

Using expert knowledge to increase realism in environmental system models can dramatically reduce the need for calibration

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Abstract

Conceptual environmental system models, such as rainfall runoff models, generally rely on calibration for parameter identification. Increasing complexity of this type of models for better representation of hydrological process heterogeneity typically makes parameter identification more difficult. Although various, potentially valuable, approaches for better parameter identification were developed in the past, strategies to impose general conceptual understanding of how a catchment works into the process of parameter identification of a conceptual model has still not been fully explored. In this study we assess the effect of imposing semi-quantitative, relational inequality constraints, based on expert-knowledge, for model development and parameter selection, efficiently exploiting the complexity of a semi-distributed model formulation. Making use of a topography driven rainfall-runoff modeling (FLEX-TOPO) approach, a catchment was delineated into three functional units, i.e. wetland, hillslope and plateau. Ranging from simplicity to complexity, three model set-ups, FLEX^A, FLEX^B and FLEX^C have been developed based on these functional units. While FLEX^A is a lumped representation of the study catchment, the semi-distributed formulations FLEX^B and FLEX^C introduce increasingly more complexity by distinguishing 2 and 3 functional units, respectively. In spite of increased complexity, FLEX^B and FLEX^C allow modelers to compare parameters as well as states and fluxes of their different functional units to each other, allowing the formulation of constraints that limit the feasible parameter space. It was shown that by allowing for more landscape-related process heterogeneity in a model, e.g. FLEX^C, the performance increases even without traditional calibration. The additional introduction of relational constraints further improved the performance of these models.

1- Introduction:

Lumped conceptual and distributed physically based models are the two endpoints of the modeling spectrum, ranging from simplicity to complexity, which here is defined as the number of model parameters. The two modeling strategies are characterized by their very own advantages and limitations. In hydrology, physically based models are typically applied under the assumptions that (a) the spatial resolution and the complexity of the model are warranted by the available data, and (b) the catchment response is a mere aggregation of small scale processes. However, these two fundamental assumptions are violated in many cases. As a result, not only the predictive power but also the hydrological insights that these models provide is limited (e.g. Beven, 1989, 2001; Grayson et al., 1992, Blöschl, 2001; Pomeroy et al., 2007; Sivapalan, 2006; McDonnell et al., 2007; Hrachowitz et al., 2013b).

In contrast, lumped conceptual models require less data for identifying model parameters. This advantage comes at the expense of considerable limitations. Representing system integrated processes, model structures and parameters are not directly linked to observable

1 quantities. Their estimation therefore strongly relies on calibration. To limit parameter
2 identifiability issues arising from calibration, these models are often oversimplified
3 abstractions of the system. If inadequately tested they may act as “mathematical marionettes”
4 (Kirchner, 2006), frequently resulting in good calibration performance. They may outperform
5 more complex distributed models (e.g. Refsgaard and Knudsen 1996; Ajami et al., 2004;
6 Reed et al., 2004), but they often fail to provide realistic representations of the underlying
7 processes, leading to limited predictive power (e.g. Freer et al., 2003; Seibert, 2003; Kirchner,
8 2006; Beven, 2006; Kling and Gupta, 2009; Andréassian et al., 2012; Euser et al., 2013;
9 Gharari et al., 2013).

10 Various strategies have been suggested in the past to allow for increased model complexity
11 and to thereby improve the physical realism of conceptual models. These strategies included
12 the attempt to incorporate different data sources in the parameter estimation process, such as
13 ground- and soil water dynamics (e.g. Seibert and McDonnell, 2002; Freer et al., 2004;
14 Fenicia et al., 2008b; Matgen et al., 2012; Sutanudjaja et al., 2013), remotely sensed
15 evaporation (e.g. Winsemius et al., 2008), snow dynamics (e.g. Parajka and Blöschl, 2008) or
16 tracer data (e.g. Vache and McDonnell, 2006; Dunn et al., 2008; Son and Sivapalan, 2007;
17 Birkel et al., 2011; Hrachowitz et al., 2013a). Alternatively, it was tried to extract more
18 information from available data, for example through the development of signatures
19 representing different aspects of the data (e.g. Gupta et al. 1998, 2008; Boyle et al., 2000,
20 2001; Madsen 2000; Fenicia et al., 2006; Rouhani et al., 2007; Khu et al., 2008; Winsemius et
21 al., 2009; Bulygina and Gupta, 2010; McMillan et al., 2011, Clark et al., 2011; Euser et al.,
22 2013; He et al., 2014; Hrachowitz et al., 2014).

23 Traditionally, parameter estimation of conceptual models relied on the availability of
24 calibration data, which, however, are frequently not available for the time period or the spatio-
25 temporal resolution of interest. A wide range of regionalization techniques for model
26 parameters and hydrological signatures were thus developed to avoid calibration in such data
27 scarce environments (e.g. Bardossy, 2007; Yadav et al., 2007; Perrin et al., 2008; Zhang et al.,
28 2008; Kling and Gupta, 2009; Samaniego et al., 2010; Kumar et al., 2010; Wagener and
29 Montanari, 2011; Kapangaziwiri et al., 2012, Viglione et al., 2013). However, it was for a
30 long time considered to be challenging to identify suitable functional relationships between
31 catchment characteristics and model parameters (e.g. Merz and Blöschl, 2004; Kling and
32 Gupta, 2009). Only recently, Kumar et al. (2010, 2013a) showed that making use of multi-
33 scale parameter regionalization (MPR) can yield global parameters which perform
34 consistently over different catchment scales. In a further study they successfully transferred
35 parameters obtained by the MPR technique to ungauged catchments in Germany and the USA
36 (Kumar et al., 2013b).

37 Related to the above discussed difficulties with parameterization, the frequent lack of
38 sufficient processes heterogeneity, i.e. complexity, in conceptual models introduces further
39 limitations to the degree of realism in these models. The concept of hydrological response
40 units (HRU) can be exploited as a strategy for an efficient tradeoff between model simplicity,
41 required for adequate parameter identifiability, and a sufficient degree of processes
42 heterogeneity. HRUs are units within a catchment, characterized by a different hydrological
43 function and can be represented by different model structures or parameters. In most cases
44 HRUs are defined based on soil types, land cover and other physical catchment characteristics
45 (e.g. Knudsen et al., 1986; Flügel, 1995; Grayson and Blöschl, 2000; Krcho, 2001; Winter,
46 2001; Scherrer and Naef, 2003; Uhlenbrook et al., 2004; Wolock et al., 2004; Pomeroy et al.,
47 2007; Scherrer et al., 2007; Schmockler-Fackel et al., 2007; Efstratiadis et al., 2008;
48 Lindström et al., 2010; Nalbantis et al., 2011; Kumar et al., 2010).

49 A wide range of studies also points towards the potential value of using topographical indices,
50 which are readily available from digital elevation models (DEM) to account for process

1 heterogeneity (e.g. McGlynn and McDonnell, 2003; Seibert et al., 2003; McGuire et al., 2005;
2 Hrachowitz et al., 2009; Jensco et al., 2009; Detty and McGuire, 2010; Gascuel-Oudoux et al.,
3 2010). As standard metrics of landscape organization, such as absolute elevation, slope or
4 curvature, as used in the catena concept (Milne, 1935; Park and Van de Giesen, 2004), are
5 often not strong enough descriptors to infer hydrological function, alternative concepts were
6 sought. The development of derived metrics such as the *Topographic Wetness Index* (Beven
7 and Kirkby, 1979) facilitated an important step forward, being at the core of TOPMODEL
8 (e.g. Beven and Kirkby, 1979; Beven and Freer, 2001b), which has proven to be a valuable
9 approach in specific environmental settings meeting the assumptions of the model. A different
10 descriptor allowing a potentially more generally applicable and hydrologically meaningful
11 landscape classification has recently been suggested by Rennó et al. (2008): the *Height Above*
12 *the Nearest Drainage* (HAND). Nobre et al. (2011) showed the hydrological relevance of
13 HAND by investigating long term groundwater behavior and land use.

14 Explicitly invoking the co-evolution of topography, vegetation and hydrology, Savenije
15 (2010) argued that catchments, as self-organizing systems, need to fulfill the contrasting
16 hydrological functions of efficient drainage and sufficient water storage to allow, in a
17 feedback process, topography and vegetation to develop the way they did. These distinct
18 hydrological functions can be associated with different landscape elements or HRUs as
19 defined by HAND and slope, such that each HRU is represented by a model structure best
20 representing its function in the ecosystem (cf. Savenije, 2010).

21 While HAND-based landscape classification can potentially show a way forward, it does not
22 solve the problem arising when moving from lumped to HRU-guided, semi-distributed model
23 formulations: multiple parallel model structures typically result in an increased number of
24 parameters, which, when not adequately constrained, may increase equifinality and thereby
25 limit predictive uncertainty (e.g. Gupta and Sorooshian, 1983; Beven, 2006; Gupta et al.,
26 2008). To better satisfy the contrasting priorities of model complexity and predictive power,
27 new strategies are sought to more efficiently utilize the modelers' understanding of the system
28 and the frequently scarce available data for constraining the feasible model- and parameter
29 space (e.g. Gupta et al., 2008; Wagener and Montanari, 2011; Singh and Bárdossy, 2012;
30 Andréassian et al., 2012; Gharari et al., 2013; Hrachowitz et al., 2013b; Razavi and Tolson,
31 2013). In contrast to earlier attempts to constrain models using multiple evaluation criteria or
32 *a priori* information on catchment properties such as land use or soil type (e.g. Koren et al.,
33 2008), the utility of a different and so far underexploited type of constraints, based on *a priori*
34 understanding of the system, has been tested in this study. The concept of topography-driven
35 conceptual modeling involves the identification of HRUs that operate in parallel. Linked to
36 the technique of regularization (e.g. Tikhonov, 1963; Engl et al., 1996), this opens the
37 possibility to impose semi-quantitative, expert knowledge based, relational constraints of
38 catchment behavior on model parameters, similar to what was suggested by Pokhrel et al.
39 (2008) and Yilmaz et al. (2008). In contrast to these studies, the suggested concept introduces
40 relations between parallel HRUs exclusively based on *hydrological reasoning* to ensure that
41 similar processes between parallel model structures are represented in an internally consistent
42 way, thereby reducing the feasible parameter space. The advantage of this method is that there
43 is only limited need to quantify the constraints or the prior parameter distributions (e.g. Koren
44 et al., 2000, 2003; Kuzmin et al., 2008; Duan et al., 2006). This could allow for a meaningful
45 and potentially more realistic representation of the system in which each model component is,
46 within certain limits, forced to do what it is designed to do, rather than allowing it to
47 compensate for data and model structural errors.

