INVITED COMMENTARY

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How can we model subsurface stormflow at the catchment scale if we cannot measure it?

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1 | INTRODUCTION

Subsurface stormflow (SSF) can be a dominant run-off generation process in humid mountainous catchments (e.g., Bachmair & Weiler, 2011; Blume & van Meerveld, 2015; Chifflard, Didszun, & Zepp, 2008). Generally, SSF develops in structured soils where bedrock or a less permeable soil layer is overlaid by a more permeable soil layer and vertically percolating water is deflected, at least partially, in a lateral downslope direction due to the slope inclination. SSF can also occur when groundwater levels rise into more permeable soil layers and water flows laterally through the more permeable layers to the stream ("transmissivity feedback mechanism"; Bishop, Grip, & O'Neill, 1990). The different existing terms for SSF in the hydrological literature such as shallow subsurface run-off, interflow, lateral flow, or soil water flow reflects

the different underlying process concepts developed in various experimental studies in different environments by using different experimental approaches at different spatial and temporal scales (Weiler, McDonnell, Tromp-van Meerveld, & Uchida, 2005). Intersite comparisons and the extraction of general rules for SSF generation and its controlling factors are still lacking, which hampers the development of appropriate approaches for modelling SSF. But appropriate prediction of SSF is essential due to its clear influence on run-off generation at the catchment scale (e.g., Chifflard et al., 2010; Zillgens, Merz, Kirnbauer, & Tilch, 2005), on the formation of floods (e.g., Markart et al., 2013, 2015) and on the transport of nutrients or pollutants from the hillslopes into surface water bodies (Zhao, Tang, Zhao, Wang, & Tang, 2013). However, a precise simulation of SSF in models requires an accurate process understanding including, knowledge about water
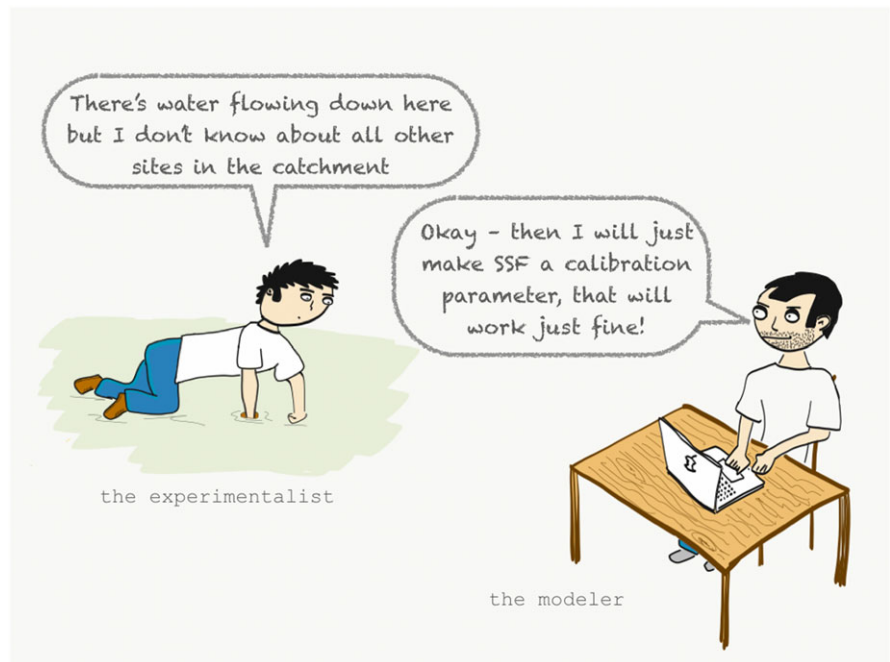
FIGURE 1 Caricature of the investigation and simulation of subsurface stormflow (SSF) (Illustration: Edoardo Martini)

pathways, residence times, magnitude of water fluxes, or the spatial origin of SSF within a given catchment because such factors determine the transport of subsurface water and solutes to the stream. But due to its occurrence in the subsurface and its spatial and temporal variability, determining and quantifying the processes generating SSF is a challenging task as they cannot be observed directly. Therefore, it is logical to ask whether we can really model SSF correctly if we cannot measure it well enough on the scale of interest (Figure 1).

This commentary reflects critically on whether current experimental concepts and modelling approaches are sufficient to predict the contribution of SSF to the run-off at the catchment scale. This applies in particular to the underlying processes, controlling factors, modelling approaches, research gaps, and innovative strategies to trace SSF across different scales.

2 | WHAT HAVE WE LEARNED FROM ALL THE EXPERIMENTAL STUDIES ABOUT SSF CARRIED OUT IN VARIOUS CATCHMENTS AT DIFFERENT SPATIAL AND TEMPORAL SCALES?

