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The effect of model complexity in simulating unsaturated zone flow processes on recharge estimation at varying time scales

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SUMMARY

Recent increases in computational power have led to the development of more advanced physically-based models which can handle a wide range of environmental processes. Although these models are very useful for increasing our understanding of unsaturated zone flow processes, their outputs usually contain high uncertainty, particularly when the level of complexity is not supported by observations. In this context, the aim of this paper is to compare the performance of three different model conceptualizations of a shallow unsaturated soil zone using the physically-based model HydroGeoSphere (HGS). To accomplish this task, we simulated actual evapotranspiration (ET), water content (WC) and discharge (D) from a weighing lysimeter for each of the conceptual models. Conceptual Model 1 considers the lysimeter as a homogeneous zone with matrix flow, while Conceptual Model 2 has an added preferential flow component. Conceptual Model 3 includes layered heterogeneity in addition to the matrix and preferential flow components. The results indicated that the model performance in reproducing daily ET, WC and D improves when we move from simple models to more complex models. A comparison between event-based, monthly, seasonal and yearly time scales indicates that the simplest conceptual model is not reliable for reproducing event-based discharges. However, it can compete with more complex models at annual scales, although the uncertainty bound for the simple model is very high. While increasing complexity from the simplest to the more complex model leads to lower uncertainty bounds and more reliable values of the lysimeter discharge at monthly and seasonal time scales, uncertainty bounds became larger when complexity increased in the most complex model. This is related to a higher number of unknown model parameters in the calibration which are not supported by the available observation datasets.

1. Introduction

Recent increases in computational power have motivated the scientific community to develop and apply more complex models of coupled environmental processes. Hydrological models, for example, have become more sophisticated in terms of the simulated unsaturated zone flow processes. Although applications of such complex models may in theory lead to increased knowledge into the governing processes, they have their own limitations such as over-parameterization when applied in practice (Perrin et al., 2001). On the other hand, simple models have proved their efficiency and applicability in hydrology, particularly in operational contexts such as rainfall-runoff (Birkel et al., 2010; Brauer et al., 2013).

Physically-based numerical simulation models are valuable tools which can be applied with a range of complexity, depending on the available data. These models have proven to be useful due to the integration of multiple hydrological processes (Brunner et al., 2012; Schwarzel et al., 2006), their applicability for areas which suffer from lack of long-term data (Bolger et al., 2011) and where the measured values of their required parameters are available (Mirus et al., 2011). However, these types of physically-based models have also been criticized for their complexity (Beven, 1993, 2006), including problems of over-parameterization and equifinality (non-uniqueness). In fact, as processes are

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simulated with greater detail, the number of parameters in physically-based models will accordingly increase. This issue is exacerbated when physically-based models are employed at large scales such as catchments where limited available data does not support the embedded complexity and therefore can have an adverse effect on prediction uncertainty (Uhlenbrook et al., 1999; van der Perk, 1997).

To overcome this limitation and fill the gap between the laboratory- and field-scale application of physically based models, weighing lysimeters can provide a valuable framework to estimate recharge. It is worth noting that lysimeters with free-drainage boundary conditions do not fully represent the real field-scale processes leading to recharge because they are disconnected from the water table and therefore capillary fringe effects are neglected. However, Abdou and Flury (2004) showed that the differences are minimal unless strong vertical structure exists among soil particles. Seneviratne et al. (2012) have also shown that the monthly streamflow is highly correlated to the monthly lysimeter discharge for a case study in Switzerland. The fact that initial and boundary conditions are well-known in a lysimeter makes them ideally suited for a variety of purposes such as estimating soil hydraulic parameters (Abbaspour et al., 1999; Durner et al., 2008), measurement of water uptake and root distribution (Schelle et al., 2013), and for estimating recharge (Kendy et al., 2003; Selle et al., 2011), which is the focus of the current study. It should be noted that we use the term "lysimeter discharge" in this text to represent the aquifer recharge. This assumption seems reasonable since the bottom of the lysimeter is within half a meter from the average water table which is measured in a nearby piezometer. Many of the published lysimeter studies, however, have neglected preferential flow while its importance under natural conditions is now well accepted (Anderson et al., 1997; Beven and Germann, 2013; Weiler and Fluhler, 2004; Zheng and Gorelick, 2003). For instance, Selle et al. (2011) showed that neglecting preferential flow in numerical simulations can bias the predictions of soil moisture and deep percolation.

