchment we see a tendency of the S-D relation to become more linear, with the exception of the lowest discharge which is dominated by sewerage.

7. Calibration of high flows

If the purpose is to obtain a model that represents flow recession and low flows well, this procedure can be considered concluded. If, in addition, the aim is to obtain a full rainfall-runoff model, one should continue improving the faster components while keeping the slow compartment unaltered.

The association of model parameters with specific hydrograph characteristics is in general not a simple task, but can be less problematic with models that are developed following a top-down approach, such as in this case. Those models are in fact developed in a way that their components aim at simulating specific features of the system response. The corresponding parameters can therefore be easily related to particular hydrograph characteristics.

In the model used and for problem at hand, we consider the parameters related to the parameterisation of *UR* and *FR* and the parameter representing the length of the transfer function that offsets the flux entering *FR* as mostly related to the representation of high flows. Therefore these parameters can be recalibrated to match the high flow portions of the hydrograph, after the slow compartment has been fixed. Here, the recalibration procedure has been applied to the following parameters: S_{fc}, L_p, β, N_{lagf} and K_f. Interception-related parameters were not recalibrated because it is assumed that the effect of interception on the hydrograph is better identifiable during periods of low flow.

The selected parameters are readjusted to minimize the objective function N_{HF} represented by the following equation:

$$N_{HF}=\frac{1}{n}\left(\sum_{i=1}^{n}\left(Q_{s,i}-Q_{o,i}\right)^2\right). \tag{9}$$

In contrast to the previous goodness-of-fit criterion, N_{HF} puts a strong weight on the high flows due to the square of the difference between observed and simulated discharge.

The effect of recalibrating high-flow related parameters for the Wark catchment is represented in Fig. 11. The first image represents the calibration after the first calibration stage; the second and third images show the effect of recalibration in the second calibration stage. The third image is the same as the second but plotted on a log scale to enhance flow recession and low flows. We can see that the recalibration of high-flow related parameters improves the simulation of high-flows, while the representation of low flows and flow recession remains almost unaltered. It is also noticeable from the second and third graph that the overall performance of the model is quite good, and the trend of the observed recession is maintained. In the third graph, the peaks in the tail are enhanced by the logarithmic scale, but, as shown on the normal scale, they are really very small, and can be caused by rain on surface water (or rain on saturated banks) which this simple model doesn't consider.

8. Discussion: is the groundwater reservoir linear?

In this study we have followed a top-down approach where, by analysing system response, we have characterised the behaviour of the "groundwater reservoir" in a simple conceptual model. The study has been applied to 8 catchments in Luxembourg, representative of different geological and physiographical conditions of this region. In most cases, despite the catchment diversities, we have determined that a linear storage-discharge relation describes the behaviour of the model reservoir appropriately. The only exception is an urbanised catchment, where a base flow is generated by a sewer system draining household water supplied from outside the catchment.

Whether these findings have a general value is difficult to state with certainty, considered the limited amount of cases that have been investigated. However, it confirms the general pattern observed world-wide that the slow groundwater component is linear and that non-linear behaviour is caused by either percolation (under wet conditions) or uptake from deeply rooted vegetation (under dry conditions).

While the validity of this work relies in the utility of a procedure that allows the reproduction of low flows and flow recession by a simple conceptual model, several questions regarding the physical interpretations of the results arise.

We may question if the "top-down" approach is a reliable tool to understanding the behaviour of the unknown underground system of the catchment. We may wonder if the results obtained are transposable to real catchment behaviour, and particularly, if the findings about the behaviour of the groundwater reservoir are realistic. If we can say something about the groundwater behaviour in the catchment, we would like to answer the question when the groundwater reservoir behaves in a particular way and, of course, why. Answering these questions is not a simple task. However, we could try to judge the relevance of this work with respect to what distinguishes a model application from the real world, and to classify both the achievements of the model and the limitations that make the physical interpretation of the results obtained less realistic.