Experimental studies on SSF generation have been carried out in different mountainous catchments with steep, well drained soils (e.g., Maimai, New Zealand [e.g., McGlynn & McDonnell, 2003]), shallow soils with bedrock outcrops (Panola, United States [e.g., van Meerveld, Seibert, & peters, 2015], and Fudoji, Japan [e.g., Uchida, Asano, Mizuyama, & McDonnell, 2004]), or catchments with periglacial drift deposits (Bohlmicke, Germany [e.g., Chifflard et al., 2008], and Ore Mountains, Germany [e.g., Heller & Kleber, 2016]). These studies have resulted in comprehensive process knowledge about SSF, which was synthesized in several reviews (e.g., Ghasemizade & Schirmer, 2013)

and have led to the identification of controlling factors of SSF like initial soil moisture content (e.g., Blume, Zehe, & Bronstert, 2009; Chifflard & Zepp, 2008; Martini et al., 2015), water table development at the soil–bedrock interface (e.g., Anderson, Weiler, Alila, & Hudson, 2010; Jost, Schume, Hager, Markart, & Kohl, 2012), preferential flow paths (e.g., Laine-Kaulio, Backnäs, Karvonen, Koivusalo, & McDonnell, 2014; Sidle, Noguchi, Tsuboyama, & Laursen, 2001; Uchida, Kosugi, & Mizuyama, 2001), hillslope characteristics (e.g., Bachmair & Weiler, 2012), drainable porosity (e.g., Weiler & McDonnell, 2006), precipitation thresholds (e.g., Hopp, McDonnell, & Condon, 2011; Kienzler & Naef, 2008a, 2008b; Peralta-Tapia, Sponseller, Tetzlaff, Soulsby, & Laudon, 2014), soil properties (e.g., Bachmair, Weiler, & Nützmann, 2009; Hopp & McDonnell, 2009), soil depth (e.g., Tromp-Van Meerveld & McDonnell, 2006a, 2006b), or bedrock topography (e.g., Freer et al., 2002). Nevertheless, little of this understanding has been incorporated into current hydrological models. As catchment hydrologists, we are particularly interested in run-off generation at the catchment scale that seems more controlled by the interplay of processes than the details of individual ones. In other words, landscape heterogeneity and process complexity at the small scale can lead to typical emergent response behaviour at the catchment scale (McDonnell et al., 2007). From this, it follows that landscape structure can inform us about the dominant run-off generation mechanisms that are most often hidden in the subsurface and therefore so difficult to observe across the entire catchment. For instance, generation of SSF on low mountain ranges in middle Europe is strongly influenced by the widespread periglacial cover beds, which are a typical example for stratified soils (Hübner, Günther, Heller, Noell, & Kleber, 2016; Hübner, Heller, Günther, & Kleber, 2015; Kleber & Terhorst, 2013; Moldenhauer, Heller, Chifflard, Hübner, & Kleber, 2013). Although in soil science the Substrate-Oriented-Soil-Evolution-Model (Lorz, Heller, & Kleber, 2011) underlines the importance of stratified soils and lithological

discontinuities as a key element controlling ecological processes, in hydrologic research, less attention has been paid to the stratification of soils as a major trigger of lateral water paths (e.g., Reinhardt-Imjela, Maerker, Schulte, & Kleber, 2018, Reiss & Chifflard, 2015, Zhang, Lin, & Doolittle, 2014). The existence of a non-linear and threshold-type response of SSF to precipitation (e.g., Ali et al., 2015; Graham, Woods, & McDonnell, 2010) adds to the challenge of both measuring and modelling this process. Indeed, the detection of these thresholds helps to classify behaviours of different hillslopes; however, the controlling factors and processes responsible for these thresholds are not yet fully clear. Therefore, it is also still unclear if these thresholds are transferable to other sites (Zhao et al., 2013).

One possible way forward would be a comprehensive site inter-comparison and an innovative strategy to compare and combine all the obtained first-order controls to assess the SSF generation. Previous attempts have provided very informative results (Bachmair, Weiler, & Troch, 2012; Uchida, Tromp-van Meerveld, & McDonnell, 2005). But on the other hand, we should ask ourselves whether it is expedient to compare all these various experimental studies investigating SSF generation carried out in different hydroclimatic regimes, at different scales or by using different experimental approaches. A better way forward might be the development of a systematic method-orientated measurement program, which combines a mixture of appropriate methods specifically targeted to the identification and characterization of SSF generation and which will be applied across well-instrumented catchments covering different spatial scales within similar environments. The experimental investigation can then focus on understanding process heterogeneity and complexity in connection with controlling factors and landscape structure. Thus, it is indispensable to develop a method-orientated research approach, which is specifically targeted to SSF generation, covers standard as well as innovative methods, and can be applied across different catchments within similar environments. This kind of standardized and systematic protocol to capture and characterize SSF will help to improve the representation of subsurface processes in spatially distributed hydrological models.

