Incorporating experimentally derived streamflow contributions into model parameterization to improve discharge prediction

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Abstract. Environmental tracers have been used to separate streamflow components for many years. They allow to quantify
10 the contribution of water originating from different sources such as direct runoff from precipitation, subsurface stormflow or groundwater to total streamflow at variable flow conditions. Although previous studies have explored the value of incorporating experimentally derived fractions of event and pre-event water into hydrological models, a thorough analysis of the value of incorporating hydrograph separation derived information on multiple streamflow components at varying flow conditions into model parameter estimation has not yet been performed. This study explores the value of such information to
15 achieve more realistic simulations of catchment discharge. We use a modified version of the process-oriented HBV model that simulates catchment discharge through the interplay of hillslope, riparian zone discharge and groundwater discharge at a small forested catchment which is located in the mountainous north of South Korea subject to a monsoon season between June and August. Applying a Monte Carlo based parameter estimation scheme and the Kling Gupta efficiency (KGE) to compare discharge observations and simulations across two seasons (2013 & 2014), we show that the model is able to provide accurate
20 simulations of catchment discharge (KGE ≥ 0.8) but fails to provide robust predictions and realistic estimates of the contribution of the different streamflow components. Using a simple framework to incorporate experimental information on the contributions of hillslope, riparian zone and groundwater to total discharge during four sub-periods, we show that the precision of simulated streamflow components can be increased while remaining with accurate discharge simulations. We further show that the additional information increases the identifiability of all model parameters and results in more robust
25 predictions. Our study shows how tracer derived information on streamflow contributions can be used to improve the simulation and predictions of streamflow at the catchment scale without adding additional complexity to the model. The complementary use of temporally resolved observations of streamflow components and modelling provides a promising direction to improve discharge prediction by representing model internal dynamics more realistically.

1 Introduction

At many catchments, particularly in temperate regions, subsurface stormflow (SSF) is an important event-scale mechanism of streamflow generation (Bachmair and Weiler, 2011; Barthold and Woods, 2015; Blume et al., 2016; Chifflard et al., 2019). SSF often occurs at hillslopes with contrasting soil hydraulic properties within the soil profile favouring lateral flow rather

5   than vertical percolation of infiltrating waters or where rising groundwater levels reach more permeable layers of the soil ("transmissivity feedback mechanism", see Bishop et al., 1990). Previous work has shown that SSF can be an important component of runoff generation at the catchment scale (Zillgens et al., 2007), adding to flood generation (Markart et al., 2015), or nutrient and contaminant transport (Zhao et al., 2013). The experimental investigation of SSF requires intensive instrumentation, and therefore only few studies have attempted to directly measure SSF on natural hillslopes (Du et al., 2016;

10   Freer et al., 2002; Tromp-Van Meerveld and McDonnell, 2006; Woods and Rowe, 1996). If direct field observations of SSF are not possible, sampling and characterizing subsurface water using tracers (soil water, shallow groundwater) can be a way forward to evaluate the relevance of SSF for streamflow generation. The tracer signatures of different water source areas or flow pathways (also called end-members) are used to compute in a mass balance approach the potential relative contributions of the sampled water sources required to result in the observed tracer signals in streamflow. Other than early approaches that

15   split streamflow into event and pre-event water (Kendall et al., 2001; Sklash et al., 1979), these approaches rely on the assumption that streamflow is a mixture of distinct water sources within the catchment. This hydrograph separation technique and more advanced multivariate statistical tools for comprehensive data sets, such as the End Member Mixing Analysis employing a principal component analysis, have extensively been used in streamflow generation studies (Brown et al., 1999; Burns et al., 2001; Christophersen and Hooper, 1992; Inamdar et al., 2013). However, the initiation, pathways, residence times,

20   quantity, or spatial origin of SSF in various landscapes are still poorly understood. Due to this lack of a general understanding of the occurrence of and controls on SSF, only few modelling studies focus on the realistic simulation of SSF (Appels et al., 2015; Chifflard et al., 2019; Hopp and McDonnell, 2009).

Conceptual models lump together the spatial heterogeneity of hydrological properties of entire catchments or hydrotopes while still considering dominant hydrological processes (Wagener and Gupta, 2005). Different streamflow components and

25   catchment internal fluxes are usually represented by the outflows of simple or modified linear reservoirs: For instance the HBV model (Hydrologiska Byrans Vattenavdelning, Lindström et al., 1997; Seibert and Vis, 2012) represents the interplay between subsurface stormflow and groundwater by a shallow groundwater reservoir with two outlets. When below a predefined threshold, only one outlet provides discharge to the stream. But when exceeding the threshold, the more dynamic second outlet releases additional water, which is one way of representing the "fill and spill" dynamics of SSF observed by Tromp-Van

30   Meerveld and McDonnell (2006). A similar procedure is used in the TOPMODEL (Beven and Kirkby, 1979; Clark et al., 2008) or the Precipitation Runoff Modeling System (PRMS, Leavesley et al., 1983; Markstrom et al., 2015) that uses a threshold to initiate subsurface stormflow (referred to by "preferential flow" in the model's manual). Physically-based models usually discretize the catchment into a grid of rectangular or triangular cells and apply physical equations, e.g., Richard's

equation or the groundwater flow equations, on each of them individually. That way they provide spatially distributed information on the flow and storage behaviour of the simulated catchments. Similar to conceptual models, many physically based models consider to contributions of different streamflow components to total catchment discharge. For instance, the WaSiM-ETH model (Schulla and Jasper, 2007) considers subsurface stormflow by calculating interflow from hydraulic

5 conductivity, river density, soil moisture and the matric potential. The SWAT model (Neitsch et al., 2011) uses a kinematic storage model to consider interflow, or the LARSIM model (Bremicker, 2000) uses the saturation deficit of the soil and a lateral drainage parameter to calculate subsurface stormflow.

In order to represent SSF correctly within conceptual and physically based models, the model parameters controlling the initiation and rate of SSF have to be estimated. However, in most of the model applications, little information about SSF model

10 parameters is available and modellers have to rely on inverse parameter assessment approaches (Vrugt et al., 2008). Due to the limited information content of discharge (Wheater et al., 1986; Ye et al., 1997), the distinction of model internal lateral flow paths like surface runoff, SSF, groundwater, etc., remains uncertain (Seibert and McDonnell, 2002). Previous work already used field observations in addition to discharge to confine model parameters and simulated processes using, for instance, hydrochemical information (Hartmann et al., 2017; Kuczera and Mroczkowski, 1998) and water isotopes (Hartmann

15 et al., 2013; Son and Sivapalan, 2007; Sprenger et al., 2015). In a multi-objective approach, Seibert and McDonnell (2002) showed that the inclusion of groundwater observations and discontinuous observations of event water contributions derived from hydrograph separation allowed for an improved confinement of simulated processes. However, a detailed analysis of the usefulness of incorporating more detailed information of experimentally derived streamflow components is, to our knowledge, not yet available.