In general, in order to be able to draw meaningful conclusions on real catchment behaviour from using a model application, one should be able to have confidence in the following aspects. First of all the model structure should reasonably represent the dominant hydrological processes in the catchment. Secondly, we should have confidence in that the calibration technique used is able to provide parameter values that are representative of the processes that those parameters characterise. Without claiming that in this application we can fully trust that these conditions apply, we can conclude that the choices made go a long way to fulfilling these requirements.

Regarding the first requirement we have chosen a parsimonious conceptual model that considers the relevant hydrological processes and reproduces key response modes of the catchment. Obviously the structure of the model may be subject to improvements and different plausible structures may yield a similar performance. The model used, however, apart from being particularly suitable for this application, appeared to give good results in terms of hydrograph simulation.

Regarding the second aspect, by calibrating low-flows and high-flows separately, we have avoided that unrealistic parameter values are obtained because certain hydrograph characteristics are favoured at the expense of others. Calibrating model parameters to match hydrograph characteristics they are designed for should assure that model components perform those operations for which they are intended.

Improvements of model structure and consistency can be achieved by using additional (orthogonal) information that can either support or invalidate the hypotheses made and allow more reasonable estimates of the internal exchanges between model compartments.

The use of a conceptual model to obtain physically interpretable results may be criticised because it is commonly assumed that conceptual models are not physically based. The need for simplifying the conceptualisation is in the first place a requirement imposed by the necessity to strike a balance between model complexity and data availability (Wagener et al., 2001). Since in this study we calibrated the model only using discharge data, we were somehow forced to consider a parsimonious model with few calibration parameters.

The use of a conceptual model, however, does not limit the interpretability of the results in physical terms. In fact, conceptual models can sometimes be better tools than physically based models to capture catchment behaviour, which may not be apparent at a hillslope scale but that becomes evident only at a larger scale of aggregation.

The reason why this is often observed may lie in the concept of self-organisation. The simplicity of the conceptual model, which contrasts with the complexity and heterogeneity we observe at the smaller scale, finds its counterpart in the dominance of averaging processes in nature which smoothens out complex, spatially distributed and highly interrelated hydraulic, morphological and ecological processes. Complex processes at smaller scales combine into an integrated response that is often simple (Savenije, 2001), as a result of self-organisation in geomorphological and ecological processes.

Within the limits of the conceptualisation used and the data available, the physical interpretation of the results of this study may be that in the Luxembourg region natural catchments behave linearly, despite differences in geological conditions, while urbanized catchments can demonstrate non-linear behaviour, due to artificially generated flow affecting the natural base flow.

Our working hypothesis is that the groundwater reservoir of a catchment is linear, or tends to become a linear reservoir. Hassanizadeh (1986) showed how Darcy's law, which was initially derived empirically, can be theoretically justified by using entropy considerations. Rodriguez-Iturbe and Rinaldo (1997) show how the landscape evolution can be explained on the basis of the principle of minimum energy expenditure and maximum entropy dissipation. We hypothesize that the process of self-organization that leads to the formation of river basin landscapes also applies underground, modelling the subsurface drainage network, and leading to the validity of the linear reservoir. Non-linear situations are of course possible, but will be due to the scale of application chosen (too small for natural averaging to take place), or to human activities influencing the natural flow regime, or to the fact that the geological formation is too young for full self-organization to have taken place.

9. Conclusions

This work describes a methodology where, by following a “top-down” philosophy, we try to infer from discharge data an appropriate conceptualisation that describes the behaviour of the subsurface drainage system of a catchment. The top-down philosophy is an approach that allows interpretation of system properties by analysing its overall response, and it offers a useful scientific framework in situations where system characteristics and its internal behaviour are unknown, as in the case of the underground drainage system of a catchment.

The part of a catchment that is responsible for the generation of the slower components of the hydrograph is conceptualised as a lumped reservoir. The response of this reservoir is determined by a storage-discharge relation that is not determined a priori, but is inferred from the data. The shape of this relation is based on a synthesized master recession curve (MRC) that represents the long-term depletion of a catchment. Subsequently a calibration procedure is followed to guarantee that during recession periods the groundwater components of the model gives a response matching the MRC. In order to prevent that the calibration procedure favours the matching of high flows over low flows, the high flows related parameters are calibrated in a separate next step.

