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INTRODUCTION TO A SPECIAL SECTION
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Special Section:
Advancing process representation in hydrologic models: Integrating new concepts, knowledge, and data

Advancing Process Representation in Hydrological Models: Integrating New Concepts, Knowledge, and Data

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Key Points:

- Data sources, such as isotopes or remote sensing, are increasingly used for enhancing model simulations and process representation
- The added value of including specific (sub-)processes in models depends on the relevance of the process in the research area
- Both top-down and bottom-up approaches are essential for reliable transfer of process knowledge to model structures

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Abstract Model fidelity and accuracy in process representations have been the crux of scientific hydrological modeling, creating a pressing need for a better linkage between the development of hydrological models and the growing number of data sources and measurement techniques. Improved representation of process dynamics in hydrological models can provide new insights into complex hydrological systems and point out less understood natural phenomena that need further investigation. This special issue includes contributions that offer potential solutions and strategies to improve and test the representation of hydrological processes. We have organized the special issue contributions into four topical categories: (a) Beyond streamflow, which looks into the power of complementary data sources in addition to traditionally used streamflow for process inference. (b) Challenge of subsurface hydrology, that reflects on lesser understood processes under the surface and their impact on the model structure. (c) Evaporation in hydrological modeling, linking ecological aspects to the hydrological functioning of the natural system. Finally, (d) top down vs. bottom up modeling approaches, relied upon for process representation analysis. The special issue and our reflection on the contributions present a snapshot of ongoing efforts for integrating new concepts, knowledge, and data in process representation in hydrological models.

1. Introduction

1.1. Motivation and Background

Model fidelity and accurate process representation at the scale of application have been the crux of [scientific] hydrological modeling. Additionally, the need to include ecological and/or anthropogenic factors pushes for a stronger synergy between the development of hydrological models and the growing volume of observational data. The advancement in process representation provides insights into the complex interactions of hydrological processes and potentially results in more reliable simulations and hence decisions. The special issue "Advancing process representation in hydrological models: Integrating new concepts, knowledge and data" in Water Resources Research is part of wider ongoing activities to reconcile the efforts for better process representation in models and in developing and applying hydrological models across scales and for multidisciplinary purposes.

This special issue is a materialization of several years of well-attended sessions at the European Geosciences Union General Assembly (2016–2021) and American Geophysical Union Fall Meeting (2016) organized by the editors of the special issue. The editors were also involved in organizing the second modeling workshop of the initiative "Improving the Theoretical Underpinnings of Hydrological Models" in Sopron, Hungary in 2018, initiated by Clark et al. (2016).

The special issue received contributions from September 2018 to June 2021. In this editorial, we discuss 29 contributions to the special issue. The authors' affiliations are spanning across 19 countries (Figure 1), and case studies in the submissions cover 11 countries. From the 29 contributions, 10 are openly accessible.

We categorize the contributions to the special issue into four major topical themes presented in the following section. We conclude the editorial with our findings and reflection.

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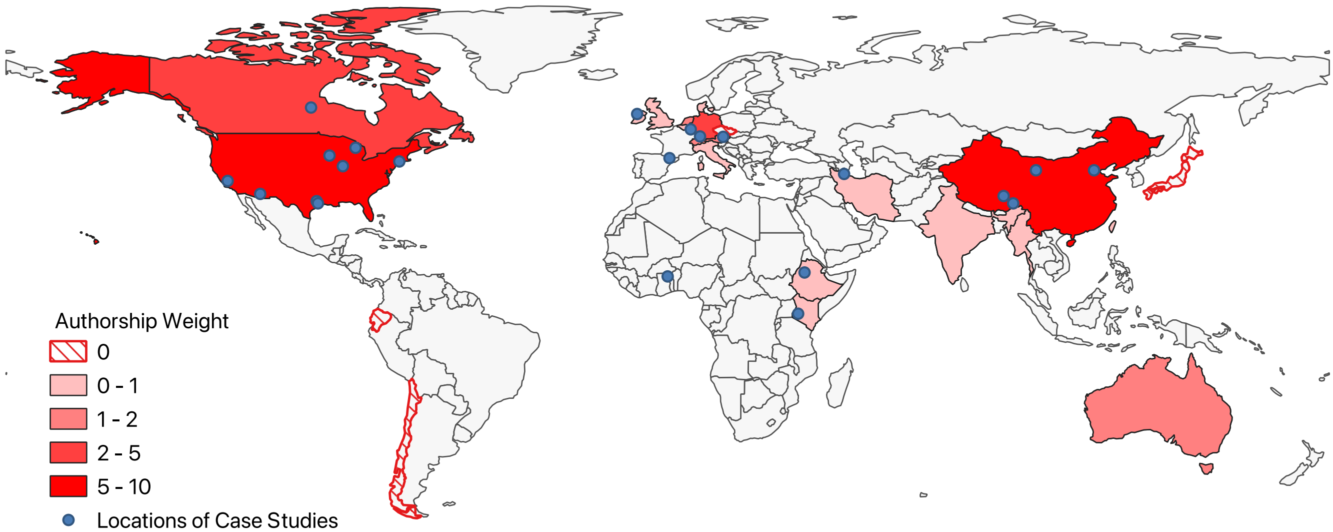