Preferential flow is one of the processes that, when applied in physically based models, can greatly increase the number of model parameters. Among the many approaches that have been suggested for preferential flow modeling (e.g., Beven and Germann (2013), Kohne et al. (2009), Simunek et al. (2003)), dual permeability (DP), which assumes that water can flow in the matrix as well as in macropores, is one approach that has been widely applied (Kohne et al., 2006; Kordilla et al., 2012; Wang et al., 2014). The DP approach can simulate peaks due to flow through macropores, as well as base flow and recessions arising from matrix flow. Although attractive, employing the DP concept to represent preferential flow in vadose zone modeling requires additional parameters, such as the fraction of macropores which cannot typically be measured in the field and therefore calibration is required.

While considerable effort has been devoted to seeking simplification strategies involving parameter and/or process lumping in environmental simulations (Shen et al., 2013; Touhami et al., 2013; Zhu and Sun, 2009), few studies have explored the effects of simplification on a model's predictive performance (Doherty and Welter, 2010; Watson et al., 2013). This issue is addressed in the current study and is, to the best of our knowledge, the first time compared temporally. We applied three different conceptual models (representing different levels of complexity) and compare them in the framework of a weighing lysimeter simulation, using the physically-based model HydroGeoSphere (HGS) (Therrien et al., 2010). Output uncertainty of each conceptual model was minimized through calibration of the parameters against actual evapotranspiration, water content and discharge. The main objective of our study is to evaluate the performance of different conceptual models in replicating the lysimeter discharge for a varying range of time scales. Specifically, we focused our research on whether process simplification and parameter reduction result in acceptable estimations of lysimeter discharge values.

In this paper, we first describe the features of our research lysimeter. We then briefly explain how DP, flow interception (Appendix A), evapotranspiration (Appendix A) and uncertainty analysis are considered in our research. Subsequently, we introduce the three different model complexities and model parameterization. We then show the performance of the three different conceptual models and discuss uncertainty of the predictions for different time scales.

2. Data and methods

2.1. Rietholzbach lysimeter

The lysimeter of our study is a free drainage lysimeter located in the Rietholzbach research catchment (Seneviratne et al., 2012), which is a pre-alpine headwater catchment of the Thur River basin in northeastern Switzerland. The average annual sums of precipitation (measured at the meteorological station at the same site) and evapotranspiration (measured with the lysimeter) in Rietholzbach are around 1450 and 560 mm, respectively (based on data from 1976 to 2007, Ewen et al. (2011)). The lysimeter belongs to the category of large lysimeters with a diameter of 2 m and a depth of 2.5 m, and is equipped with TDR sensors for measuring water content (soil moisture). These sensors are located at depths of 5, 15, 25, 35, 55, 80, and 110 cm from the top of the lysimeter. However, due to inconsistency in soil moisture data, the water content values at depths of 35 and 110 cm were not included in the simulations. The lysimeter has been back-filled with gleyic cambisol (clay loam) in 1974 with surrounding soil. Whether the soil is layered or structured is unknown. In fact, this is one of the reasons we included different levels of complexity in our modeling experiment. The surface of the lysimeter is covered with grass to reflect the surrounding natural conditions of the vegetation (structure, cutting, fertilization). Using a dye tracer, Menzel and Demuth (1993) found preferential flow in the Rietholzbach lysimeter, confirmed by Vitvar et al. (1999) by application of ^{18}O isotopes. However, to the knowledge of the authors, no quantitative modeling of this fast flow in the Rietholzbach lysimeter has been reported.

2.2. Model setup

In order to evaluate different levels of complexity and the effect of increasing model parameters on predictive uncertainty, three different conceptual models were analyzed within the framework of the HGS model. In conceptual model 1 (C1) with 7 parameters, it was assumed that the lysimeter consists of only matrix flow without any explicit component to represent flow in macropores (Fig. 1a). However, in order to allow fast flow, the matrix hydraulic conductivity was given a wider range of variation during calibration (Elci and Molz, 2009). Conceptual model 2 (C2) with 13 parameters was set similar to C1 with the same calibration dataset, with the only difference being that DP was added to C2 in order to include preferential flow (Fig. 1b). This model represents mainly the effect of adding complexity through including *additional processes*. Conceptual model 3 (C3) includes 25 parameters and was distinguished from C2 by adding heterogeneity consisting of four layers of soil, each represented by soil moisture data at different depths (Fig. 1c). Model C3 mainly represents the effect of adding complexity through including *additional parameters*.