The main conclusions of this work can be summarized as follows:

1. While the MRC is extracted directly from discharge data, it is still necessary to go through a calibration procedure to guarantee that the response of the groundwater components of the model matches the observed behaviour of the catchment during recession periods.

2. The response of the catchment captured by the MRC can in most cases be reproduced by a linear reservoir that empties while a recharge flux (or an upward flux) is taken into account.

3. Even if this study is limited to a few catchments, and there are clear limitations that restrict the physical interpretation of the results, our hypothesis is that in general the groundwater reservoir of the catchment is linear. We suppose that non-linear situations may be due to the scale of application (too small for the natural averaging to take place), or to artificial disturbances (altering natural base flow production), or to geological formations being relatively young so that self-organization of the natural environment has not yet fully developed.

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Table 1. Physiographic characteristics of the selected catchments. SH: schists, SS: sandstone, MR: marls, LS: limestone.

Catchment	Outlet	Area (km^2)	Cultivated land (%)	Grassland (%)	Forested land (%)	Urbanized land (%)	Geologic units
Wark	Ettelbruck	81.5	24	30	42	4	SH, SS
Schwebich	Useldange	30	16	51	31	2	SS, MR
Attert	Useldange	247	29	35	32	4	SH, MR, SS
Wiltz	Winseler	102.5	34	34	25	7	SH
Eisch	Hagen	49.8	41	35	18	6	MR
Petrusse	Luxembourg	44.9	12	42	22	24	MR. SS
Alzette	Hesperange	288	27	26	29	18	LS, MR
Alzette	Pfaffenthal	356	25	27	28	20	LS, MR, SS

Table 2. Model parameters and units.

Parameter	Units
I_c	–
$I_{\max}$	mm
S_{fc}	mm
L_p	–
β	–
D	–
$P_{\max}$	mm/h
N_{lagf}	h
N_{lags}	h
K_f	h^{-1}

Table 3. Linearity of the storage-discharge relation.

Catchment	R^2 initial	R^2 final
Wark	0.97	0.99
Schwebich	0.86	0.95
Attert	0.91	0.96
Wiltz	0.99	0.99
Eisch	0.97	0.98
Petrusse	0.79	0.87
Alzette-Hes	0.95	0.98
Alzette-Pfaf	0.96	0.97

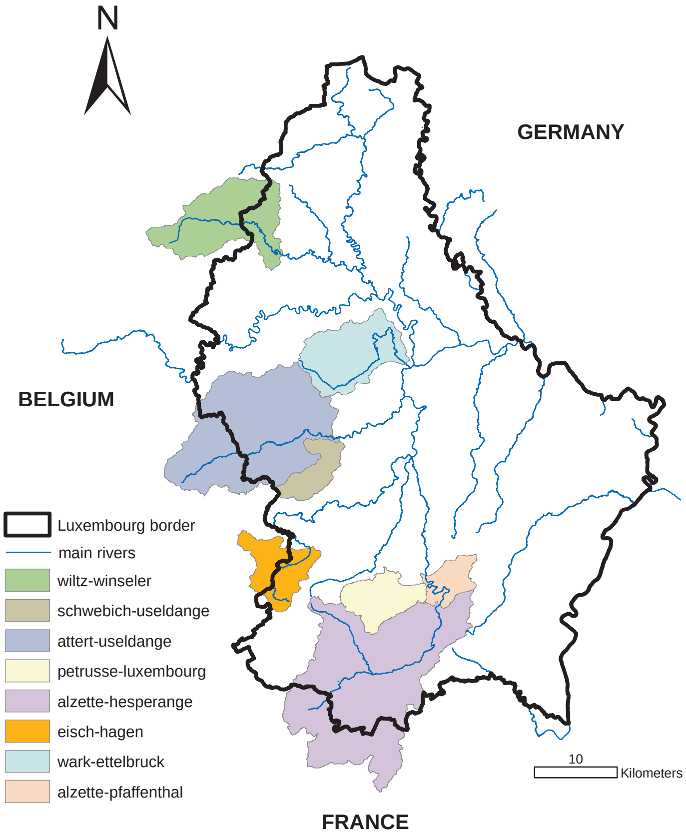

Fig. 1. Location of the subcatchments in the Grand-Duchy of Luxembourg.

