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What can we learn from multi-data calibration of a process-based ecohydrological model?

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We assessed whether a complex, process-based ecohydrological model can be appropriately parameterized to reproduce the key water flux and storage dynamics at a long-term research catchment in the Scottish Highlands. We used the fully-distributed ecohydrological model EcH_2O, calibrated against long-term datasets that encompass hydrologic and energy exchanges, and ecological measurements. Applying diverse combinations of these constraints revealed that calibration against virtually all datasets enabled the model to reproduce streamflow reasonably well. However, parameterizing the model to adequately capture local flux and storage dynamics, such as soil moisture or transpiration, required calibration with specific observations. This indicates that the footprint of the information contained in observations varies for each type of dataset, and that a diverse database informing about the different compartments of the domain, is critical to identify consistent model parameterizations. These results foster confidence in using EcH_2O to contribute to understanding current and future ecohydrological couplings in Northern catchments.

1. Introduction

Numerical models are crucially important in the environmental sciences: models can complement and integrate theory and empirical data by incorporating testable hypotheses and by extending knowledge at spatial and/or temporal scales inaccessible to current observation methods. In particular, process-based models seek to explicitly represent the "*state variables and fluxes that are theoretically observable and can be used in the closure of assumed forms of the laws of conversation of mass, energy, and momentum at temporal scales characterizing the underlying physical processes*" (adapted from Fatichi et al., 2016). In contrast to conceptual and empirical approaches, physically-based models facilitate investigation of specific variables at local, process-specific scales (e.g., Endrizzi et al., 2014; Manoli et al., 2017; Niu and Phanikumar, 2015; Pierini et al., 2014). Additionally, a fully-distributed description of the simulation domain opens the possibility for tracking intra-system patterns and dynamics (e.g. Maxwell and Condon, 2016; Pierini et al., 2014), a task much less accessible to coarser spatial representations (i.e., lumped or semi-distributed models). Combining these two methodological choices with physically-based, fully-distributed models is thus a way to disentangle feedbacks and non-linear dynamics across fundamentally different processes (e.g. Drewry et al., 2010; Tague, 2009), and better predict system behaviour outside recorded environmental conditions (Seibert, 2003; Uhlenbrook et al., 1999). These tools are of particular relevance for the emerging field of critical zone science (National Research Council, 2012), which seeks integrated understanding of ecological, geological, geomorphological and pedological processes within a framework of hydrological partitioning (Brooks et al., 2015).

Within the field of hydrology the issue of appropriate model complexity is a focus of ongoing discussion. The corollary of expanding process-based approaches towards an "universal model" is an inevitable increase in complexity as explicit descriptions of additional system characteristics are added (e.g. topography, soil texture, tree height, canopy density etc.) (Band et al., 2001; Maxwell and Condon, 2016). Arguing that many of these numerous parameters cannot be appropriately measured,

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some fear that evolution of complex multi-disciplinary models only layer up unavoidable uncertainty and are prone to equifinality, whereby several combinations of parameter values –realistic or not– yield comparable performance (e.g. Beven and Binley, 1992; Beven and Freer, 2001; McDonnell et al., 2007).

The utility of measurements to help constrain the model solution space and identify feasible model configurations has been an increasingly central issue in hydrological model calibration. Sufficiently informative observations are necessary to ensure that the goodness of model-data fit attained effectively translates into physically-sound information for the internal model parameters; i.e., getting the right answers for the right reasons (Beven and Binley, 1992; Kirchner, 2006). The problem of equifinality—a particular case of *underdetermination* (Duhem, 1954)—is apparent when stream discharge is the only monitored variable available for calibration. Unfortunately, this remains the most common situation. The widespread use of streamflow time series to calibrate and validate models has spurred the development of elaborate single and multiple-criteria goodness-of-fit metrics (Kling et al., 2012; Krause et al., 2005; Legates and McCabe, 1999; Madsen, 2003; van Werkhoven et al., 2009) and calibration algorithms (Duan et al., 1992; Gupta et al., 1998; Sorooshian and Dracup, 1980; Tang et al., 2007; Tolson and Shoemaker, 2007) directed toward extracting a maximum of information content from this type of data (He et al., 2015; Rouhani et al., 2007; Shafii et al., 2017).