20 This study explores the value of experimentally derived streamflow components to identify the increase in accuracy of simulated streamflow components at the catchment scale. We use a modified version of the process-oriented HBV model and Monte Carlo based parameter estimation framework to (1) obtain acceptable simulations of total streamflow at the catchment outlet and (2) incorporate experimentally derived information on the contributions of the hillslope, riparian zone and groundwater to total streamflow into model parameter estimation. By iteratively adding this information to the parameter

25 estimation, we can quantify the impact of the additional data on parameter identifiability and on the uncertainty of discharge simulations during variable flow conditions. We apply our approach at a well-instrumented test site in the monsoonal mountainous north of South Korea during two consecutive seasons.

2 Test catchment: site characteristics, measurements and hydrograph separation results

Our test catchment is located in a mountainous area in the northeast of South Korea (N38.2051°, E128.1816°). The forested

30 headwater catchment has an area of ~16 ha, with elevations ranging from 368 to 682 m a.s.l. and a mean slope of 24° (Lee et al., 2016). Its soils consist mostly of cambisols with a loamy texture and an average thickness of 0.6 m. A deciduous stand dominates at elevations above 450 m (61% of the entire area), whereas lower elevations are dominated by a coniferous stand

(39% of the entire area). Precipitation data in daily resolution from a weather station of the Korea Meteorological Administration (station no. 594, located approx. 3 km northeast of the study site; https://www.kma.go.kr) was obtained for the years 2013 and 2014. In addition, monthly precipitation data from this station was available for the period 1997-2012. South Korea experiences the East Asian summer monsoon during the months June, July and August (JJA). Mean annual precipitation

5   was 1273 mm (1997-2014), with on average 60% of it occurring from June through August. In 2013, annual precipitation was 1313 mm (JJA: 897 mm), whereas 2014 was much drier with an annual precipitation of 699 mm (JJA: 364 mm).

Discharge was measured at the outlet of the catchment during 2013 and 2014 (Fig. 1). In 2013 among others, throughfall, streamflow at the catchment outlet, hillslope soil water (20 to 40 cm depth, sampled with suction lysimeters) and riparian zone soil water (20 to 40 cm depth, sampled with suction lysimeters) were sampled regularly between early June and mid-August

10   (for detailed information on methodology please refer to Payeur-Poirier, 2018). A range of geochemical tracers (calcium, magnesium, nitrate, sulphate), electrical conductivity EC and δ^2H were analysed in the water samples. These were used for a simple three-component two-tracer hydrograph separation. As overland flow was not observed during the field work and also direct channel interception was considered to be negligible, we defined three end members, i.e. three water sources potentially contributing to streamflow: hillslope soil water, riparian zone soil water, and groundwater (streamflow hydrochemical

15   signature before the onset of the monsoon, i.e. baseflow). The general procedure of hydrograph separation relies on several assumptions: (1) streamflow can be described as a linear mixture of the end members, (2) the end members have characteristic and differing tracer concentrations, i.e. typical signatures, (3) end member concentrations are time-invariant, and (4) tracers behave conservatively (Hooper et al., 1990). Various pairings of the six tracers were explored using bivariate plots, where the concentrations of two tracers in the end members and streamflow are plotted against each other. If streamflow can be well

20   described by a mixture of the three selected end members, streamflow concentrations will fall within the bounds of the triangle that is created by the tracer concentrations of the three end members. Mixing ratios between the three selected end members were calculated using mass balances for water and the two tracers:

25
$$1 = f_1 + f_2 + f_3$$
$$c_{s1} = f_1 c_{11} + f_2 c_{21} + f_3 c_{31} \tag{1}$$
$$c_{s2} = f_1 c_{12} + f_2 c_{22} + f_3 c_{32}$$

Where c_{sj} means concentration of tracer j in streamwater, c_{ij} is concentration of tracer j in end member i, and f_i is fractional contribution of end member i to streamflow. By rearranging these three equations, the three unknowns f_1, f_2 and f_3 can be

30   determined.

The analysis of the end member tracer concentrations revealed that end member concentrations varied over time, i.e. assumption (3) was not met. Based on the temporal behaviour of the end member concentrations, weekly precipitation amounts and the discharge response, we delineated four periods over the course of the sampling period, for which we calculated mean end member concentrations: baseflow (pre-monsoon), wet-up, main monsoon, and drying-up. In the following text, these

periods are called the "monsoon periods". We used these mean end member concentrations for calculating mixing ratios. By performing the hydrograph separation for individual periods, we tried to account for the time-variant behaviour of end member signatures (see for an early example Ogunkoya and Jenkins, 1993). The tracer pairs Mg/EC, NO₃/Mg and Ca/δ2H all resulted in very similar mixing ratios per monsoon period, and we report in Table 1 the mean of calculated mixing ratios from these

5   three pairings per monsoon period. Per our definition, pre-monsoon, i.e. baseflow, streamflow concentrations were used as proxy for groundwater; therefore, during the pre-monsoon period, groundwater constitutes 100% of streamflow. During the subsequent monsoon periods, however, the change in mixing ratios indicates that the relative contribution of water from the hillslopes and the riparian zones to streamflow increased markedly for the main monsoon and drying-up period.

Table 1: Relative contributions to streamflow (based on three-component hydrograph separation) of groundwater, hillslope soil
10   **water, and riparian zone soil water during baseflow (09.06.-22.06.2013), wet-up (23.06.-06.07.2013), main monsoon (07.07.-27.07.2013) and drying-up (28.07.-17.08.2013) of the 2013 monsoon season.**