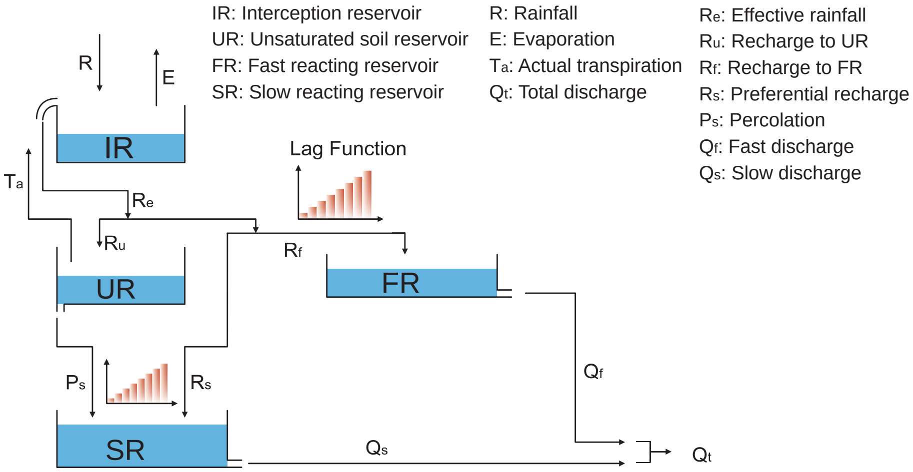

Fig. 2. Structure of the FLEX hydrological model.

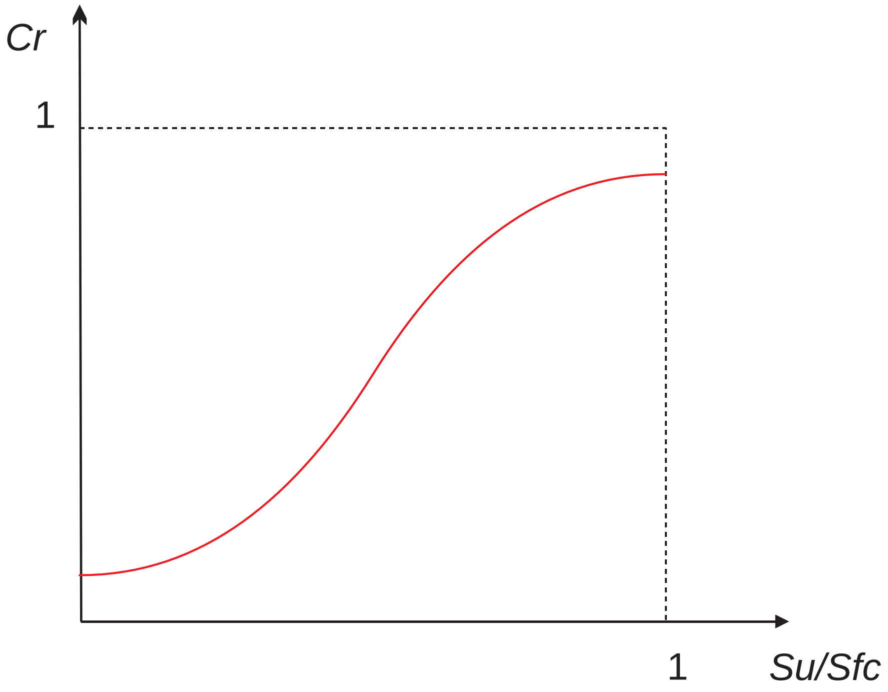

Fig. 3. C_r–S_u functional relationship.