However, the information contained in streamflow time series is often insufficient to inform the parameterization of physically based models. Parameter values that represent physical properties of the catchment are usually poorly identified and become very sensitive to boundary conditions (Maneta et al., 2007). The situation deteriorates as more complex models incorporate increasingly detailed descriptions of catchment functioning. To constrain parameters of components associated with different subdomains of the model (ecological, surface, subsurface, etc.) it is desirable—but often impractical—to diversify data sources (Fang et al., 2013; Larsen et al., 2016; Rajib et al., 2016; Thorstensen et al., 2015). Combining different types of observations reduces information redundancy and provides direct insights into the different groups of physical processes represented in the model (Clark et al., 2011; Fatichi et al., 2016). A data-extensive approach to model calibration makes the choice of performance metrics easier because the information contained in observations is more directly related to the model compartment being calibrated (e.g. Birkel et al., 2014). Information diversity, however, brings other issues related to the assimilation of observations with diverse characteristics during calibration: some are technical e.g. combining spatio-temporal scales and associated uncertainties, while others are more fundamental to modelling, e.g. parameters compensating for model imperfections (Clark and Vrugt, 2006), or overlapping constraints and thus, possibly "pulling" the model in different directions (Efstratiadis and Koutsoyiannis, 2010). In other research fields, this approach is exemplified by the current efforts and associated challenges in assimilating multiple types of carbon cycle data to optimise Earth system models (Kaminski et al., 2013; Peylin et al., 2016).

The ecohydrology of high-latitude, energy-limited landscapes has traditionally been understudied despite the global ecological importance of this region. Since studies of plant-water couplings across disciplines gained momentum in the late 90s (Bonell, 2002), research efforts in ecohydrology have been primarily conducted in environments where water scarcity (Newman et al., 2006) or permanent presence (e.g., wetlands (Rodriguez-Iturbe et al., 2007)) makes hydrology an obvious, critical control upon how plants distribute and compete. Only recently, efforts have been directed towards understanding the specific ecohydrological processes of boreal, energy-limited regions (e.g. Cable et al., 2014) While there have been process-based model developments dedicated to the hydrology of high-latitude environments (e.g. Endrizzi et al., 2014; Kuchment et al., 2000; Lindström et al., 1997; Pomeroy et al., 2007), most model applications in these regions lack an explicit implementation of vegetation dynamics (e.g. Ala-aho et al., 2017a), and thus, cannot finely capture ecosystem imprints on water partitioning at the catchment scale.

High-latitude regions comprise mixed temperate forests, boreal forests and tundra, covering nearly 20% of the continental land mass (Tetzlaff et al., 2015a). These regions are subject to rapid climate change, with significant regional to global-scale implications (Hinzman et al., 2013), including shifts in precipitation regime and snow-mediated water balance (Bintanja and Andry, 2017; Jiménez Cisneros et al., 2014) and associated implications for runoff generation (Peterson et al., 2002; Zhang et al., 2014). While such environmental change has been observed to alter water pathways and flow regimes (Dye and Tucker, 2003; McClelland et al., 2006; Tetzlaff et al., 2013) and ecosystem dynamics (Naito and Cairns, 2015; Piao et al., 2008), further work is needed to identify the underlying mechanisms. Reasons for the limited understanding so far lie in the fine-scale landscape heterogeneity and the implications for spatial variation in energy inputs, as well as the logistical difficulties of collecting data in comparatively remote areas (Pomeroy et al., 2013; Tetzlaff et al., 2013), and the alarming recent decline in long-term monitoring of northern catchments (Laudon et al., 2017). However, we need to understand such processes and the related uncertainties of water cycling in these regions, while ongoing/projected biome shifts (e.g., (Beck et al., 2011; Williams et al., 2007)) call for particular scrutiny of ecosystem influence on water availability (Law, 1956) and vice-versa.

In this study, our main aim was to investigate to what extent a data-extensive approach to calibration can constrain the range of behavioural configurations of a highly-parameterized, physically-based model, such that the achieved parameter sets can be used as falsifiable hypotheses of the internal functioning of the catchment. For this, we used a distributed ecohydrologic model (EcH$_2$O, see (Maneta and Silverman, 2013) that integrates a kinematic hydrologic and energy balance model, with a vegetation dynamics model. The model is calibrated using several combinations of data types covering a range of ecohydrological variables collected at a long-term experimental northern montane catchment. We ask the following questions through our modelling experiments, *1)* what are the physical insights gained across ecohydrological processes? *2)* how valuable are the information contents brought by the different constraining datasets? Addressing these questions will help building a robust ecohydrological modelling framework dedicated to critical zone functioning in high-latitude environments.

2. Material and methods

2.1. Study site

The Bruntland Burn (Fig. 1) is a small catchment (3.2 km^2) located in the eastern Scottish Highlands (57°8′N 3°20′W). It is a headwater of the River Dee, which provides drinking water for the city of Aberdeen (250,000 people), ecosystem services such as an Atlantic salmon fishery, and has EU conservation designations. The region receives around 1100 mm of average annual precipitation (P), distributed quite evenly throughout the year, although November–February and June–August are usually wettest and driest periods, respectively. Less than 5% of P occurs as snowfall. The climatic water balance is energy-limited, with 400 mm of annual Potential Evapotranspiration (PET). The mean annual