Streamflow component	Baseflow	Wet-up	Main monsoon	Drying-up
Groundwater F_{GW} [%]	100	100	50	38
Hillslope soil water F_{SSF} [%]	0	0	40	47
Riparian zone soil water F_{RZ} [%]	0	0	10	15
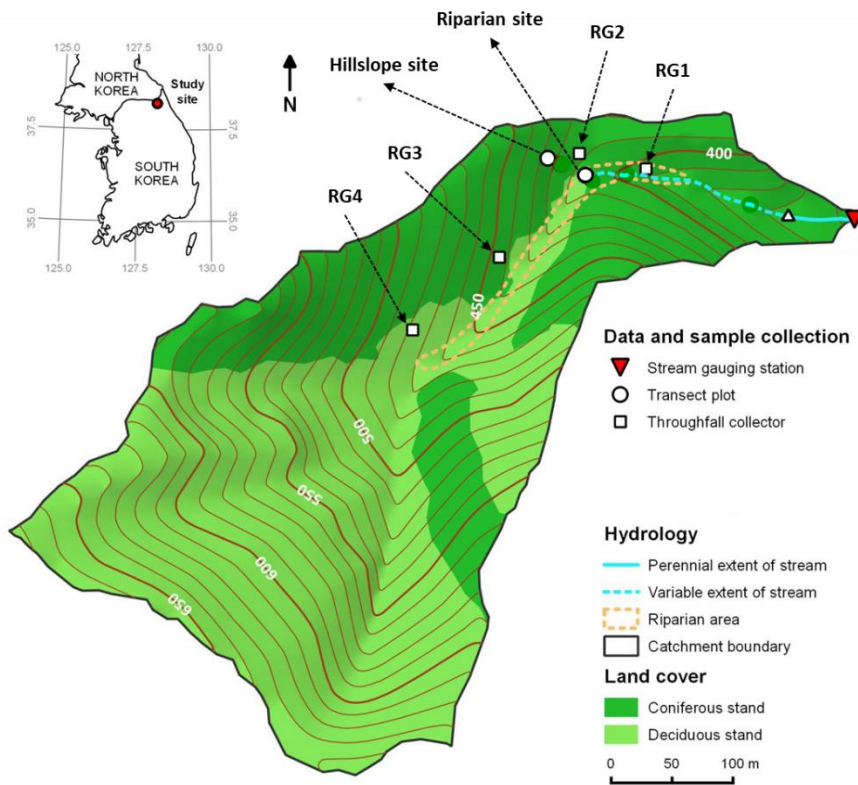
Figure 1: Location and detailed map of the test catchment and sampling setup.

3 Methods

We used a process-based lumped model to simulate the storage and flow dynamics of the hillslope, the riparian zone and the groundwater for different periods of the 2013 monsoon season by separate subroutines. We used a Monte Carlo approach to create 2,000,000 simulation time series, which we iteratively confined using performance criteria of discharge and the mixing

5   ratios estimated by tracer-based three component hydrograph separation (Table 1). At each step, we quantify the sensitivity of model parameters to learn about the information content of the discharge observations and hydrograph separation results considered in the confinement procedure. We finally compare the uncertainty of the simulated streamflow components with and without using the hydrograph separation results and, using independent discharge observations of the 2014 monsoon season, quantify how much the inclusion of experimentally derived streamflow components can reduce prediction uncertainty.

10   **3.1 The model**

We use a modified version of the HBV model (Beck et al., 2010; Seibert and Vis, 2012). The model was modified to include the riparian zone similar to Seibert et al. (2003) and simplified by removing the snow routine and considering only two reservoirs that simulate the contributions of the hillslope, the riparian zone and groundwater to total discharge with eight model parameters (Figure 2, Table 2). The first storage receives all precipitation [mm/d] and calculates actual evapotranspiration

15   [mm/d] from potential evaporation [mm/d] (Penman-Wendling approach, DVWK, 1996; Wendling et al., 1991) by multiplication with an evaporation factor f_{Evap} [-] $(0 \leq f_{Evap} \leq 1)$:

$$f_{Evap}(t) = \frac{V_S(t)}{F_C \cdot L_P} \tag{2}$$

with V_S [mm] as the soil storage at time t, F_C [mm] the field capacity, and L_P [-] as an evaporation shape factor. A wetness factor f_{Wet} derived from soil saturation and a shape factor β [-] determines the fraction of precipitation that percolates through

20   the soil:

$$f_{Wet}(t) = \left(\frac{V_S(t)}{F_C} \right)^{\beta} \tag{3}$$

The remaining part of precipitation $[1 - f_{wet}(t)]$ is added to the soil storage. Soil percolation is added to the water stored in reservoir one, $V_I(t)$ [mm], which is drained by groundwater discharge Q_{GW} [mm/d] and hillslope discharge (sometimes referred to by subsurface storm flow or interflow) Q_{HS} [mm/d] when a maximum groundwater storage U_{GW} [mm] is exceeded:

25
$$Q_{GW}(t) = \frac{V_I(t)}{K_{GW}} \tag{4}$$

$$Q_{HS}(t) = \begin{cases} \frac{V_1(t) - U_{GW}}{K_{HS}} & if \ V_1(t) \geq U_{GW} \\ 0 & if \ V_1(t) < U_{GW} \end{cases}$$

(5)

where K_{GW} [d] and K_{HS} [d] are the storage constant of the groundwater and the hillslope, respectively, and U_{GW} [mm] is the maximum groundwater storage. Hillslope discharge is fed into reservoir two, which represents the riparian zone until riparian zone storage $V_2(t)$ exceeds it maximum capacity U_{RZ} [mm]. Discharge of the riparian is therefore defined as

$$Q_{RZ}(t) = \begin{cases} \dfrac{V_2(t)}{K_{RZ}} & if\ V_2(t) < U_{RZ} \\[2ex] \dfrac{U_{RZ}}{K_{RZ}} & if\ V_2(t) = U_{RZ} \end{cases} \qquad (6)$$