48 The objectives of this paper are thus to test the hypothesis if the use of semi-distributed,
49 conceptual models, representing HRUs defined by hydrologically meaningful, topography-
50 based landscape classification combined with model constraints (1) can increase model

1 internal consistency and thus the level of process realism as compared to lumped model set-
2 ups, (2) can increase the predictive power compared to lumped model set-ups and (3) can
3 reduce the need for model calibration by the use of expert knowledge based on relations
4 between parameters, fluxes and states.

6 **2- Study area and data:**

8 The outlined methodology will be illustrated and tested with a case study using data of the
9 Wark catchment in the Grand Duchy of Luxembourg. The catchment has an area of 82 km²
10 with the catchment outlet located downstream of the town of Ettelbrück at the confluence
11 with the Alzette River (49.85° N, 6.10° E, Figure 1). With an annual mean precipitation of
12 850 mm yr⁻¹ and an annual mean potential evaporation of 650 mm yr⁻¹ the annual mean runoff
13 is approximately 250 mm yr⁻¹. The geology in the northern part is dominated by schist while
14 the southern part of the catchment is mostly underlain by sandstone and conglomerate.
15 Hillslopes are generally characterized by forest, while plateaus and valley bottoms are mostly
16 used as crop land and pastures, respectively. Drogue et al. (2002) quantified land use in the
17 catchment as 4.3% urban areas, 52.7% agricultural land and 42.9% forest. In addition they
18 reported that 61% of catchment is covered by permeable soils while the remainder is
19 characterized by lower permeability substrate. The elevation varies between 195 to 532 m,
20 with a mean value of 380 m. The slope of the catchment varies between 0-200%, with a mean
21 value of 17 % (Gharari et al., 2011).

22 The hydrological data used in this study include discharge measured at the outlet of the Wark
23 catchment, potential evaporation estimated by the Hamon equation (Hamon, 1961) with
24 temperature data measured at Luxembourg airport (Fencia et al., 2008a); and precipitation
25 measured by three tipping bucket rain gauges located at Reichlange. The temporal resolution
26 used in this study is 3 h.

28 **3- FLEX-TOPO framework:**

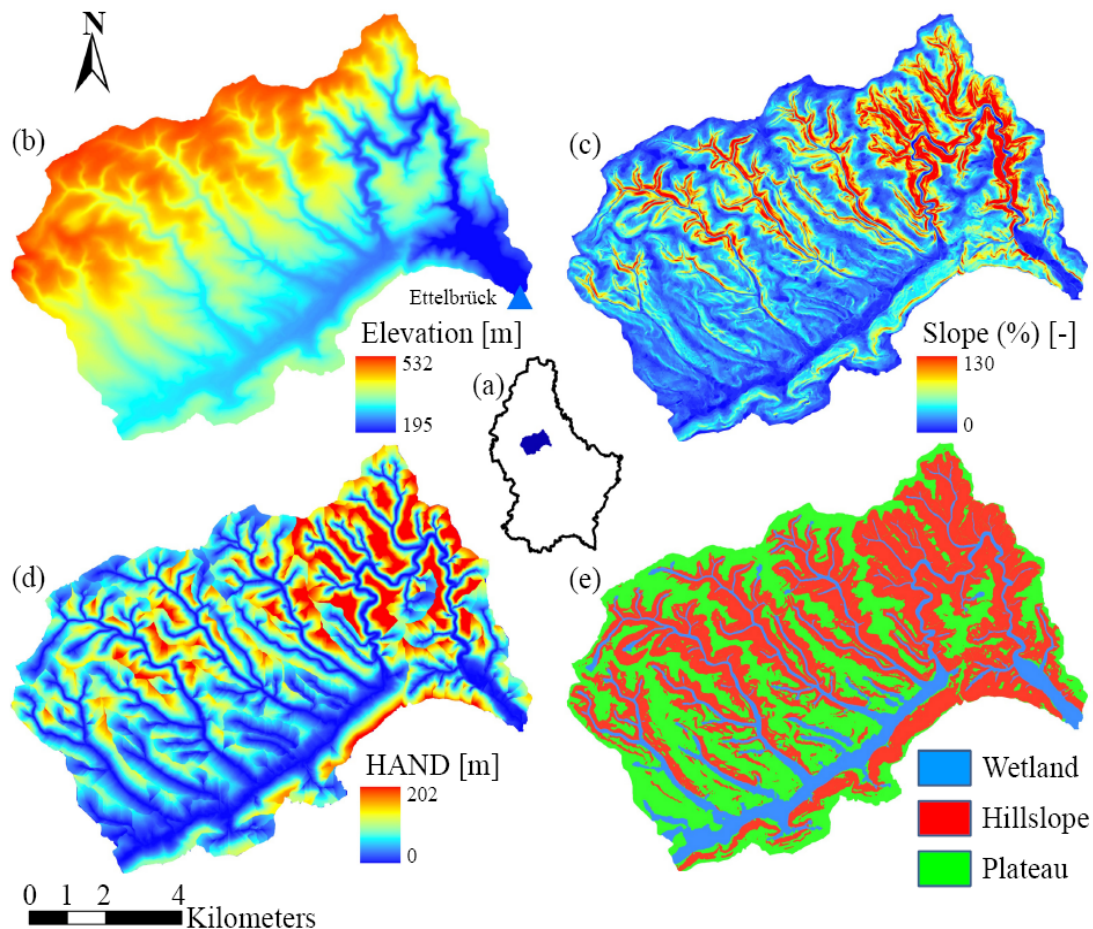
30 Realizing the potential of “reading the landscape” in a “*systems approach*” (cf. Sivapalan,
31 2003), Savenije (2010) argued that due to the co-evolution of topography, soil and vegetation,
32 all of which define the hydrological function of a given location, an efficient, hydrologically
33 meaningful descriptor of topography together with land use could be used to distinguish
34 different HRUs. HAND, which can be loosely interpreted as the hydraulic head at a given
35 location in a catchment, may be such a descriptor as it potentially allows for meaningful
36 landscape classification (e.g. Rennó et al., 2008). It was argued previously (Gharari et al.,
37 2011) that, in Central European landscapes, HAND can efficiently distinguish between
38 wetlands, hillslopes and plateaus. These are landscape elements that may also be assumed to
39 fulfill distinct hydrological functions (HRUs) in the study catchment (Savenije, 2010).
40 Wetlands, located at low elevations above streams, are characterized by shallow ground water
41 tables with limited fluctuations. Due to reduced storage capacity between ground water table
42 and soil surface, potentially exacerbated by the relative importance of the capillary fringe,
43 wetlands tend to be saturated, and thus connected, earlier during a rainfall event than the two
44 other landscape elements with arguably higher storage capacity, thus frequently becoming the
45 dominant source of storm flow during comparably dry periods (e.g. Seibert et al., 2003;
46 McGlynn et al., 2004; Molenat et al., 2005; Blume et al., 2008; Anderson et al., 2010;
47 Kavetski et al., 2011). The dominant runoff process in wetlands can therefore be assumed to
48 be saturation overland flow. In contrast, forested hillslopes, landscape elements with steeper
49 slopes than the wetlands or plateaus, require a balance between sufficient storage capacity and
50 efficient drainage to develop and maintain the ecosystem (Savenije, 2010). A dual system

1 combining sufficient water storage in the root zone and efficient lateral drainage through
2 preferential flow networks, controlled by a suite of activation thresholds as frequently
3 observed on hillslopes (e.g. Hewlett, 1961; Beven and Germann, 1982; Sidle et al., 2001;
4 Freer et al., 2002; Weiler et al., 2003; McNamara et al., 2005; Tromp van Meerveld and
5 McDonnell, 2006a, 2006b; Zehe and Sivapalan, 2009; Spence, 2010) can be seen as the
6 dominant mechanism. Finally, plateaus are landforms with low to moderate slopes and
7 comparably deep ground water tables. In absence of significant topographic gradients and due
8 to the potentially increased unsaturated storage capacity, it can be hypothesized that the
9 primary functions of plateaus are sub-surface storage and groundwater recharge (Savenije,
10 2010). Although plateaus may experience infiltration excess overland flow in specific
11 locations, the topographical gradients may not be sufficient to generate surface runoff
12 connected to the stream network (Liu et al., 2012). In the FLEX-TOPO approach the
13 proportions of the hydrologically distinct landscape units, i.e. HRUs, in a given catchment
14 need to be determined on the basis of topographical and land cover information. Subsequently
15 suitable model structures and parameterizations (read constitutive functions) will be assigned
16 to the different HRUs (Clark et al., 2009; Fenicia et al., 2011; Hrachowitz et al., 2014). The
17 integrated catchment output, i.e. runoff and evaporative fluxes, can then be obtained by
18 combining the computed proportional outputs from the individual HRUs. Note that the three
19 landscape classes tested for suitability in this study, i.e. wetland, hillslope and plateau
20 together with their assumed dominant runoff process are designed for the Wark catchment
21 and are likely to be different for other environmental settings (e.g. Gao et al., 2014).

22 23 **3-1- Landscape classification:**

24
25 As the objective of FLEX-TOPO is to efficiently extract and use hydrologically relevant
26 information from worldwide readily available topographic data, i.e. DEMs, the *Height Above*
27 *the Nearest Drainage* (HAND; Rennó et al., 2008; Nobre et al., 2011; Vannamettee et al.,
28 2014) is a potentially powerful metric to classify landscapes into HRUs with distinct
29 hydrological function, as discussed above. Testing a suite of HAND-based classification
30 methods Gharari et al. (2011) found that results best matching observed landscape types could
31 be obtained by using HAND together with the local slope. Based on a probabilistic
32 framework to map the desired HRUs which were then compared with in-situ observations
33 they obtained a threshold for HAND and slope of approximately 5 m and 11 % for the Wark
34 catchment. Following that, wetlands were defined to be areas with $HAND \leq 5$ m. Areas with
35 $HAND > 5$ m and local slopes > 11 % were classified as hillslopes, while areas with $HAND >$
36 5 m and slope ≤ 11 % were defined as plateaus. The HAND and slope map of the study
37 catchment together with the classified landscape entities (wetland, hillslope and plateau) are
38 presented in Fig. 1. The proportion of the individual HRUs wetland, hillslope and plateau are
39 15%, 45% and 40% respectively.