3 | ARE THE EXISTING HYDROLOGICAL WATERSHED MODEL CONCEPTS REFLECTING SSF ADEQUATELY?

The simulation of catchment-scale run-off generation and the associated water balance in the unsaturated zone, including SSF, strongly varies with respect to the model concept and spatial scale of prediction. Methods range from detailed physically based approaches such as the Richards' equation (Beven & German, 2013) or the kinematic wave method (e.g. Flügel & Smith, 1999) to less complex conceptual models such as the Soil Conservation Service Curve Number methods. The conceptual models do not require detailed process knowledge, but we make the claim that for the development of process-based hydrological models, a good understanding of the generation of SSF and the incorporation of process knowledge is essential (e.g.,

Bachmair, Weiler, & Nützmann, 2010; McGuire, Weiler, & McDonnell, 2007; Zhu & Lin, 2009). However, parametrizing the experimentally identified and quantified SSF knowledge at the catchment scale is a problem, as at this scale, the spatial heterogeneity of soil properties and the spatial organization of the specific pathways in the subsurface are largely undeterminable (Lin & Zhou, 2008). And even if information on all model parameters was available at the catchment scale, the question posed by Tromp-van Meerveld and Weiler (2008, p. 25) "How much model complexity is needed to explain the observed subsurface flow response […]?" still remains unsolved. Indeed, it could be that the process complexity (e.g., matrix and preferential flow) and the natural variability of environmental properties (e.g., soil properties) collapse to a relatively simple functional relationship between a functional trait (e.g., soil moisture patterns) and catchment-scale run-off response (McDonnell et al., 2007).

Hydrogeophysical methods may have the potential to identify subsurface flow paths (e.g., Angermann et al., 2017; Binley et al., 2015) or, at least, soil heterogeneity (Martini et al., 2017), but their use is mostly limited to the hillslope scale (Vereecken et al., 2015). Here, subsurface flow paths are more likely to be connected over shorter rather than longer distances, which leads to higher effective flow velocities (e.g., Anderson, Weiler, Alila, & Hudson, 2009; Wienhöfer & Zehe, 2014). Preferential flow processes should be taken into account when calculating SSF in rainfall–run-off models at the catchment scale, but the representation of preferential flow is a particular challenge for all model concepts (e.g., Gerke, Germann, & Nieber, 2010; Hartmann, 2016). It would require model parameters (such as macropore density) at high temporal and spatial resolution, something that we can only determine at the scale of a soil column or a plot (e.g. Rinderer & Seibert, 2012). In addition, the spatial discretization (e.g., control volume or pixel) required if these approaches are used at the catchment scale is often in the order of tens to hundreds of metres and thus one or two orders of magnitude larger than the scale at which these physical relations (e.g., Richards' equation) originally have been developed. So it is doubtful that these models can still be referred to as "physically based" (Köhne, Köhne, & Šimůnek, 2009). In order to incorporate hydrological heterogeneity at scales larger than the plot or hillslope, hydrological models have used certain simplifications and assumptions. For instance, TOPMODEL (Beven et al., 1979) is based on the assumption that under steady-state flow conditions, the slope of the groundwater table is parallel to the slope of the surface topography. Only then is the topographic index derived from a digital elevation model such as the Topographic Wetness Index (Beven & Kirkby, 1979) a good proxy to estimate the groundwater table across a catchment. Other models, such as PDM (Probability Distributed Model, Moore, 2007) or VarKarst-R (Hartmann et al., 2015; Hartmann, Gleeson, Wada, & Wagener, 2017), implement subsurface heterogeneity by using Pareto functions.

Although these approaches are useful modelling concepts for capturing flow in the saturated zone, they do not explicitly incorporate SSF processes (Rinderer, van Meerveld, & Seibert, 2014; Seibert, Bishop, Rodhe, & McDonnell, 2003). Therefore, new modelling concepts are necessary, which explicitly incorporate the process

knowledge and first-order controls of SSF that were obtained in many experimental studies at various spatial scales. In addition, new ways have to be found to parameterize rainfall–run-off models adequately to calculate SSF at scales larger than a soil column or an experimental plot. Instead of continuing to investigate the process complexity of SSF with more and more experimental studies at different sites, we call for a concerted, method-orientated experimental approach carried out in accordance with the new approaches to include SSF explicitly in catchment-scale rainfall–run-off models. We thus generate process knowledge based on a systematic measurement program, which in turn allows us to parameterize and calibrate SSF modules in rainfall–run-off models at the catchment scale.

4 | CAN WE REALLY VERIFY SIMULATED SSF?