5   Catchment discharge is obtained by summarizing over Q_{GW}, Q_{HS} and Q_{RZ} at each time t and rescaling them to [m³/s] using the catchment area (16 ha). Re-scaling the catchment discharge for each time step t, we can express each streamflow component in [%]. Similar to preceding work that compared simulated and tracer derived streamflow contributions (Robson et al., 1991, 1992), we can now compare the model's simulations to the results of the streamflow separation analysis (section 2).
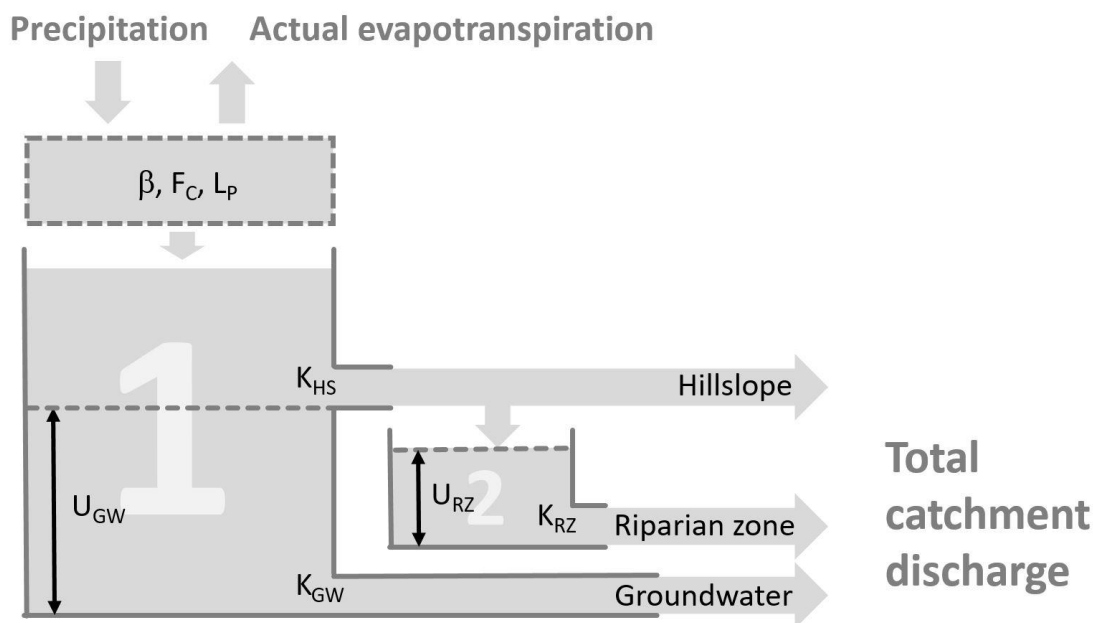
Figure 2: Structure of the modified HBV model. The three components hillslope, riparian zone and groundwater sum up to total catchment discharge.

The model operates at a daily temporal resolution to simulate the monsoon seasons of 2013 and 2014 after a warm-up period of 3.5 years. Precipitation data from a nearby meteorological station of the Korean Meteorological Administration (see section
15   2) and from a global product (Global Land Data Assimilation System GLDAS, Rodell et al., 2004), corrected with the observations from the local weather station, were used to complete the missing observations before the 2013 monsoon season and between the two monsoon seasons. Since reliable hydrograph separation results are only available for the 2013 monsoon

season, we use this year for model calibration, while we use the monsoon season of 2014, when only discharge observations are available, for the validation of the model.

3.2 Step-wise parameter estimation and quantification of information content of observations

Similar to the Generalized Likelihood Uncertainty Estimation (GLUE) framework (Beven and Binley, 1992), we use a "soft

5 rules" approach to estimate model parameters and their sensitivities that allows the consideration of different types of observations (Chang et al., 2020; Hartmann et al., 2017; Sarrazin et al., 2018). We apply a Monte Carlo parameter sampling to obtain 2,000,000 model realisations derived by uniform sampling of model parameters within their predefined ranges (Table 2). For each run, we calculate the model performance concerning observed catchment discharge by the Kling Gupta efficiency KGE_Q (Gupta et al., 2009), that indicates flawless simulations with a value of one and simulations worse than the simple

10 average of the observations with a value of -0.41 (Knoben et al., 2019), and the deviation of observed and simulation contributions of groundwater F_{GW} [%] and midslope discharge F_{HS} [%] over all four monsoon periods defined in Table 1. In a three-step procedure, we remove those model realisations that perform poorly against discharge or streamflow component observations with rather soft thresholds for F_{GW} and F_{HS} to account for the comparably large uncertainties of multi-component streamflow separation (Genereux, 1998).

1. We reduce the sample by discarding all simulations that perform badly in terms of observed total streamflow by removing all simulations with $KGE_Q < 0.8$.
2. We further reduce the sample be removing all simulations whose F_{HS} show more than 20% deviation compared to the hydrograph separation estimates.
20 3. We further reduce the sample be removing all simulations whose F_{GW} show more than 20% deviation compared to the hydrograph separation estimates. Since the contributions of the hillslope, groundwater and the riparian zone sum up to 100%, riparian zone contributions are implicitly considered in this last step.

To quantify the information content provided through adding more and more information along the three parameter

25 confinement steps, we quantify the strength of reduction of the initial sample of 2,000,000 and the change of the distribution of each model parameter at each individual step. If discharge observations or one of the hydrograph separation streamflow components has a high information content, a strong decrease of the initial sample and a substantial change of a large number of model parameters should be found.

3.3 Quantification of uncertainty of simulated model internal fluxes and discharge

30 We quantify simulation uncertainty of discharge by the mean and standard deviations of KGE_Q, obtained by using only observed discharge or both observed discharge and the hydrograph separation results for parameter confinement for the calibration period in 2013 and the validation period in 2014. Similarly, to quantify the simulation uncertainty of simulated

internal fluxes (hillslope discharge, groundwater discharge and riparian zone discharge), we compare their simulated means and standard deviations, that were obtained by using only observed discharge or by both observed discharge and the hydrograph separation results for parameter confinement, with the hydrograph separation derived streamflow components during the four time periods of the 2013 sampling period. We do the same for the 2014 monsoon season but since there are no reliable

5   hydrograph separation results available for this year, we only analyse the simulated mean and standard deviation of the simulated streamflow contributions for both calibrations. If the hydrograph separation derived from streamflow components provides new information for parameter estimation, it will result in a reduction of uncertainty of simulated fluxes and discharges in both years, and an increase of KGE_Q of the 2014 predictions should be found.

4 Results

10 **4.1 Step-wise parameter estimation and quantification of information content of observations**

When iteratively applying the three rules for parameter confinement, we observe a substantial decrease of the initial sample of 2,000,000 parameter sets (Figure 3). Extracting only those with $KGE_Q \geq 0.8$ reduces the sample to less than 10% (137,137 parameter sets left). Adding the observed streamflow components to the calibration procedure results in a further reduction of the sample. Discarding all parameter sets that deviate more than 20% from the observed hillslope contributions, results in 555