40



1
2
3 Figure 1- (a) Location of the Wark catchment in the Grand Duchy of Luxembourg, (b) digital
4 elevation model (DEM) of the Wark catchment with cell size of $5\text{ m} \times 5\text{ m}$ [m], (c) local
5 slopes (%) in the Wark catchment derived from a DEM with resolution of $5\text{ m} \times 5\text{ m}$ [-], (d)
6 HAND of the Wark Catchment derived from a DEM with resolution of $5\text{ m} \times 5\text{ m}$ [m], (e) the
7 classified landscape units wetland, hillslope and plateau using the combined HAND and slope
8 thresholds of 5 m and 11%, respectively (from Gharari et al., 2011).
9

10 3-2- Model setup:

11
12 In this study a lumped conceptual model of the Wark catchment, hereafter referred to as
13 FLEX^A, is used as similar lumped conceptual models are frequently used in catchment
14 hydrology (e.g. Merz and Blöschl, 2004; Clark et al., 2008; Perrin et al., 2008; Seibert and
15 Beven, 2009; Fenicia et al., 2013). The above discussed concept of FLEX-TOPO (Savenije,
16 2010) is thereafter tested with a stepwise increased number of parallel landscape units
17 (FLEX^B, FLEX^C), thereby increasing the conceptualized process heterogeneity and thus the
18 model complexity. The core of the three model set-ups is loosely based on the FLEX model
19 (Fenicia et al., 2006).
20

21 **3-2-1-FLEX^A:** This model set-up represents the catchment in a lumped way. The FLEX^A
22 model structure consists of four storage elements representing interception, unsaturated, slow
23 (i.e. groundwater) and fast responding reservoirs (i.e. preferential flow and saturation
24 overland flow). A schematic illustration of FLEX^A is shown in Fig. 2a. The water balance and
25 constitutive equations used are given in Table 2.

1
2 **3-2-1-1-Interception reservoir (S_I):** The interception reservoir is characterized by its
3 maximum storage capacity (I_{\max} [L]). After precipitation (P [$L T^{-1}$]) enters this reservoir the
4 excess precipitation, hereafter referred to as effective precipitation (P_e [$L T^{-1}$]), is distributed
5 between the unsaturated (S_U), slow (S_S) and fast (S_F) reservoirs.
6

7 **3-2-1-2-Unsaturated reservoir (S_U):** The unsaturated reservoir is characterized by a
8 parameter that loosely reflects the maximum soil moisture capacity in the root zone ($S_{U,\max}$
9 [L]). Part of the effective precipitation (P_e) enters the unsaturated zone according to the
10 coefficient C_r , which here is defined by a power function with exponent β [-], reflecting the
11 spatial heterogeneity of thresholds for activating fast lateral flows from S_F . This coefficient C_r
12 will be 1 when soil moisture (S_U) is lower than a specific percentage of maximum soil
13 moisture capacity ($S_{U,\max}$) defined by relative soil moisture at field capacity (F_c [-]), meaning
14 that the entire incoming effective precipitation (P_e) at a given time step is stored in the
15 unsaturated reservoir (S_U). The soil moisture reservoir feeds the slow reservoir through matrix
16 percolation (R_p [LT^{-1}]), expressed as a linear relation of the available moisture in the
17 unsaturated zone (S_U) and the maximum percolation capacity (P_{per} [LT^{-1}]). The reverse
18 process, capillary rise (R_c), feeds the unsaturated reservoir from the saturated zone. Capillary
19 rise (R_c [LT^{-1}]) has an inverse linear relation with the moisture content in the unsaturated zone
20 and is characterized by the maximum capillary rise capacity (C [LT^{-1}]). Soil moisture is
21 depleted by plant transpiration. Transpiration is assumed to be moisture constrained when the
22 soil moisture content is lower than a fraction L_p [-] of the maximum unsaturated capacity
23 ($S_{U,\max}$). When the soil moisture content in the unsaturated reservoir is higher than this
24 fraction (L_p) transpiration is assumed to be equal to the potential evaporation (E_{pot} [LT^{-1}]).
25

26 **3-2-1-3- Splitter and transfer functions:** The proportion of effective rainfall which is not
27 stored in the unsaturated zone, i.e. $1-C_r$, is further regulated by the partitioning coefficient (D
28 [-]), distributing flows between preferential groundwater recharge (R_S [$L T^{-1}$]) to S_S and water
29 that is routed to the stream by fast lateral processes from S_F (e.g. preferential flow or
30 saturation overland flow, R_F). Both fluxes are lagged by rising linear lag functions with
31 parameters N_{lagf} and N_{lags} , respectively (e.g. Fenicia et al., 2008b).
32

33 **3-2-1-4-Fast reservoir (S_F):** The fast reservoir is a linear reservoir characterized by reservoir
34 coefficient K_F .
35

36 **3-2-1-5-Slow reservoir (S_S):** The slow reservoir is a linear reservoir characterized by a
37 reservoir coefficient K_S .
38

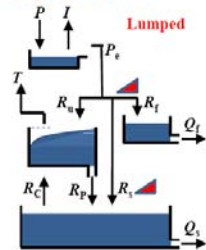
39 **3-2-2-FLEX^B:** As discussed above, a range of process studies suggested that wetlands can
40 frequently exhibit storage-discharge dynamics that are decoupled from other parts of a
41 catchment, in particular due to their typically reduced storage capacity and closeness to the
42 stream. FLEX^B explicitly distinguishes wetlands from the rest of the catchment, the
43 “remainder” (i.e. hillslopes and plateaus), which is represented in a lumped way, to account
44 for this difference. The FLEX^B model set-up therefore consists of two parallel model
45 structures which are connected with a common groundwater reservoir (Figure 2b), similar to
46 what has been suggested by Knudsen et al. (1986). One major difference between the two
47 parallel structures is that capillary rise is assumed to be a relevant process only in the wetland,
48 while it is considered negligible in the remainder of the catchment due to the deeper
49 groundwater. Further, since the wetlands are predominantly ex-filtration zones of potentially
50 low permeability, preferential recharge is considered negligible in wetlands. The areal

1 proportions of wetland and the remainder (i.e. hillslope and plateau) of the catchment are 15%
 2 and 85%, respectively (Gharari et al., 2011).

3
 4 **3-2-3-FLEX^C**: This model set-up offers a complete representation of the three HRUs in the
 5 study catchment: wetland, hillslope and plateau (Figure 2c). The formulation of the wetland
 6 module in FLEX^C is identical to the one suggested above for FLEX^B. The hillslope HRU is
 7 represented by a model structure resembling the FLEX^A set-up. Plateaus are assumed to be
 8 dominated by vertical fluxes, while direct lateral movement in the form of Hortonian overland
 9 flow is considered negligible compared to those generated from hillslope and wetland HRUs.
 10 Therefore the plateau model structure does not account for these fast fluxes. Analogous to
 11 FLEX^B, the FLEX^C set-up is characterized by one single groundwater reservoir linking the
 12 three dominant HRUs in this catchment. The individual proportions of wetland, hillslope and
 13 plateau are 15%, 45% and 40%, respectively (Gharari et al., 2011). The proportions of these
 14 HRUs are used to compute the total discharge based on the contribution of each landscape
 15 unit.

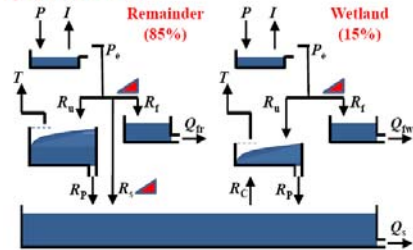
16 The connection between the parallel structures of FLEX^B and FLEX^C is through the surface
 17 drainage network (the stream network) and through the slow (groundwater) reservoir.

(a) FLEX^A



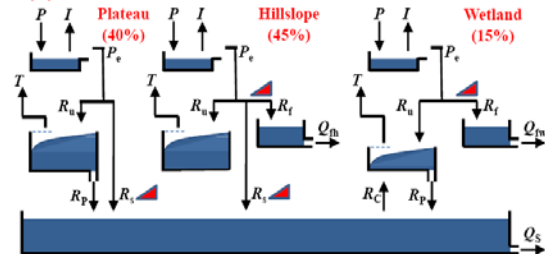
18
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(b) FLEX^B



20
 21

(c) FLEX^C



22
 23

Figure 2- The model structures for (a) FLEX^A, (b) FLEX^B and (c) FLEX^C.