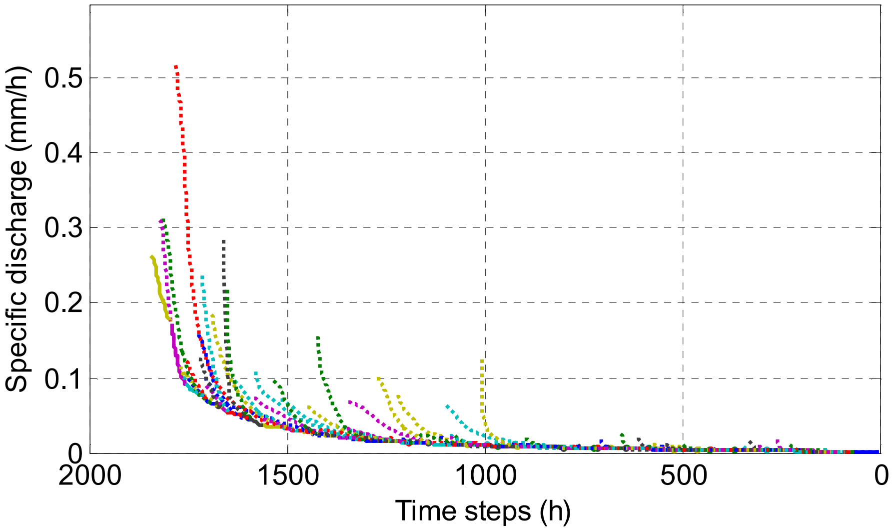

Fig. 4. Graphical representation of a Master Recession Curve for the Wark catchment.

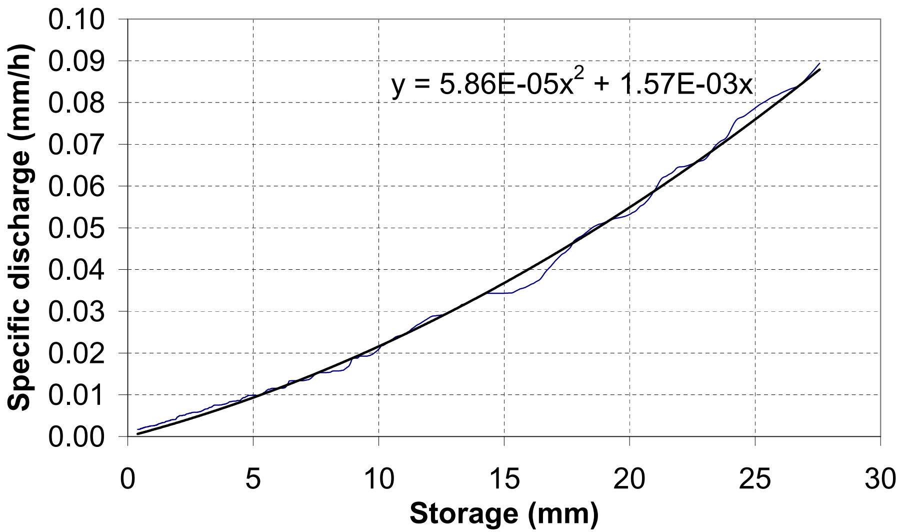

Fig. 5. Initial estimate of the storage-discharge relation.

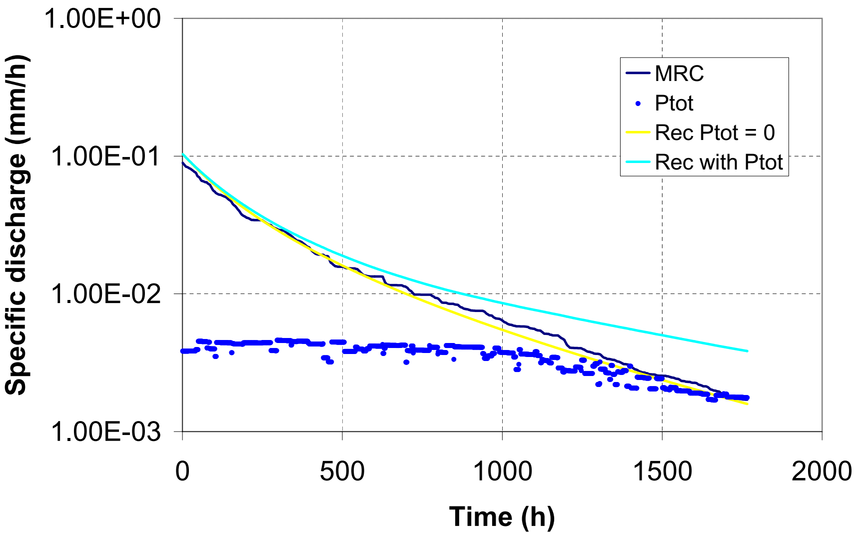

Fig. 6. Master recession curve, total exchange to *SR* (P_{tot}) and recession curves from SR in different recharge conditions.