15 remaining parameter sets and in 29 parameter sets when the groundwater contributions (implicitly the riparian zone contributions, too) are finally added. Despite being only average values over the four sub-periods of the 2013 sampling period, the incorporation of the hydrograph separation derived streamflow contributions results in a reduction by more than three orders of magnitude, while the discharge observations, although using a high value of 0.8 of the KGE_Q criterion, only reduced the sample by slightly less than one order of magnitude.
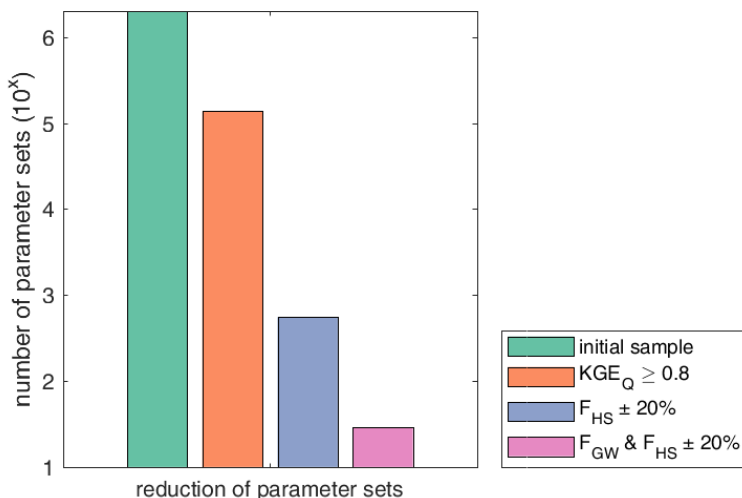
Figure 3: Iterative reduction of the initial sample of 2,00,000 parameter sets using the KGE$_Q$ and hydrograph-separation derived streamflow contributions for the individual years 2013 and 2014, as well as for both years together

The influence of the parameter confinement procedure using observed discharge and streamflow components is also visible

5   through the changes of the distribution of each of the parameters occurring at each of the confinement steps (Figure 4). When only discharge is considered in the first step of the confinements (KGE$_Q \geq 0.8$), some model parameter distributions shift away from the mean of the normalized range, e.g. L_P, K_{HS}, or K_{GW}, but only one of them, F_C, shows a confinement of its 25th and 75th percentile, which indicates a reduction of uncertainty. When the sample is further confined by the observed streamflow contributions of the hillslope, a few more parameters shift away from the mean, e.g. β and U_{GW}, but three more parameters,

10   K_{HS}, K_{GW} and K_{RZ}, show confined uncertainties. When finally adding the groundwater contributions (and implicitly the riparian zone contributions), all model parameters show a clear shift of their distributions away from the mean, for most of them going along with a reduced uncertainty indicated by narrowing 25th and 75th percentiles. We find the same results when calculating the mean and standard deviations of the model parameters for the confinement by discharge only and the confinement by discharge and the observed streamflow contributions (Table 2).

15   **Table 2: Parameters of the modified HBV model, description, units, and boundaries for parameter estimation (see below), and the model performances and simulated streamflow components for the four delineated monsoon periods (see Table 1) when confining the initial parameter sample by discharge only, and by discharge and observed streamflow contributions for the calibration in 2013 and the validation in 2014**

Parameter	Description	Unit	Lower boundary	Upper boundary	KGE$_Q \geq 0.8$	F$_{GW}$ & F$_{HS}$ ± 20%
β	Shape factor	[-]	1	10	5.6 ± 2.6	4.9 ± 2.6
F_C	Maximum storage in hillslope soil	[mm]	0	250	98.2 ± 58.2	54.5 ± 59.3
L_P	Threshold for reduction of evaporation	[-]	0.3	1	0.7 ± 0.2	0.7 ± 0.2
$log10\ K_{HS}$	Recession coefficient (hillslope)	[d-1]	-5	0	-1.4 ± 1.5	-0.3 ± 0.1
$log10\ K_{GW}$	Recession coefficient (groundwater)	[d-1]	-5	0	-1.6 ± 1.7	-1.6 ± 0.5
U_{GW}	Maximum groundwater storage	[mm]	0	250	114.6 ± 68.4	100 ± 74.6

$log10\ K_{RZ}$	Recession coefficient (riparian zone)	[d-1]	-5	0	-2.6 ± 1.5	-1.6 ± 0.7
U_{RZ}	Maximum riparian zone storage)	[mm]	0	100	48.2 ± 28.9	36.9 ± 22.9
2013						
KGE_Q	model performance concerning discharge	[-]	∞	1	0.84 ± 0.02	0.82 ± 0.02
$F_{GW,BF}$	simulated groundwater contribution during baseflow	[-]	0	1	0.74 ± 0.35	0.97 ± 0.06
$F_{GW,WU}$	simulated groundwater contribution during wet-up	[-]	0	1	0.74 ± 0.38	0.99 ± 0.03
$F_{GW,,MM}$	simulated groundwater contribution during main monsoon	[-]	0	1	0.59 ± 0.46	0.36 ± 0.03
$F_{GW,DU}$	simulated groundwater contribution during drying-up	[-]	0	1	0.61 ± 0.45	0.46 ± 0.08
$F_{HS,BF}$	simulated hillslope contribution during baseflow	[-]	0	1	0.01 ± 0.07	0.00 ± 0.00
$F_{HS,WU}$	simulated hillslope contribution during wet-up	[-]	0	1	0.11 ± 0.28	0.00 ± 0.00
$F_{HS,MM}$	simulated hillslope contribution during main monsoon	[-]	0	1	0.33 ± 0.42	0.57 ± 0.03
$F_{HS,DU}$	simulated hillslope contribution during drying-up	[-]	0	1	0.27 ± 0.39	0.32 ± 0.04
$F_{RZ,BF}$	simulated riparian contribution during baseflow	[-]	0	1	0.25 ± 0.34	0.03 ± 0.06
$F_{RZ,WU}$	simulated riparian contribution during wet-up	[-]	0	1	0.14 ± 0.28	0.01 ± 0.03
$F_{RZ,MM}$	simulated riparian contribution during main monsoon	[-]	0	1	0.08 ± 0.2	0.07 ± 0.03
$F_{RZ,DU}$	simulated riparian contribution during drying-up	[-]	0	1	0.11 ± 0.26	0.21 ± 0.09
2014						
KGE_Q	model performance concerning discharge	[-]	∞	1	-0.98 ± 1.54	0.02 ± 0.39
$F_{GW,MS}$	simulated groundwater contribution monsoon season*	[-]	0	1	0.75 ± 0.28	0.87 ± 0.09
$F_{HS,MS}$	simulated hillslope contribution during monsoon season*	[-]	0	1	0.04 ± 0.1	0.02 ± 0.01
$F_{RZ,MS}$	simulated riparian contribution monsoon season*	[-]	0	1	0.21 ± 0.25	0.11 ± 0.09