24

25 Table 1- Uniform prior parameter distributions for the three model set-ups

	Unit		FLEX ^B		FLEX ^C		
			wetland	remainder	wetland	hillslope	plateau
I_{max}^*	mm	Interception storage for forest	2-5				
		Interception storage for grassland and pasture	1-3				

$S_{u,max}$	mm	Maximum unsaturated storage	0-500	0-100	0-500	0-100	0-500	0-500
β	-	Soil moisture distribution exponent	0-5	0-5	0-5	0-5	0-5	0-5
L_p	-	Transpiration coefficient	0.5	0.5	0.5	0.5	0.5	0.5
F_C	-	Relative soil moisture at field capacity	0-0.3	0	0-0.3	0	0-0.3	0-0.3
D	-	Partitioning fast and slow reservoir	0-1	0	0-1	0	0-1	1
C	mm(3h) ⁻¹	Maximum capillary rise rate	0	0-0.3	-	0-0.3	-	-
P_{per}	mm(3h) ⁻¹	Maximum percolation rate	0-0.5	0-0.5	0-0.5	0-20.5	0	0-0.5
N_{lagf}	3h	Lag time for flux to fast reservoir	1-7	1-3	1-5	1-3	1-5	-
N_{lags}	3h	Lag time for preferential recharge	1-7	-	1-7	-	1-7	1-7
K_F	(3h) ⁻¹	Fast reservoir coefficient	0-1	0-1	0-1	0-1	0-1	-
K_S	(3h) ⁻¹	Slow reservoir coefficient	0.005-0.05	0.005-0.05	-	-	0.005-0.05	-

1 *Inferred from Breuer et al., 2003

2

3 Table 2- Water balance and constitutive equations used in FLEX^A

Interception reservoir	$\frac{dS_I}{dt} = P - I - P_e$ (1)	$I = \begin{cases} E_{pot} & S_I > 0 \\ 0 & S_I = 0 \end{cases} \quad (2)$ $P_e = \begin{cases} 0 & S_I < I_{max} \\ P & S_I = I_{max} \end{cases} \quad (3)$
Unsaturated reservoir	$\frac{dS_U}{dt} = R_u - T - R_p + R_C$ (4)	$R_u = C_r P_e \quad (5)$ $C_r = \begin{cases} 1 - \left[\frac{(S_u - S_{u,max} F_C)}{(S_{u,max} - S_{u,max} F_C)} \right]^\beta & S_u \geq S_{u,max} F_C \\ 1 & S_u < S_{u,max} F_C \end{cases} \quad (6)$ $T = K_T (E_{pot}) \quad (7)$ $K_T = \begin{cases} \left[\frac{S_u}{S_{u,max} L_p} \right] & S_u < S_{u,max} L_p \\ 1 & S_u \geq S_{u,max} L_p \end{cases} \quad (8)$ $R_p = [S_u / S_{u,max}] P_{per} \quad (9)$ $R_C = [1 - (S_u / S_{u,max})] C \quad (10)$
Fast reservoir	$\frac{dS_F}{dt} = R_{F,lag} - Q_F$ (11)	$R_F = (1 - D)(1 - C_r) P_e \quad (12)$ $R_{F,lag} = R_F * N_{lagf} \quad (13)$ $Q_F = K_F S_F \quad (14)$
Slow reservoir	$\frac{dS_S}{dt} = R_{S,lag} - Q_S + R_p - R_C$ (16)	$R_S = D(1 - C_r) P_e \quad (17)$ $R_{S,lag} = R_S * N_{lags} \quad (18)$ $Q_S = K_S S_S \quad (19)$

4 * is the convolution operator.

5

6 3-3- Introducing realism constraints in selecting behavioral parameter sets:

7

8 With increasing process heterogeneity from FLEX^A over FLEX^B to FLEX^C, the respective
9 model complexities and therefore the number of calibration parameters also increase. This, in
10 the frequent absence of sufficient suitable data to efficiently constrain a model, typically leads
11 to a situation where parameters have increased freedom to compensate for errors in data and
12 model structures, as recently reiterated by Gupta et al. (2008). In this study, two

1 fundamentally different types of model constraints were applied to test their value for
 2 reducing equifinality in complex model set-ups, *parameter constraints* and *process*
 3 *constraints*.

4 **3-3-1-Parameter constraints:**

6 Inequality conditions between parameters of parallel model units, hereafter referred to as
 7 *parameter constraints*, were imposed *before* each model evaluation run. These *a priori*
 8 constraints ensure that the individual parameter values for the same process in the parallel
 9 units, reflect the modeler's perception of the system. For example, it can be argued that the
 10 maximum interception capacity (I_{\max}) of a forested HRU needs to be higher than that of a not
 11 forested one. In the absence of more detailed information this does not only allow overlapping
 12 prior distributions but it also avoids the need for quantification of the constraints themselves.
 13 In the following, a set of parameter constraints imposed on the different model structure are
 14 listed. The applicability of each parameter constraint for every model structure is summarized
 15 in Table 3. The subscripts w, h and p indicate parameters for wetland, hillslope and plateau,
 16 respectively.

18 **3-3-1-1-Interception:**

20 Different land cover proportions of individual landscape units, here wetlands, hillslopes and
 21 plateaus, can be used to define the relation between interception thresholds (I_{\max}) of these
 22 individual units. The land uses are defined as two general classes for this case study, forested
 23 areas and grass or pasture-land areas. The maximum interception capacity (I_{\max}) for each
 24 landscape entity can be estimated from the proportion of land-use classes and their maximum
 25 interception capacities, selected from their respective prior distributions as given in Table 1:
 26

$$27 \quad I_{\max,w} = a_w I_{\max,forest} + b_w I_{\max,cropland} \quad (20)$$

$$28 \quad I_{\max,h} = a_h I_{\max,forest} + b_h I_{\max,cropland} \quad (21)$$

$$29 \quad I_{\max,p} = a_p I_{\max,forest} + b_p I_{\max,cropland} \quad (22)$$

30 The proportions of forested area are indicated with a_w , a_h and a_p for wetland, hillslope and
 31 plateau and are fixed at 42%, 60% and 29%, respectively. The proportions of cropland and
 32 grass land areas are indicated by b_w , b_h and b_p for wetland, hillslope and plateau and are fixed
 33 at 58%, 40% and 71%, respectively. Moreover the parameter sets which are selected for
 34 maximum interception capacity of forest are expected to be higher than crop- or grassland:

$$35 \quad I_{\max,cropland} < I_{\max,forest} \quad (23)$$

37 **3-3-1-2- Lag functions:**

38 Preferential recharge (R_s) is routed to the slow reservoir by a lag function. Due to a deeper
 39 groundwater table on plateaus it can be assumed that the lag time for R_s is longer for plateaus
 40 than for hillslopes. It can also be assumed that the lag function used for fast reservoir for
 41 hillslopes is longer than for wetlands due to the on average higher distance of and therefore
 42 longer travel times from hillslopes to the stream.

$$43 \quad N_{lags,w} \leq N_{lags,h} \leq N_{lags,p} \quad (24)$$

3-3-1-3-Soil moisture capacity:

Wetlands have shallower groundwater tables than the other two landscape entities in this study. Therefore the unsaturated zone of wetland should have a lower maximum soil moisture capacity ($S_{U,max}$) than hillslopes and plateaus. Moreover, as hillslopes in the study catchment are predominantly covered with forest, it can, due to the deeper root zone of forests, be expected that the maximum unsaturated soil moisture capacity ($S_{U,max}$) in the root zone of hillslopes is deeper than the other two landscape entities.

$$S_{U,max,w} < S_{U,max,p} < S_{U,max,h} \quad (25)$$

3-3-1-4-Reservoir coefficients:

The reservoir coefficient of the wetland fast reservoir (K_F) is assumed to be higher than reservoir coefficient of the hillslope fast reservoir as, once connectivity is established, the flow velocities of saturation overland flow in wetlands are assumed to exceed the integrated flow velocities of preferential flow networks (cf. Anderson et al., 2009). Likewise, the reservoir coefficient of the slow reservoir should be lower than both wetland and hillslope fast reservoirs.

$$K_S < K_{F,h} < K_{F,w} \quad (26)$$

The reservoir constraints can be applied to all models while the other constraints can only be applied to FLEX^B and FLEX^C.

3-3-2-Process constraints:

In contrast to the parameters constraints discussed above, which are set *a priori*, *process constraints* are applied *a posteriori*. Only parameters which generate model flux and state dynamics in agreement with the modeler's perception of these dynamics are retained as feasible. Hence, while with the use of parameter constraints there is no need to run the model for rejected parameter sets, here it is necessary to run the model to evaluate it with respect to the process constraints.

Process constraints are defined for dry and wet periods as well as for peak-, high- and low flows. Here wet periods were defined to be the months from November to April, while the dry periods in the study catchment occur between May and October. The thresholds for distinguishing between high and low flow were chosen to be 0.05 and 0.2 mm(3h)⁻¹ respectively for dry and wet periods. Furthermore, events during which discharge increases with a rate of more than 0.2 mm(3h)⁻² are defined as peak flows. Note that in the following the subscripts peak, high and low indicate peak-, high- and low flows. The applicability of each process constraint for every model structure is summarized in Table 3.

3-3-2-1-Transpiration:

Transpiration typically exhibits a clear relationship with the normalized difference vegetation index (NDVI, Szilagyi et al., 1998). Therefore the ratios between NDVI values of different landscape units can serve as constraints on modeled transpiration obtained from the individual parallel model components. A rough estimation of the ratio between transpiration from plateau and hillslope can be derived from LANDSAT 7 images. For this ratio seven cloud free images were selected (acquisition dates of 20/4/2000, 6/3/2000, 11/9/2000, 18/2/2001,

6/3/2001, 26/3/2001 and 29/8/2001). The ratio of transpiration between hillslope and plateau (R_{trans}) can be estimated by assuming a linear relation (Szilagyi et al., 1998) with slope of α and intercept zero between transpiration and mean NDVI for each landscape unit (μ_{NDVI}).

$$R_{trans} = \frac{\alpha \mu_{NDVI,h}}{\alpha \mu_{NDVI,p}} = \frac{\mu_{NDVI,h}}{\mu_{NDVI,p}} \quad (27)$$

Mean ($\mu_{R_{trans}}$) and standard deviation ($\sigma_{R_{trans}}$) of the transpiration ratio (R_{trans}) can be used to estimate acceptable limits of the transpiration ratios for hillslope and plateau.

Therefore the annual transpiration can be confined between two values as follows:

$$\mu_{R_{trans}} - \sigma_{R_{trans}} < \frac{\int T_h dt}{\int T_p dt} < \mu_{R_{trans}} + \sigma_{R_{trans}} \quad (28)$$

Based on the mean ($\mu_{R_{trans}} = 1.2$) and standard deviation ($\sigma_{R_{trans}} = 0.2$) of the seven LANDSAT 7 images used the following process constraint on transpiration from hillslope (T_h) and plateau (T_p) was imposed:

$$1.0 < \frac{\int T_h dt}{\int T_p dt} < 1.4 \quad (29)$$

Similar constraints can be imposed between transpiration fluxes from wetland, hillslope or plateau; however, the spatial resolution of LANDSAT 7 data with resolution of 30 meters is coarser than the required 20-meter DEM resolution for distinguishing wetlands from other landscape entities (Gharari et al., 2011).