Rainfall–run-off models are used for studies that are either investigative or predictive (Blöschl & Sivapalan, 1995). In both cases, the simulated SSF is mainly calibrated and validated based on single rainfall–run-off events (e.g., artificial sprinkling experiments) for which tracer hydrological data and information on specific run-off components are available (e.g., Markart et al., 2015; Uhlenbrook, Roser, & Tilch, 2004). However, it is obvious that these single events with steady-state conditions are not sufficient to capture the whole range of SSF response that depends on factors such as initial conditions and rainfall intensities and is often threshold dependent. Furthermore, the quality of a run-off model is still assessed by comparing modelled and observed total run-off measured at a gauge often situated at the catchment outlet. This is not expedient for studying the generation of SSF. However, currently, SSF in both types of rainfall–run-off models (investigative and predictive) is still an unvalidated parameter, which is adjusted (calibrated) to fit the model output against available discharge observations. The assumption is that if the model discharge fits the discharge observations satisfyingly, SSF is also simulated correctly. This is not necessarily true, particularly when considering changes in SSF contributions over the course of an event. High frequency measurements of chemical tracers and stable water isotopes (e.g., ^{18}O and ^2H) in streams and soils have the potential to gain better insights into SSF (e.g., Mueller et al., 2014; Sprenger et al., 2018). However, this comes with additional challenges: for soil water isotope data, the choice of the sampling method (e.g., wick sampler and suction cups) predetermines whether the more tightly bound or the more mobile soil water is extracted (Landon, Delin, Komor, & Regan, 1999). Even the choice of laboratory has been shown to influence the results of isotope analysis (Orlowski et al., 2018). In addition, hydrochemical signatures that can give insights into the biogeochemical-hydrological process links at different spatial scales (e.g., McKnight, Burns, Barnard, & Gabor, 2015; Ponton, West, Feakins, & Galy, 2014) are promising approaches to identify subsurface flow networks. The use of such "tracers" (e.g., N, DOC, ^{13}C, ^{15}N, and microbial communities; Blume & van Meerveld, 2015; Sanderman, Lohse, Baldock, & Amundson, 2009; Sebestyen et al., 2008), their chemical characteristics (e.g., biodegradable organic carbon and excitation emission matrix; Barnard, Burns, McKnight, Gabor, & Brooks, 2014; Burns, 2014; Hood, Williams, & McKnight, 2005), and their depth distribution in soils (Gabor, Eilers, McKnight, Fierer, & Anderson, 2014; Hassouna, Massian, Dudal, Pech, & Theraulaz, 2010; Wynn, Harden, & Fries, 2006) in combination with traditional tracers (e.g., ^{18}O, ^2H, and SiO_2) may offer new opportunities for testing hydrological models. Nevertheless, limited consideration has been given to assimilating these approaches into rainfall–run-off models (Ebert, McKnight, Lajtha, Hartnett, & Jaffe, 2013).

5 | CONCLUSIONS

Existing empirical studies have revealed different facets of SSF across catchments in different environments. Nevertheless, deficits still exist in the capability to use this knowledge to generalize our process understanding on subsurface flow dynamics at the catchment scale. This might be due to the fact that a generally accepted organizational framework for site intercomparison is not yet available. We have to consider whether such a framework is absolutely necessary or approaches based on a few representative monitoring sites and an upscaling approach based on landscape structure seem a promising way forward.

Nevertheless, many catchment hydrological models do not even consider SSF, whereas the more detailed, physically based models that do so are difficult to parameterize or validate without spatial information on catchment states (e.g., soil properties) and dynamics (e.g., antecedent soil moisture). The run-off response at the catchment scale is also most likely not dominated by the same detailed processes that we observe at the point or plot scale but instead by an emergent behaviour that results from an interplay between small-scale and large-scale processes. So how can we simulate subsurface flow at the catchment scale if we cannot even measure it?

We advocate for a more systematic design of future empirical studies on SSF across a range of representative landscapes which are concerned with the need not only to improve process understanding but also to develop new modelling approaches. Instead of model validation on the basis of single rainfall–run-off events for which tracer hydrological data and hydrometric measurements of selected run-off components are available at a single gauged trench, it is instead necessary to continuously monitor subsurface run-off components at the catchment outlet as well as on its hillslopes with high temporal resolution over longer time spans. We see great potential in exploiting the potential of distributed sensor networks and new tracers or combination of tracers that can give direct or indirect information on SSF. To address this concern, we need to collaborate with colleagues from neighbouring disciplines that have developed biogeochemical methods that can also be highly informative for SSF (e.g., microbial communities and nanoparticles as tracers). These new types of datasets will bring us one step further towards knowing what, where, and when to measure and how complex our models need to be in order to make our SSF simulations more realistic than they are today.

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