* from 01.04.2014 to 30.09.2014 (same as in Figure 5h)
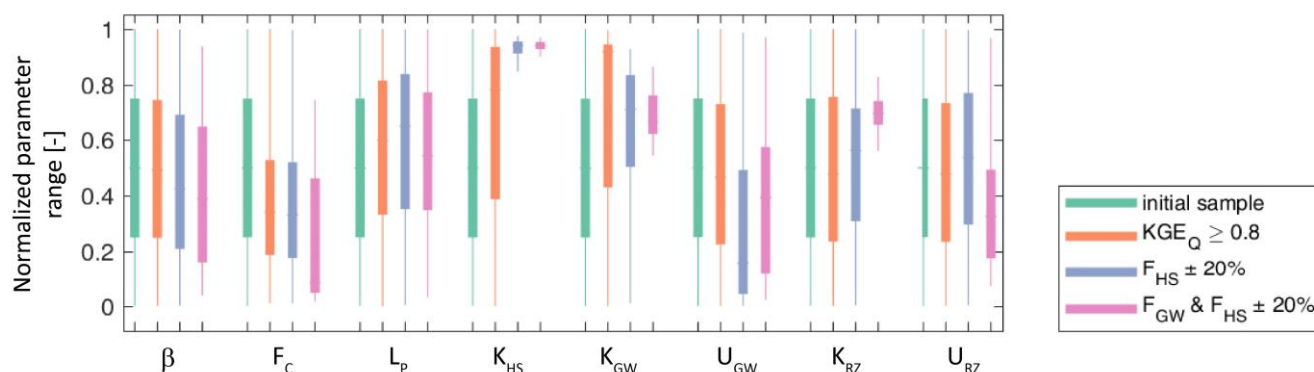
Figure 4: Initial parameter distribution and their modification along the three parameter estimation steps for the individual years 2013 and 2014, as well as for both years together. Boxes indicate the range between the 25th and 75th percentile, lower and upper whiskers show the 5th and 95th percentile, respectively.

4.2 Quantification of uncertainty of simulated model internal fluxes and discharge

Using only $KGE_Q \geq 0.8$ to confine the parameter sample, an average KGE_Q of 0.84 with a relatively low standard deviation of 0.02 is found for the calibration period in 2013 (Table 2), which also results in an acceptable visual agreement between simulations and observations (Figure 5g). Adding the observed streamflow contributions to the parameter confinement results in a similar mean KGE_Q (0.82), standard deviation (0.02), and visual agreement. However, when looking at the simulated streamflow contributions of the calibration by discharge only, we find that the standard deviations are large compared to the mean simulated contributions of groundwater, hillslope discharge and riparian zone discharge across all four monsoon periods (Table 2). Visualizing the entire range of their uncertainties (Figure 5a,c,e), we can see that simulated groundwater and riparian

zone contribution could range from 0% to 100%. The same is true for the hillslope contributions during wet-up, main monsoon and drying up. Only during drier periods, hillslope contributions to discharge are limited and sometimes fall down to 0%. Adding the observed streamflow contributions to the parameter confinement reduces the simulation uncertainty of all three streamflow components for the four monsoon periods in 2013 as indicated by their strongly reduced standard deviations in

5 Table 2 and by the narrower ranges around the observations of their simulations in Figure 5a,c,e. The strong dominance of the groundwater streamflow component during the baseflow and wet-up periods is well represented, as well as the onset of hillslope discharge during the main monsoon and the drying period, when the contributions of the riparian zone to streamflow gradually increase. The simulations also indicate that hillslope discharge mostly replaces groundwater in the main monsoon and the drying up, while before and after the monsoons season, streamflow is comprised by an interplay of groundwater and

10 riparian zone discharge. The comparison of simulations and observations also indicates that strong variations of streamflow components occur even within the monsoon periods, especially during the main monsoon and the drying-up (Figure 5a,c,e).
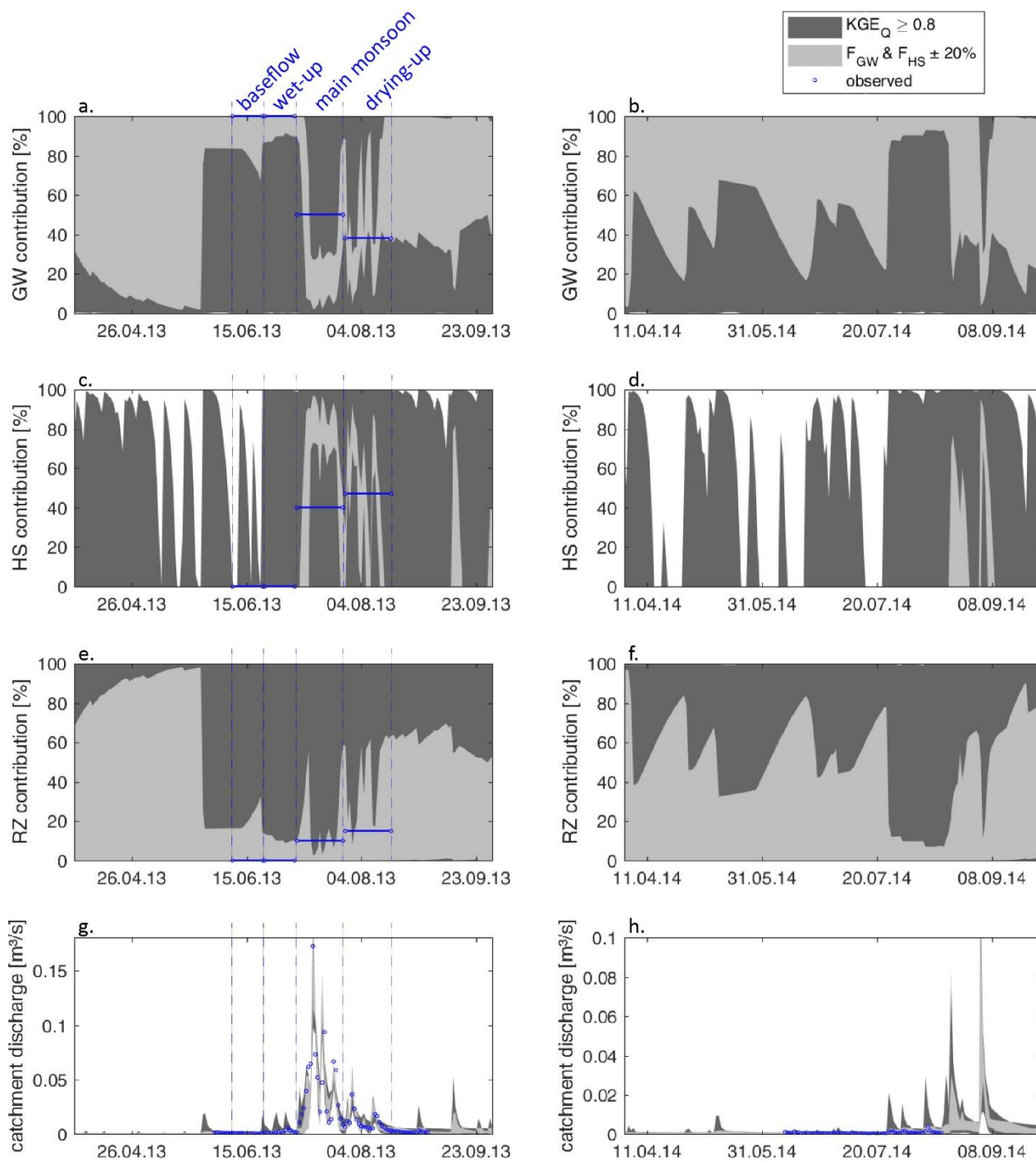
Figure 5: Simulated time series of groundwater discharge, subsurface stormflow, riparian zone discharge, and total catchment discharge (bottom to top) by using discharge (KGE$_Q$) only and by using F$_{SSF}$ and F$_{GW}$ during both years for parameter estimation.