3-3-3-2-Runoff coefficient:

The runoff coefficient is a frequently used catchment signature (e.g. Sawicz et al., 2011; Euser et al., 2013) and can be used as a behavioral constraint (e.g. Duan et al., 2006; Winsemius et al., 2009). In this study the runoff coefficients of dry and wet periods as well as the annual runoff coefficient were used. Parameters that result in modeled runoff coefficients that substantially deviate from the observed ones are therefore discarded. In case of absence of suitable runoff data, the long-term mean annual runoff coefficient can be estimated from the regional Budyko curve using for example the Turc-Pike relationship (Turc, 1954; Pike, 1964; Arora, 2002). However in this study the runoff coefficients of each individual year, and their respective dry and wet periods was used and determined the mean and standard deviation of the runoff coefficients for these periods. Here, as a conservative assumption, the limits are set to three times the standard deviation around the mean runoff coefficient. Note that the runoff coefficient is the only process constraint that is not related to model structure in this study and can therefore also be applied to the lumped FLEX^A set-up.

$$\frac{\int Q_m dt}{\int P dt} < 0.43 \quad (30)$$

$$\frac{\int Q_m dt}{\int P dt} > 0.16 \quad (31)$$

$$\frac{\int Q_{m,dry} dt}{\int P_{dry} dt} < 0.36 \quad (32)$$

$$\frac{\int Q_{m,dry} dt}{\int P_{dry} dt} > 0 \quad (33)$$

$$\frac{\int Q_{m,wet} dt}{\int P_{wet} dt} < 0.71 \quad (34)$$

$$\frac{\int Q_{m,wet} dt}{\int P_{wet} dt} > 0.40 \quad (35)$$

3-3-3-3-Preferential recharge:

The slow reservoir can be recharged by both preferential and matrix percolation from the unsaturated reservoirs. Here, hillslopes and plateaus contribute to the slow reservoir by preferential recharge. It can be assumed that in a realistic model setup the long term contribution volume of preferential recharge ratio between hillslope and plateau should not be unrealistically high or low. For example, it can be assumed unrealistic that the ratio is zero or infinity, meaning that one landscape unit is constantly feeding the slow reservoir while another one is not contributing at all. To avoid such a problem, a loose and very conservative constraint was imposed on the ratio of contribution of the two fluxes.

$$0.2 < \frac{\int R_{s,h} dt}{\int R_{s,p} dt} < 5 \quad (36)$$

3-3-3-4-Fast component discharge:

During dry periods, hillslopes and plateaus can exhibit significant soil moisture deficits, limiting the amount of fast runoff generated from these landscape elements. In contrast, due to their reduced storage capacity, wetlands are likely to generate fast flows at lower moisture levels, thus dominating event response during dry periods (cf. Beven and Freer, 2001a; Seibert et al., 2003; Molenat et al., 2005; Anderson et al., 2010; Birkel et al., 2010). It can thus be assumed that peak flows during dry periods the fast component of wetlands ($Q_{f,w,dry,peaks}$) contributes to runoff more than the fast component of hillslopes ($Q_{f,h,dry,peaks}$). In contrast, high flows during wet periods are predominantly generated by fast reaction from hillslopes ($Q_{f,h,wet}$; $Q_{f,h,wet,high}$) rather than of wetland ($Q_{f,w,wet}$; $Q_{f,w,wet,high}$). This process constraint is also applied to FLEX^B.

$$\frac{\int Q_{f,h,dry,peaks} dt}{\int Q_{f,w,dry,peaks} dt} < 1 \quad (37)$$

$$\frac{\int Q_{f,h,wet,high} dt}{\int Q_{f,w,wet,high} dt} > 1 \quad (38)$$

$$\frac{\int Q_{f,h,wet} dt}{\int Q_{f,w,wet} dt} > 1 \quad (39)$$

Table 3 - The applicability of different parameter and process constraints for the three different model structures, FLEX^A, FLEX^B and FLEX^C.

	Parameter constraints				Process constraints			
	3-3-1-1- Interception	3-3-1-2- Lag functions	3-3-1-3- Soil moisture capacity	3-3-1-4- Reservoir coefficients	3-3-2-1- Transpiration	3-3-3-2- Runoff coefficient	3-3-3-3- Preferential recharge	3-3-3-4- Fast component discharge
FLEX ^A				×		×		
FLEX ^B	×	×	×	×		×		×
FLEX ^C	×	×	×	×	×	×	×	×

3-3-4-Calibration algorithm and objective functions:

Based on uniform prior parameter distributions as well as on the parameter- and process constraints the model was calibrated using MOSCEM-UA (Vrugt et al., 2003). The use of constraints in common calibration algorithms such as MOSCEM-UA, penalizing the objective function(s) based on the number of unsatisfied constraints, may lead to non-smooth objective functions. This can potentially cause instabilities in the search algorithm or generating invalid results. A recently developed stepwise search algorithm was therefore used for finding parameter sets which satisfy both parameter- and process constraints (Gharari et al., this issue). These parameter sets were then used as initial sampling parameter sets for MOSCEM-UA instead of the traditionally used Latin Hypercube sampling strategy.

The models were evaluated on the basis of three different objective functions to emphasize different characteristics of the system response: (i) the Nash-Sutcliffe efficiency of the flows (Nash and Sutcliffe, 1970; E_{NS}), (ii) the Nash-Sutcliffe efficiency of the logarithm of the flows ($E_{NS,log}$) and (iii) the Nash-Sutcliffe efficiency of the flow duration curve ($E_{NS,FDC}$). These criteria evaluate the models' ability to simultaneously reproduce high flows, low flows and flow duration curves respectively. While the year 2001 was used as warm up period, the model set-ups were constrained and calibrated for the year 2002-2005 and validated for year 2006-2009 (see below) and vice versa (see Supplementary Information).

3-4-Model validation and parameter evaluation:

To assess the value of incorporating parameter and process constraints in increasingly complex models a four-step procedure as outlined below was followed.

3-4-1- Evaluating models with “constrained but uncalibrated” parameter sets:

Firstly, all parameter sets which satisfy all the applied constraints were evaluated based on their ability to reproduce the observed hydrograph. Hereafter these parameter sets are referred to as *constrained but uncalibrated* parameter sets because they were obtained *without any calibration* on the observed hydrographs. Based on the retained, feasible parameter sets, the mean performance of the three *constrained but uncalibrated* models FLEX^A, FLEX^B and FLEX^C, for the three objective functions (E_{NS} , $E_{NS,log}$, $E_{NS,FDC}$) together with their uncertainty ranges for both the calibration and the validation periods are compared. FLEX^A, FLEX^B and FLEX^C have an increasing number of constraints. It was thus tested whether the higher complexity models also result in better model performance and how the predictive uncertainty is affected by increased complexity and model realism. To investigate how well the hydrographs generated with parameters satisfying all constraints match the observed hydrograph, the 95% uncertainty intervals of simulated hydrographs based on these parameter sets were generated for the three models. The uncertainty was estimated on the basis of the area indicated by 95% uncertainty intervals based on simulated hydrographs.

To further study the effect of constraints on the performance and uncertainty of constrained but un-calibrated parameter sets, three benchmark models have been considered whereby no

1 constraint is present. This simply means the models can produce any possible output without
2 any restriction on parameters, fluxes and states. However the percentages of each landscape
3 for model FLEX^B and FLEX^C remains intact.

6 **3-4-2- Evaluating models with “constrained and calibrated” parameter sets:**

8 In the second step, the three models FLEX^A, FLEX^B and FLEX^C have been calibrated within
9 the parameter space which satisfied all the imposed parameter and process constraints. The
10 models were calibrated using a multi-objective strategy (E_{NS} , $E_{NS,log}$, $E_{NS,FDC}$). The obtained
11 Pareto optimal model parameters are in the following referred to as *constrained and*
12 *calibrated*.

13 Uncertainty intervals were evaluated based on the constrained and calibrated Pareto members.
14 The uncertainty was estimated on the basis of the area of the uncertainty bands.

15 As in the previous section, the models here are compared to calibrated but unconstrained
16 benchmarks.

18 **3-4-3- Comparison of model performance and uncertainty for “constrained but un- 19 calibrated” and “constrained and calibrated” parameter sets:**

21 To assess the added value of incorporating constraints in higher complexity models, the
22 performance and uncertainties of the three models FLEX^A, FLEX^B and FLEX^C were
23 compared for both the “constrained but un-calibrated” and the “constrained and calibrated”
24 case during calibration and validation periods.

26 **3-4-4- Comparison of modeled hydrograph components for different model structures:**

28 One of the main reasons for imposing constraints on model parameters is to ensure the
29 realistic internal dynamic of a model. Comparing different fluxes contributing to the modeled
30 hydrograph can give an insight into the performance of imposed constraints on the model.
31 The effect of imposing behavioral constraints on fast and slow components of the three
32 models structures, FLEX^A, FLEX^B and FLEX^C is compared visually. The fast component of
33 lumped model, FLEX^A, is compared with fast components of FLEX^B which are wetland and
34 remainder of catchment and fast components of FLEX^C which are wetland and hillslope. This
35 visual comparison is based on normalized average contribution of each component for Pareto
36 optimal parameter sets in every time step.

39 **4- Results and discussion**

41 **4-1- Evaluating the performance of constrained but uncalibrated parameter sets:**

43 The median and the 95% uncertainty intervals of the performance of modeled hydrographs for
44 *constrained but uncalibrated* parameter sets is presented in Table 4 for the 2002-2005
45 calibration and 2006-2009 validation periods together with their benchmarks (unconstrained).
46 The lumped FLEX^A model has only one parameter and one process constraint, i.e. the
47 reservoir coefficient and the runoff coefficient, respectively. Hence, this model is free within
48 the limits of this relatively weak condition, resulting in a wide range of feasible parameter
49 sets, many of which cannot adequately reproduce the system response. As a consequence, the

1 overall performance is poor ($E_{NS,median}=0.18$, $E_{NS,log,median}=0.05$, $E_{NS,FDC,median}=0.39$) (Table 4,
2 Figure 3).

3 FLEX^B, run with the set of *constrained but uncalibrated* parameters shows a substantial
4 improvement in overall performance ($E_{NS,median}=0.56$, $E_{NS,log,median}=0.33$, $E_{NS,FDC,median}=0.87$)
5 compared to FLEX^A, as FLEX^B not only allows for more process heterogeneity but, more
6 importantly, it is conditioned with an increased number of constraints.