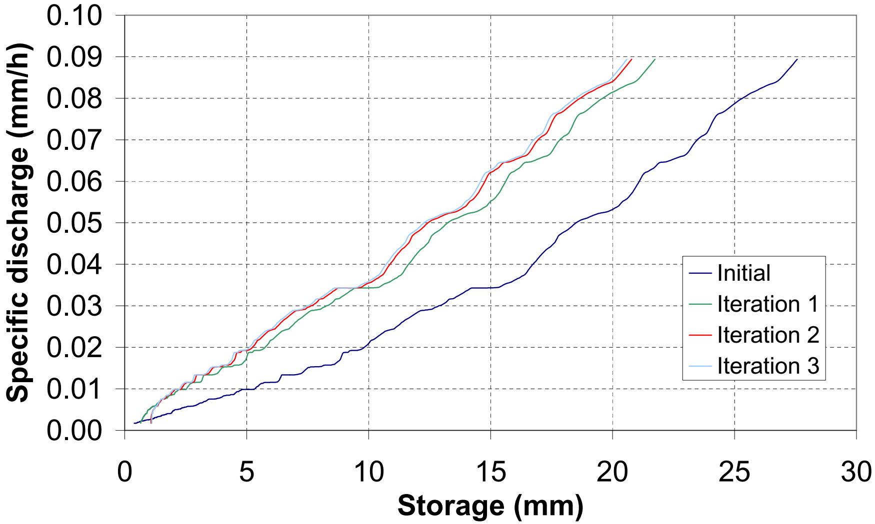

Fig. 7. Recalculation of the storage-discharge relation.

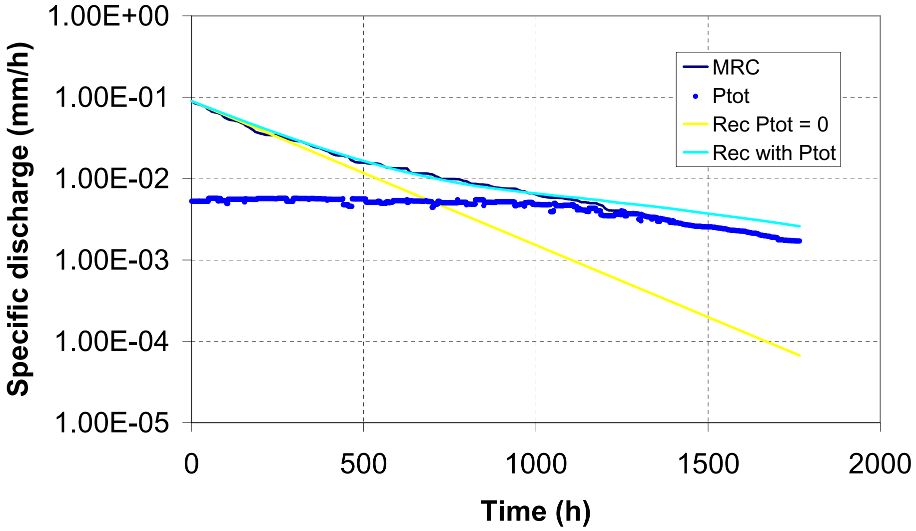

Fig. 8. Master recession curve, total exchange to *SR* (P_{tot}) and recession curves from *SR* in different recharge conditions.