During the validation in 2014, simulation performance of discharge decreases for both calibration steps, including discharge observations only and including observed discharge and streamflow components (Table 2). Using only discharge observations, a very poor simulation quality (KGEQ=-0.98) is found with a standard deviation of 1.54 indicating a very high simulation uncertainty. When using both, discharge and streamflow components for calibration, a much better performance is found

5 (KGEQ=0.02), which is well above the KGE that would be obtained when using just the average observations to predict discharge (-0.41) and which has a much smaller simulation uncertainty indicated by a standard deviation of 0.09, which is confirmed when comparing simulated and observed time series (Figure 5h). Although there are no observations of the streamflow components available for the validation year 2014, we can still see that the simulation uncertainty of all three components indicated by their standard deviations is generally high over the whole simulation period when only discharge is

10 used for calibration and reduced by more than a third when the stream contributions are considered in the calibration (Table 2). Similar to the calibration year 2013, we see that the interplay between groundwater and the riparian zone is much better defined and that the short but pronounced initiation of hillslope discharge is much better represented when both observed discharge and stream flow components are used for calibrations (Figure 5b,d,f).

5 Discussion

5.1 Realism of model simulations

We use a simple approach to incorporate streamflow contributions derived from environmental tracers into our simulation approach that compares simulated streamflow contributions and tracer-derived streamflow contributions instead of simulating tracer transport directly. That way, no additional uncertainty was introduced due to additional model parameters to consider transport (Birkel and Soulsby, 2015). Despite its simple structure, the model easily achieves performances of KGE $\geq$ 0.8 with

20 more than 130,000 parameter sets (out of initially 2,000,000, Figure 2) indicating adequateness of its structure for simulating the hydrology of our small forested mountainous catchment. Such good performance could be expected since similar models like the HBV model or similar modifications of the HBV model performed already well at similar landscapes (Chen et al., 2018; Seibert et al., 2003; Uhlenbrook et al., 1999). Including the observed streamflow contributions results in a further substantial reduction of the initial parameter sample to 29 parameter sets and in a slight decrease of overall discharge simulation

25 performance. Such further reduction of the parameter sample is due to the increased difficulty to simulate adequately and simultaneously both discharge and streamflow contributions and was already found in previous studies that investigated the influence of additional information in a GLUE-like approach (Hartmann et al., 2017; Mudarra et al., 2019).

Likewise, a decrease of simulation uncertainty concerning discharge going along with incorporating additional information into parameter estimation has already been observed (Kuczera and Mroczkowski, 1998; Seibert and McDonnell, 2002; Son

30 and Sivapalan, 2007). This mostly went along with an increased identifiability of model parameters and prediction skill, which is also found in this study. Using only discharge for model parametrization, a mean KGE of -0.98 in the validation year of 2014 is found (Table 2). The parameter sets obtained from using both discharge and observed streamflow contributions result

in a mean KGE of 0.02. Compared to the performances of KGE ≥ 0.8 that we obtained during the calibration in year 2013, this appears to be a strong decrease but it is substantially better than using the mean of discharge observations for prediction (that would result in KGE=-0.41; Knoben et al., 2019). Also, while the discharge observations in the calibration year 2013 cover the entire stream response to the monsoon season (maximum observed discharge > 0.15 m³/s, Figure 5), the validation data set

5   stops before the onset of the late and weak monsoon events in late August that produced increased discharge observations (observed discharges < 0.004 m³/s, Figure 5). Hence, the decrease of performance can also partially be explained by the challenge of predicting low flows with a calibration that covers the entire variability of streamflow (Nicolle et al., 2014).

5.2 Identification of model parameters and processes

The acceptable multi-variate performance of the model in the calibration period and the still acceptable performance found in

10   the validation period gives us reason to believe that our approach provides interpretable results. Incorporating observed streamflow contributions into parameter estimation results in reduced parameter uncertainty for all model parameters except for L_P (remains the same) compared to the parameter estimation using discharge only (Table 2). The iterative inclusion of observations into the parameter estimation procedure allows assessing the information content of each data type. When discharge only is considered, changes of the distributions of parameters L_P, K_{HS}, or K_{GW}, and F_C change (Figure 4), confirming

15   the well-known fact that only four to six model parameters can be identified when calibrating a model with discharge observations only (Jakeman and Hornberger, 1993; Wheater et al., 1986; Ye et al., 1997). When the experimental information of the contributions of the hillslope subsurface flow to streamflow is added, more parameters change their distributions indicating that additional information is added to the parameter estimation. We can see that this is most pronounced for K_{HS}, which controls the discharge dynamics of the hillslope, and K_{GW} and U_{GW} that indirectly control hillslope discharge by

20   triggering it after saturation of the groundwater storage (Figure 2). Adding the observed streamflow contributions of groundwater (and implicitly information about the riparian zone contributions as all three together sum up to 1), we see a further increase of sensitivity for K_{GW}, which is indicated by a further narrowing of its 25th and 75th percentile. Most prominently, K_{RZ} and U_{RZ} show substantial confinement indicating the new information about streamflow contributions added more information about riparian zone and groundwater dynamics.