7 The additional process heterogeneity and constraints allowed by FLEX^C, results in the highest
8 overall performance for all three objective functions ($E_{NS,median}=0.66$, $E_{NS,log,median}=0.36$, $E_{NS,$
9 $FDC,median}=0.93$) (Table 4, Figure 3).

10 These results clearly illustrate that the imposed relational constraints force the model and its
11 parameters towards a more realistic behavior, which significantly improves model
12 performance. Additionally, the comparison of result of the three models with their
13 unconstrained benchmarks (Table 4) clearly shows that the incorporation of constraints
14 improves the median performance and 95% uncertainty intervals of all the models by
15 rejecting parameter sets that violate the constraints and cannot reproduce certain aspects of the
16 response patterns. In addition, the comparison between the unconstrained benchmark models
17 themselves suggests that more complex model structures improve the performance, implying
18 that model structures themselves already contain a considerable degree of information even in
19 absence of any constraints or calibration attempts.

20 The 95% uncertainty areas mapped by simulated hydrographs indicate that FLEX^C, which
21 might be expected to produce the highest uncertainty interval due to its complexity, is
22 providing a lower uncertainty compared to FLEX^B. Although FLEX^C cannot outperform
23 FLEX^A in terms of a narrower uncertainty interval in the validation period, overall
24 performance of this model is better than FLEX^A as discussed earlier (Table 4, Figure 3).

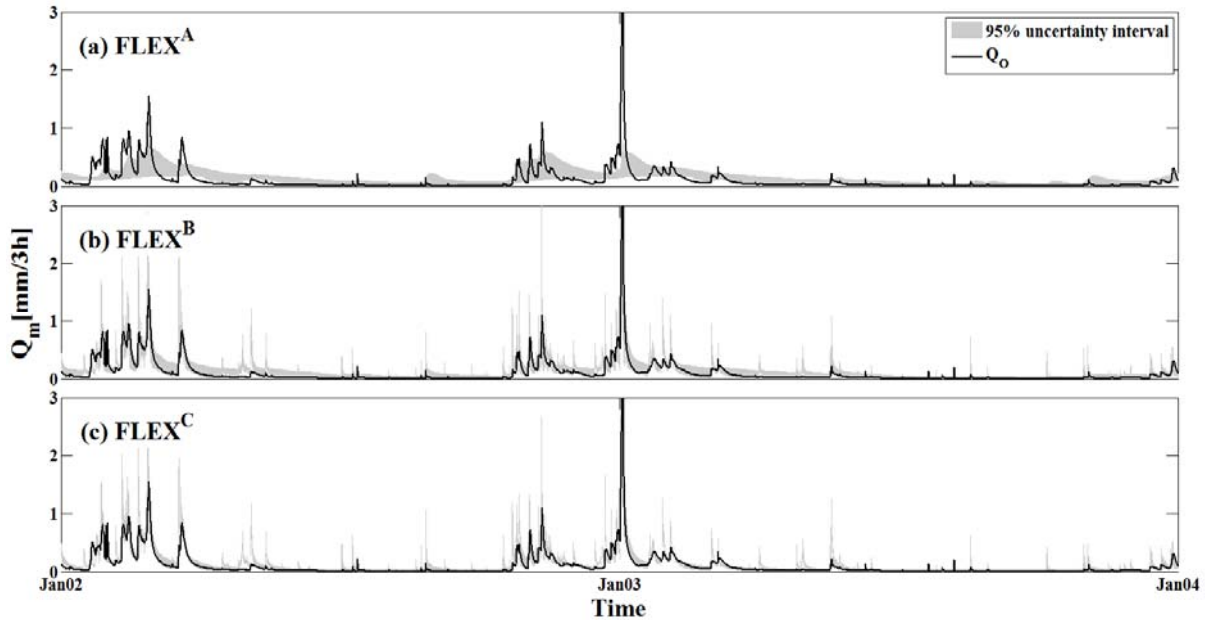
25 Flipping calibration and validation gave equivalent results, which are, for brevity, provided in
26 the Supplementary material (Table S1; Figure S1).

27 Table 4- The median model performances (in brackets their corresponding 95% uncertainty
28 intervals) and the area spanned by the 95% uncertainty interval of hydrograph derived from
29 uncalibrated parameter sets which satisfy the complete set of constraints for the three model
30 set-ups FLEX^A, FLEX^B and FLEX^C, for the three modeling objectives (E_{NS} , $E_{NS,log}$, $E_{NS,FDC}$)
31 in the calibration (2002-2005) and validation (2006-2009) periods. The italic values indicate
32 performance and 95% uncertainty interval of hydrograph for the unconstrained benchmark
33 models.
34

		E_{NS}			$E_{NS,log}$			$E_{NS,FDC}$			95% uncertainty area [mm]
FLEX ^A	Cal	0.18	[0.09	0.29]	0.05	[-0.40	0.49]	0.39	[0.25	0.69]	1325
		<i>0.16</i>	<i>[-0.16</i>	<i>0.30]</i>	<i>0.10</i>	<i>[-1.11</i>	<i>0.51]</i>	<i>0.35</i>	<i>[-0.12</i>	<i>0.67]</i>	1814
FLEX ^B	Cal	0.23	[0.12	0.39]	0.29	[-0.02	0.59]	0.45	[0.28	0.76]	1243
	Val	<i>0.18</i>	<i>[-0.37</i>	<i>0.39]</i>	<i>0.29</i>	<i>[-2.53</i>	<i>0.56]</i>	<i>0.38</i>	<i>[-0.35</i>	<i>0.76]</i>	1888
FLEX ^B	Cal	0.56	[0.00	0.73]	0.33	[-1.36	0.65]	0.87	[0.66	0.95]	1827
		<i>0.44</i>	<i>[-1.03</i>	<i>0.72]</i>	<i>0.07</i>	<i>[-3.06</i>	<i>0.60]</i>	<i>0.77</i>	<i>[0.05</i>	<i>0.93]</i>	2615
FLEX ^B	Cal	0.52	[-0.06	0.77]	0.45	[-1.15	0.73]	0.89	[0.62	0.99]	2042
	Val	<i>0.45</i>	<i>[-1.44</i>	<i>0.76]</i>	<i>0.30</i>	<i>[-3.50</i>	<i>0.73]</i>	<i>0.81</i>	<i>[0.08</i>	<i>0.97]</i>	2993
FLEX ^C	Cal	0.66	[0.22	0.75]	0.36	[-2.37	0.70]	0.93	[0.82	0.96]	1274
		<i>0.54</i>	<i>[-0.24</i>	<i>0.75]</i>	<i>0.34</i>	<i>[-2.30</i>	<i>0.69]</i>	<i>0.86</i>	<i>[0.60</i>	<i>0.94]</i>	2015

		0.67	[-0.06	0.80]	0.50	[-0.33	0.74]	0.95	[0.88	0.99]	1294
	Val	0.59	[-0.11	0.79]	0.58	[-2.89	0.75]	0.93	[0.65	0.99]	2287

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Figure 3- The observed hydrograph and the 95% uncertainty interval of the modeled hydrograph derived from the complete set of *constrained but un-calibrated* parameter sets for the three different model set-ups (a) FLEX^A, (b) FLEX^B and (c) FLEX^C for two years (2002-2003) of calibration.

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4-2- Evaluating the performance of *constrained and calibrated* parameter sets:

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The comparison of the *constrained and calibrated* model set-ups shows that all three models set-ups can reproduce the hydrograph similarly well (Table 5, Figure 4). FLEX^A exhibits a slightly better calibration performance, based on $E_{NS,log}$, compared to the other two model set-ups. This can partly be attributed to the lower number of parameters which leads, with the same number of samples, to a more exhaustive sampling of the parameter space and a smoother identification of Pareto optimal solutions. In addition, FLEX^A has the lowest number of imposed constraints, i.e. only the runoff coefficient and one parameter constraints, compared to FLEX^B and FLEX^C. This allows the model more freedom in exploiting the parameter space to produce mathematically good fits between observed and modeled system response in the calibration period.

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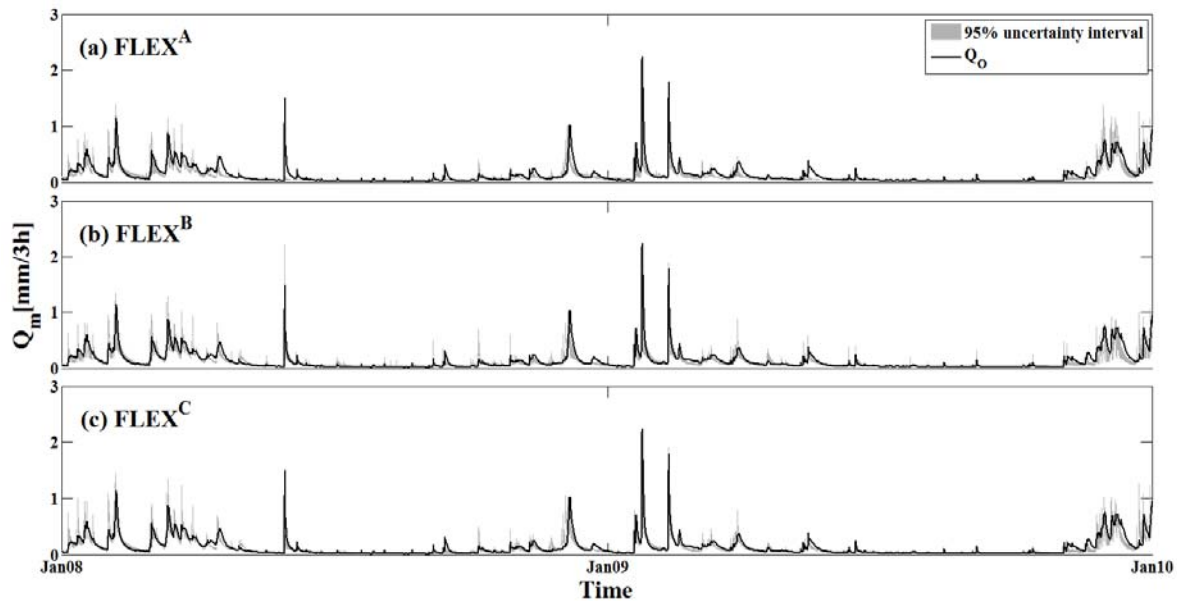
For the validation period, arguably more important for model evaluation, as in contrast to the calibration period, it gives information on model consistency (cf. Klemes, 1986; Andréassian et al., 2009; Euser et al., 2013) and predictive uncertainty, the performances of the three model set-ups exhibit quite different patterns (Table 5). The simplest model, the lumped FLEX^A, is characterized by performance deterioration from calibration to validation. In contrast, FLEX^B and FLEX^C exhibit a performance improvement in the validation period. Although the increase in performance is subjected to the nature of the forcing and observed discharge data in calibration and validation period, and formally no meaningful comparison between Nash-Sutcliffe efficiencies for different periods can be made, these results nevertheless indicate that the more complex model structure together with its constraints

1 performs more stable outside the calibration period. When flipping the calibration and
 2 validation periods the difference between model performance in calibration and validation is
 3 not as strong (Supplementary material, Table S2). A possible explanation could be that the
 4 observed data quality is not informative enough for calibration (period 2002-2005).
 5 Constraints then prevent the model to over-fit and thus enable the models to maintain a more
 6 reliable performance outside the calibration period. On the contrary, if the calibration period
 7 is informative (period 2006-2009), constraints may not affect performance outside the
 8 calibration period that much. However constraints remain necessary to reduce model
 9 uncertainty both during calibration and validation. In addition to formal performance and
 10 uncertainty measures, it can be seen visually in Figure 4 that FLEX^C can adequately predict
 11 the high flows during a dry period, while FLEX^A misses most of the peaks.