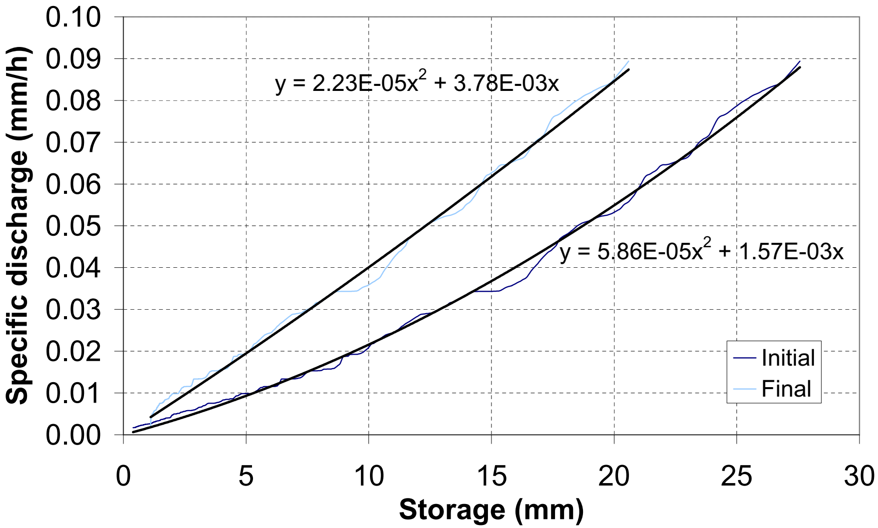

Fig. 9. Initial and final estimate of the storage-discharge relation.

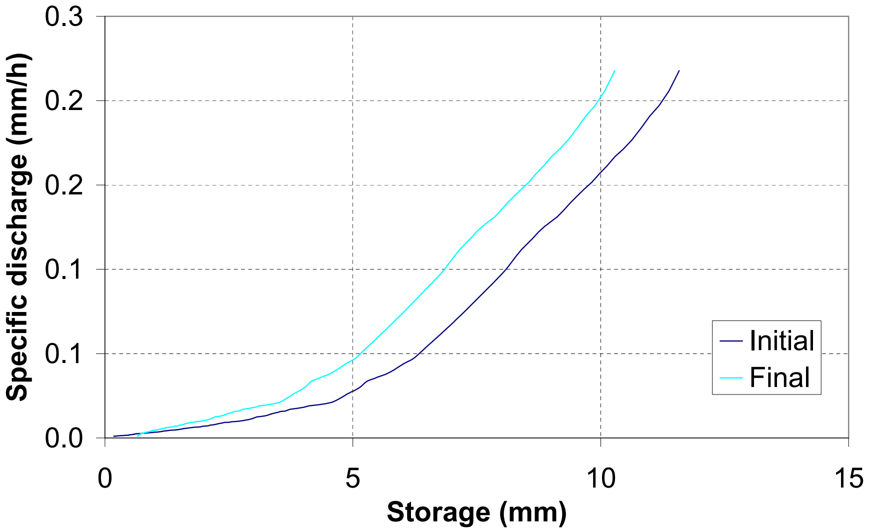

Fig. 10. Storage-discharge relation for the Petrusse catchment.

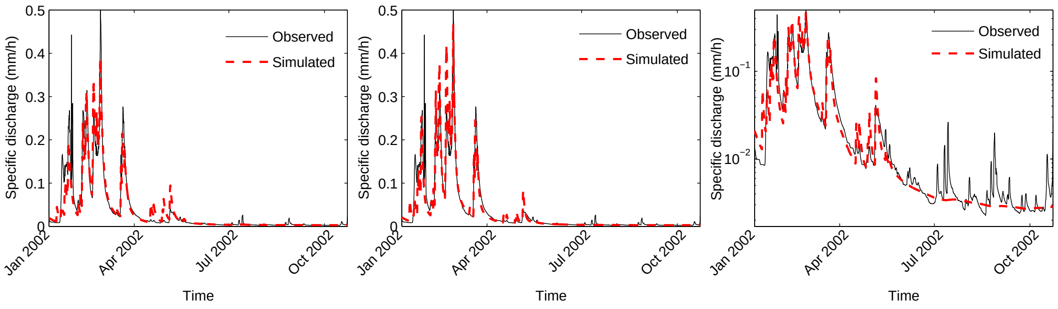

Fig. 11. Effect of recalibration of high-flows related parameters.