25   Previous work with a model that simulated discharge and solute transport already showed that added information through environmental tracers can be linked to their origin in the hydrological system and respective model parameters (Hartmann et al., 2017). Our results indicate that even without the explicit inclusion of solute transport in the model, similar linkages between observations of streamflow contributions and model parameters that control the dynamics of their origin, hillslope, groundwater or riparian zone, could be found. These relationships are plausible and can be regarded as validation of the realism

30   of the model (Hartmann et al., 2013). By including discharge and observed streamflow components into parameter estimation without adding more complexity to the model, we achieve desirable levels of model parameter identifiability (all nine parameters) and prediction uncertainty (Birkel and Soulsby, 2015). The resulting parameters express the effective properties of our test catchment with thin soil (F_C= 54.5 mm ± 59.3 mm) and fast percolation of water towards the hillslope and

groundwater storages through a high value of β (4.9 ± 2.6). The value of L_P (0.7 ± 0.2) indicates that plant water uptake through forest cover is efficient even below saturation of the soil. The groundwater storage can store more than double of the soil while the riparian zone storage is about 15 mm smaller (Table 2). With around 0.5 d^{-1}, K_{HS} indicates fast hillslope dynamics after initiation, while with both at around 0.025 d^{-1}, K_{GW} and K_{RZ} are reacting slowly. The scales of the three parameters are

5   comparable to the parameters identified by Uhlenbrook et al. (1998), who found 0.1 − 0.35 d^{-1} and 0.02 − 0.05 d^{-1} for their simulated interflow and groundwater dynamics, respectively.

5.3 Benefits of including observed streamflow contributions for streamflow prediction

The uncertainty of the simulated streamflow contributions obtained by discharge during the same period show considerable uncertainty allowing for contributions of groundwater and the riparian zone from 0% - 100% throughout the entire simulation

10   period of 2013 (Figure 5ac) despite high performance in simulating discharge (Figure 5g, Table 2). Just for the hillslope contributions, the calibration by discharge only indicates possible contributions <100% during the baseflow period but shows the same uncertainty as the simulated groundwater and riparian zone contributions when the wet-up begins (Figure 5e). This strong uncertainty of the three simulated streamflow contributions despite high discharge simulation performance is a text book example of the equifinality problem (Beven, 2006; Perrin et al., 2001) that is known to result in poor prediction

15   performance as we also found in this study when using discharge for parameter estimation only. With the observed streamflow contributions considered in the calibration, the simulated time series of all three contributions, groundwater, hillslope and riparian zone, become more distinguishable especially during the main monsoon and the drying up period of the 2013 monsoon (Figure 5ace). We clearly see that the simulated groundwater contribution dominates discharge in the baseflow and wet-up periods following the observed contribution of groundwater. At the same time, the riparian zone contributions confine

20   themselves to their observed values close to 0%. During the main monsoon and the drying-up, the observed contributions of the hillslope are -on average- enveloped by the model simulations resulting in a substantial decrease of the groundwater contributions.

Strongly different model internal behaviour that results in almost the same discharge performance was also observed by Seibert and McDonnell (2002) who showed with a similar model that two completely different model setups can produce very similar

25   discharge simulation performance. Among different types of hard and soft data, they also showed the value of observed streamflow contributions for reducing model parameter uncertainty but only focusing on two streamflow components (new water and old water) at peak discharge for six separate rainfall runoff events (McDonnell et al., 1991). In our study, we distinguish three different streamflow components temporally disaggregated over four periods that resulted in parameter uncertainty reductions that could be attributed to the respective flow and storage processes at their origin (subsection 5.2). In

30   addition, using the monsoon year of 2014, we can show the discharge prediction performance of the model increased and simulation uncertainty decreased when the streamflow contributions are considered during parameter estimation (Figure 5h, Table 2). This is due to the improved representation of the three flow components in the model that indicate, likewise to the monsoon period in 2013, that the model could have over-estimated the contribution of the riparian zone and under-estimated

the contributions of groundwater, as well as it could have miss-predicted the onset and ceasing of the hillslope contributions to discharge. Such decrease of predictive uncertainty was also revealed in other studies (Hartmann et al., 2017; Son and Sivapalan, 2007) but, to our knowledge, it has not yet been achieved using more than two experimentally separated streamflow components and not yet without accepting additional uncertainty through the incorporation of transport routines into the model.

5 ## 6 Conclusions

The value of environmental tracers in improving the realism and prediction skills of hydrological models has been tested and proved in many previous studies. However, few studies were able to include them without adding more complexity to their models due to the conclusion of transport routines. Our study shows that, by directly comparing simulated and experimentally derived streamflow contributions, information derived from environmental tracers can be considered without adding transport

10 routines to our model. Considering the contribution of three streamflow components, namely the hillslope, the riparian zone and groundwater, at four separate periods during a strong change of hydrological boundary conditions, we provide strong indication that it is worth considering the temporal dynamics of components that express more than just pre-event and event water in the model. Including this information in our stepwise parameter estimation procedure, we obtain increased parameter sensitivities and und decreased simulation uncertainty in the validation period compared to using discharge only for calibration.

15 Incorporating the contributions of different components iteratively, we can show that they increase the identifiability of parameters related to the dynamics of their origin (e.g., the hillslope flow and storage dynamics when hillslope contributions to streamflow are considered). Considering all three observed streamflow components, we can identify all nine model parameters compared to just five parameters when using discharge only for calibration. Consequently, the uncertainty of predicted streamflow in 2014 decreases along with an increased precision of predicted streamflow components.

20 Our study adds to the large body of preceding work that provides evidence for the usefulness of incorporating auxiliary data into model calibration. In particular, it shows that the full potential of incorporating streamflow contributions obtained by environmental tracers has not yet been explored. On the one hand, including estimated streamflow contributions from multiple sources (not just event and pre-event water) allows enhanced improvement of the simulation of model internal processes, especially those that are seldom monitored such as hillslope contributions through subsurface stormflow (Chifflard et al.,

25 2019). On the other hand, considering the dynamics of those streamflow contributions over time provides a more thorough distinction between realistic and unrealistic parameters combinations. We see that among the four periods that we considered, the observations for the baseflow and wet-up periods are well enveloped by the simulations. But the temporal resolution of observed streamflow contributions during the main monsoon and the drying-up period seem to be too coarse as the simulations show much higher temporal variability (while their average seems to follow the observed contributions). Hence, further efforts

30 may involve the monitoring and integration into the model of streamflow components at a higher temporal resolution. Furthermore, separating contributions of streamflow components of different origin, our approach might be suitable for parameterization of hillslope processes in more complex and spatially distributed models (Fan et al., 2019).

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8 Code/Data availability

Data and model code will be published at https://github.com/KarstHub when the paper is accepted.

9 Author contribution

AH designed and implemented the modelling part and drafted large parts of the paper. JLPP collected the experimental data. LH applied the hydrograph separation and drafted the study site description. All authors contributed in improving and finalizing the manuscript.

10 Competing interests

There are no competing interests.

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