12
 13 Table 5- The median model performances (in brackets their corresponding Pareto uncertainty
 14 intervals) and the area spanned by the uncertainty interval of the hydrograph derived from the
 15 Pareto optimal solutions of the *constrained and calibrated* model set-ups FLEX^A, FLEX^B and
 16 FLEX^C for the three modeling objectives (E_{NS} , $E_{NS,\log}$, $E_{NS,FDC}$) in the calibration and
 17 validation periods. The italic values indicate performance and 95% uncertainty interval of
 18 hydrograph for the benchmark models (without any constraints).

		E_{NS}	$E_{NS,\log}$	$E_{NS,FDC}$	95% uncertainty area [mm]
FLEX ^A	Cal	0.71 [0.51 0.83] <i>0.71 [0.51 0.84]</i>	0.80 [0.70 0.85] <i>0.79 [0.68 0.85]</i>	0.97 [0.95 0.99] <i>0.97 [0.95 0.99]</i>	709 732
	Val	0.63 [0.45 0.78] <i>0.63 [0.46 0.78]</i>	0.73 [0.65 0.80] <i>0.73 [0.63 0.80]</i>	0.95 [0.93 0.97] <i>0.95 [0.93 0.97]</i>	844 870
FLEX ^B	Cal	0.75 [0.50 0.80] <i>0.74 [0.51 0.80]</i>	0.71 [0.40 0.79] <i>0.72 [0.46 0.82]</i>	0.96 [0.92 0.98] <i>0.96 [0.92 0.98]</i>	790 826
	Val	0.76 [0.32 0.82] <i>0.72 [0.45 0.82]</i>	0.79 [0.63 0.85] <i>0.78 [0.48 0.84]</i>	0.97 [0.93 1.00] <i>0.96 [0.94 0.99]</i>	999 986
FLEX ^C	Cal	0.74 [0.53 0.82] <i>0.74 [0.48 0.82]</i>	0.72 [0.47 0.81] <i>0.71 [-0.17 0.83]</i>	0.96 [0.92 0.98] <i>0.96 [0.90 0.98]</i>	763 864
	Val	0.78 [0.45 0.82] <i>0.73 [0.42 0.83]</i>	0.83 [0.72 0.85] <i>0.78 [-0.05 0.85]</i>	0.99 [0.98 1.00] <i>0.98 [0.95 0.99]</i>	927 1047

19
 20



1
2 Figure 4- The observed hydrograph and the 95% Pareto uncertainty interval of the modeled
3 hydrograph for constrained and calibrated parameter sets for the three different model set-ups
4 (a) FLEX^A, (b) FLEX^B and (c) FLEX^C for the two years (2008-2009) of validation period.
5

6 **4-3- Comparison of “constrained but uncalibrated” and “constrained and calibrated”
7 models:**
8

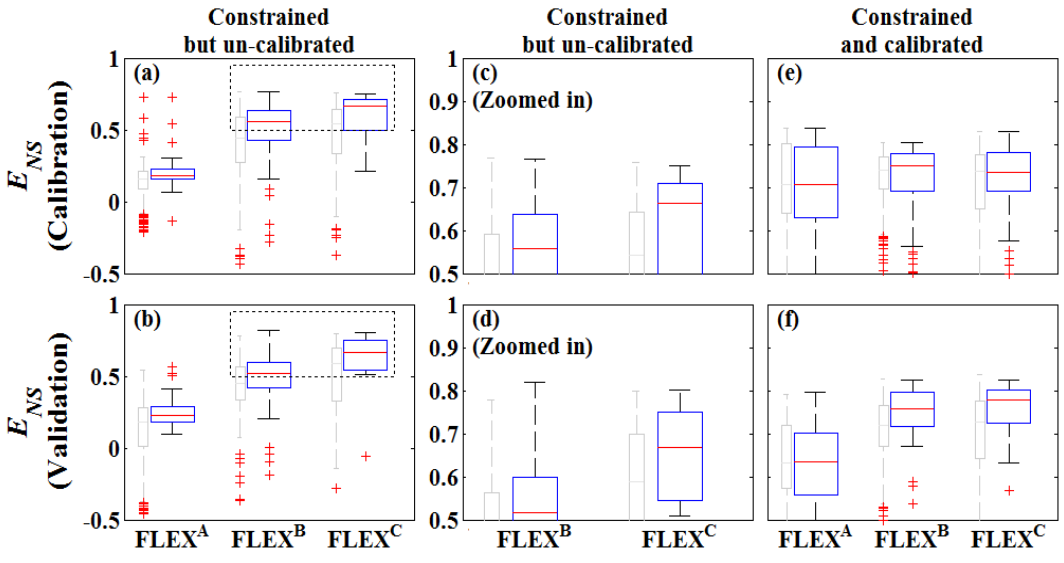
9 The following comparison of the performances of FLEX^A, FLEX^B and FLEX^C for
10 “constrained but uncalibrated”, “constrained and calibrated” and their unconstrained
11 benchmarks is focused on E_{NS} only, for the reason of brevity (Figure 5, gray box plots
12 indicate the benchmark models). In Figures 5a and 5b the model performances based on the
13 “constrained but un-calibrated” parameter sets, that satisfy the full set of constraints, are
14 shown for the calibration and validation periods. As discussed in detail above, although un-
15 calibrated, increasing the number of constraints from FLEX^A to FLEX^C increases the overall
16 performance of the models while reducing uncertainty (Figures 5c and 5d; note that these are
17 zoom-ins). Further, comparison to the uncalibrated benchmarks, suggests that improving the
18 model structure based on landscape units in itself substantially increases the performance of
19 the model. However additional constraints will eventually reduce the uncertainty and improve
20 the performance (Figure 5a and 5b).

21 Figure 5e compares model performance based on *constrained and calibrated* parameter sets
22 for the calibration period. When comparing the individual model performances of the
23 constrained and calibrated models during the validation period (Figure 5f), it can be seen that
24 FLEX^A not only shows the strongest performance deterioration compared to the calibration
25 period but also that FLEX^A is also the model with the poorest performance in the validation
26 period. This implies that although FLEX^C is the most complex model, the realism constraints
27 together with landscape related structure imposed on this model generate the most reliable
28 outputs when used for prediction, i.e. in the validation period. When the calibration and
29 validation periods are switched, the performance of FLEX^C remains comparable to above,
30 although in this case FLEX^A performs best during validation (see supplementary material
31 Figure S5). This strongly underlines that the widely accepted notion of complex models
32 necessarily being subject to higher predictive uncertainty is not generally valid when the
33 feasible parameter space can be constrained based on assumptions of realistic functionality of
34 a catchment. As explained earlier, this also indicates that when the data of the calibration

1 period are not sufficiently informative, imposing constraints will force the model to perform
 2 better outside the calibration period.

3 In addition, a second crucial aspect was revealed by comparing “constrained but un-
 4 calibrated” and “constrained and calibrated” models. It can be seen that constrained but
 5 uncalibrated FLEX^C, shows significant improvement in performance approaching the
 6 performance of the calibrated lumped model, FLEX^A. Interestingly, it was found that in
 7 validation the *constrained but uncalibrated* FLEX^C can, depending on the performance
 8 measure used and the information content of the calibration period (i.e. climatic variability
 9 and data quality), reach the performance level of the *constrained and calibrated* FLEX^A
 10 (Figs.5 and S5). This highlights the value of semi- and non-quantitative hydrological expert
 11 knowledge for finding suitable model parameter sets for ungauged basins.

12



13 Figure 5- Model performance (E_{NS}) based on *constrained but uncalibrated* (a-d) and
 14 *constrained and calibrated* (e-f) parameter sets for calibration (2002-2005) and validation
 15 (2006-2009) periods for the three different model set-ups FLEX^A, FLEX^B and FLEX^C. Note
 16 that (c) and (d) are zoom-ins of (a) and (b) and the gray box-plots represent the unconstrained
 17 benchmark models. The box plots indicate the median value in red and 25% and 75% quartile.
 18 Whiskers represent the 1.5 times the interquartile range (IQR) and the red crosses show
 19 outliers.
 20

21

22 **4-4- Comparison of flow contributions from different model components:**

23

24 The comparison of the fluxes generated from the individual model components in the three
 25 model set-ups helps to assess to which degree the model internal dynamics reflect the
 26 modeler’s perception of the system and thus to a certain degree the realism of the models.

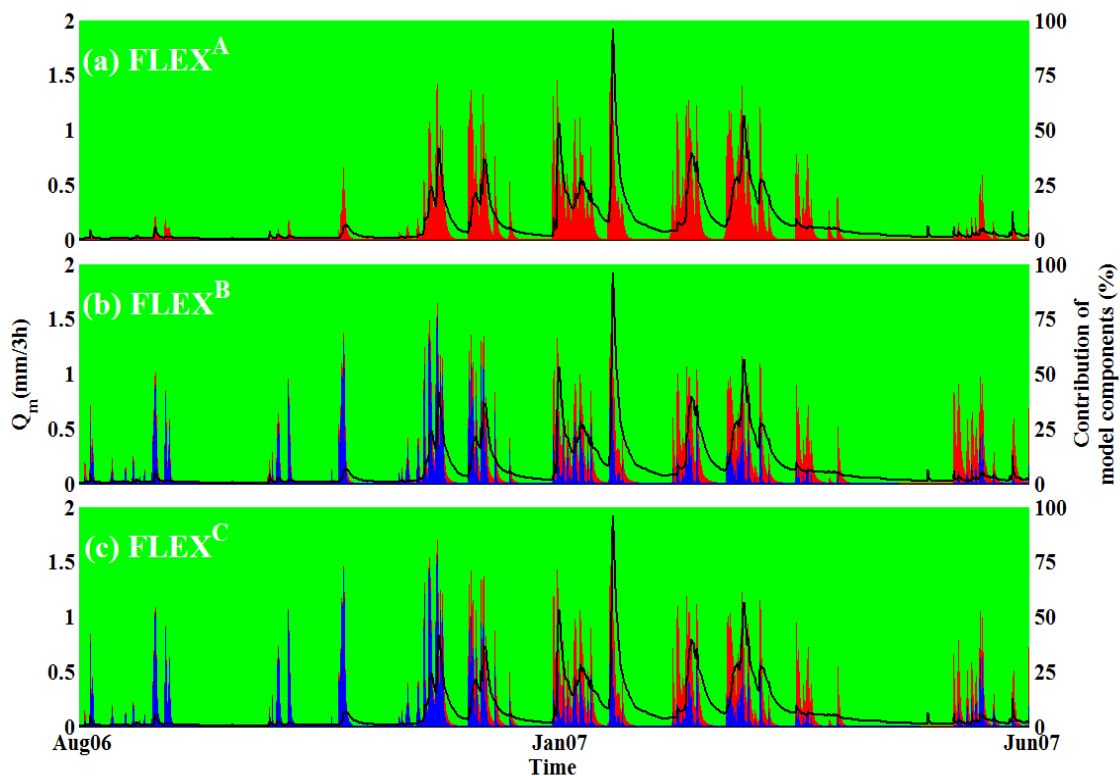
27 Fast and slow responses of each tested model set-up have been visually illustrated in Fig. 6.
 28 Predominance of slow responses of all the three models are indicated by green color;
 29 predominance of fast responses of FLEX^A, fast responses of the remainder of the catchment
 30 of FLEX^B and fast responses of hillslope of FLEX^C is indicated by red color; wetland fast
 31 responses of FLEX^B and FLEX^C are indicated by predominance of blue color.

32 The colors in Fig. 6 are an illustration using three colors (red, green and blue) for the models’
 33 responses based on their weight of contribution to the modeled runoff. As it can be seen in

1 Fig.6a the fast component of FLEX^A is dominant just during peak flows and even the
 2 recession shortly after peak flows are accounted for mainly by ground water. Analysis of the
 3 individual model components computed by Pareto optimal parameter sets (not shown here for
 4 brevity), indicates that some Pareto optimal parameters can generate peak flows by
 5 predominant contributions from slow responses while fast reaction tends to be inactive during
 6 these events.

7 In accordance with the perception of the system that wetlands are predominantly responsible
 8 for peak flows during dry conditions, Fig.6b and c show that wetland fast responses in FLEX^B
 9 and FLEX^C control the rapid response during wetting up periods (dry to wet transition),
 10 before hillslope fast processes become more important at higher moisture levels. When the
 11 system is saturated the hillslope contribution to modeled runoff becomes significantly higher
 12 compared to the wetland response. Note that the response of the wetland may not correspond
 13 well to individual events, as a consequence of the fact that the corresponding constraint was
 14 set for an aggregated period.

15



16

17 Figure 6- Comparison between mean proportions of Pareto members for model components
 18 of the three model set-ups in part of the validation periods (August 2006- June 2007) (a)
 19 FLEX^A, (b) FLEX^B, and (c) FLEX^C. The green color indicates the relative contribution of the
 20 slow reservoir for the three different models. Red indicates relative contribution from the fast
 21 components, i.e. fast reservoir in FLEX^A, fast reservoir of the remainder of the catchment in
 22 FLEX^B and fast reservoir of hillslope of FLEX^C. The blue color indicates the relative
 23 contribution of fast wetland component of FLEX^B and FLEX^C.

24

25 **4-5- Wider implications:**

26

27 The results of this study quite clearly indicate that discretizing the catchment into
 28 hydrological response units (HRUs) and incorporating expert knowledge in model
 29 development and testing is a potentially powerful strategy for runoff prediction, even where

1 insufficient data for model calibration (e.g. Koren et al., 2003; Duan et al., 2006; Winsemius
2 et al., 2009) or only comparatively unreliable regionalization tools are available (e.g. Wagener
3 and Wheater, 2006; Bárdossy, 2007; Parajka et al., 2007; Oudin et al., 2008; Laaha et al.,
4 2013). It was found that the performance and the predictive power of a comparatively
5 complex uncalibrated conceptual model, based on posterior parameter distributions obtained
6 merely from relational, semi- and non-quantitative realism constraints inferred from expert
7 knowledge, can approach or even be as efficient as the calibration of a lumped conceptual
8 model (Fig. 5, Supplementary material Figure S3).

9 Typically it is expected that, if not warranted by data, models with higher complexity suffer
10 from higher predictive uncertainty. As stated by Beven (2001): “More complexity means
11 more parameters, more parameters mean more calibration problems, more calibration
12 problems will often mean more uncertainty in the predictions, particularly outside the range of
13 the calibration data”. Thus, more parameters would allow better fits of the hydrograph but
14 would not necessarily imply a better and more robust understanding of catchment behavior or
15 more reliable predictions.

16 A complex model may include many processes, i.e. hypotheses, which can usually not be
17 rigorously tested with the available data. However, a wide range of previous studies has
18 demonstrated that hydrologically meaningful constraints can help to limit the increased
19 uncertainty caused by incorporating additional processes, i.e. parameters (e.g. Yadav et al.,
20 2007; Zhang et al., 2008; Kapangaziwiri et al., 2012). These studies generally include a large
21 set of catchments and try to relate model parameters to catchment characteristics. Although
22 regional constraints are important, the importance of expert knowledge on the catchment
23 scale, which leads to better understanding of hydrological behavior is highlighted in this
24 study.

25 In a similar attempt, Pokhrel et al. (2008, 2012) demonstrated use of regularization for model
26 parameters and reduction of model parameter space dimensionality by linking model
27 parameters using super-parameters to catchment characteristics. However, no explicit
28 hydrological reasoning is typically applied for such “regularization rules” (e.g. Pokhrel et al.,
29 2012). On the other hand, Kumar et al. (2010, 2013) parameterize and successfully
30 regionalize their models using empirical transfer functions with global parameters, developed
31 from extensive literature study and iterative testing in a large sample of catchments In
32 contrast, the use of relational parameter- and process constraints, as presented in this study, is
33 based on semi-quantitative, hydrologically explicit and meaningful reasoning avoiding the
34 need for empirical transfer functions to link catchments characteristics and model parameters.

35 Including prior knowledge for parameters of physically-based models for estimating runoff in
36 ungauged basins was quite successfully investigated in the past (e.g. Otte and Uhlenbrook
37 2004, Vinegradov et al., 2011, Fang et al., 2013, Semenova et al., 2013). These studies
38 specifically indicate that calibration can be replaced by prior information which is a
39 significant contribution to Predictions in Ungauged Basins (PUB). While physically-based
40 models need detailed information of catchment behavior for model parameters, the here
41 proposed semi-distributed conceptual modeling framework, exploiting relational constraints,
42 can be more efficiently set up using the least prior information necessary. In this study, the
43 performances and uncertainties of the three tested model set-ups for *constrained but*
44 *uncalibrated* parameters indicate the potential of the presented FLEX-TOPO framework for
45 Predictions in Ungauged Basins (PUB). Hence, this framework can efficiently use expert
46 knowledge for improving model parameter value selection in complex conceptual
47 hydrological models, not only to increase model performance but also to reduce model
48 predictive uncertainty even in the absence of calibration.

1 It should be kept in mind that the conclusion of this study remains at this point only valid for
2 the study catchment. To generalize the findings of this study more rigorous tests should be set
3 up (Andréassian et al., 2009) which expand this presented concept for different time series of
4 a catchment and also a larger set of catchments such as in recent work of Gao et al. (2014)
5 and Hrachowitz et al. (2014). Some further challenges that remain, include the need to
6 formulate generic constraints for any catchment based on available data in an automated
7 procedure. Likewise it will be necessary to develop a better understanding of model
8 sensitivities to different constraints and of the effectiveness and reliability of individual
9 constraints. It is also emphasized that the constraints introduced in this study are based on the
10 authors' subjective understanding of catchment behavior and can and should be discussed
11 further. However, we would like to stress the notion that reaching an agreement on the
12 relations between parameters and fluxes in different landscape units is potentially much easier
13 than finding the most adequate parameter values together with associated uncertainties for a
14 conceptual model based on field observations or available data on geology or soil types.

15 **5- Conclusion:**

16
17
18 In this study it was tested if a topography-driven semi-distributed formulation of a catchment-
19 scale conceptual model, conditioned by expert knowledge based relational parameter- and
20 process constraints, can increase the level of process realism and predictive power while
21 reducing the need for calibration.

22 It was found that:

- 23 (1) The performance of models, although uncalibrated, improves by accounting for different
24 topography-based hydrological response units, even if this introduces additional complexity.
- 25 (2) Imposing relational parameter and process constraints improves the performance of
26 uncalibrated models and reduces their uncertainty. This illustrates the potential value of the
27 combined use of higher complexity models and relational constraints for prediction in
28 ungauged basins, where no time series are available for model calibration.
- 29 (3) Due to the reduced feasible parameter space, the search for behavioral parameter sets
30 focuses on the feasible parameter space only.
- 31 (4) Imposing constraints prevents the model from over-fitting on calibration time series and
32 therefore enables the model to more reliably perform outside the calibration period.

33
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