Figure 1. Geographic distribution of contributing authors and location of case studies. The authorship contribution per country is calculated based on the summation of primary (first) affiliation of each author of all contributions, distributing a unit value equally between the authors of each publication. Red hash marks the countries that are not the primary first affiliations (with the contribution of 0). Dots identify the location of the case studies.

2. Topical Themes

2.1. Beyond Streamflow

Streamflow quantities as an integrated metric of processes across catchments or basins are commonly used for model calibration. However, identifying individual processes from streamflow can be challenging, hence additional data sources are required to improve the representation of processes within models.

The benefit of using additional data sources at the large scale is shown by using remote sensing products (Dembélé et al., 2020; Huang et al., 2020; Soylu & Bras, 2021). Dembélé et al. (2020) improved the simulated spatial patterns of a semi-distributed hydrological model with on hydrological information from satellite observation (ESA CCI, GRACE) and hydrologic model-based simulation of evaporation (GLEAM and MODIS). Huang et al. (2020) combined water levels from satellite altimetry (Jason-2) with river width data from Landsat and water levels from measurement stations. The latter two data types were used to illustrate the potential of prospect data from the SWOT mission (Surface Water and Ocean Topography). The authors showed that an improvement streamflow estimation was achieved even when using limited portion of available remote sensing data. Their finding emphasizes the value of satellite-based water level data for predictions in ungauged basins. Last but not least, Soylu and Bras (2021) provided an algorithm to derive shallow groundwater data using spaceborne soil moisture observations combined with a Hydrus-1D model.

Isotope data have been used to improve representations of flow pathways and storage compartments (Evaristo et al., 2019; Holmes et al., 2020). Evaristo et al. (2019) linked soil moisture conditions and the evapotranspiration process by using isotopes to quantify the age of the water that various species of plants transpire. Isotope tracers were used in Holmes et al. (2020) for a process-specific calibration of the model isoWATFLOOD™. A multi-objective optimization calibration strategy for streamflow and isotopes led to improvement in the simulation of hydrological states and fluxes, in particular of evapotranspiration and soil moisture storage, and provided a better representation of landscape controls on the hydrological system. Isotope-based model optimization led to lower evaporation and higher transpiration (while the total evapotranspiration remains unaffected). Moreover they concluded that lateral flow is originated predominantly from deeper soil, which resulted in an increase in base-flow and a decrease of inter-flow.

The multi-objective calibration with additional data such as isotopes (Holmes et al., 2020) or remote sensing products (Dembélé et al., 2020) lead to a small decrease in the performance of streamflow, but a significant increase of the accuracy in representing individual processes: The benefit for the process representation highly compensates the reduction in streamflow performance metric. When the model structure can accommodate and assimilate additional information, the spatio-temporal variability of internal fluxes and states can be improved.

Széles et al. (2020) contributed to a better linkage of field observations to models. They demonstrated how a large amount of additional field observations can be integrated into a hydrological model (HBV) in a small catchment in Austria (66 ha). By step-wisely adding information of three different processes, namely snow cover, soil moisture, and runoff generation, model performance was improved for these processes simultaneously.

While the above studies show the crucial importance of additional data beyond streamflow, streamflow is becoming central again when data are collected with crowd-sourced approaches - a new way of informing models with additional and distributed information. The presented crowd-sourced approaches collect water level and water temperature variables (Avellaneda et al., 2020; Weeser et al., 2019). In both studies, the benefit of using a low-cost and relatively easily applicable method was emphasized. Avellaneda et al. (2020) differentiated between streamflow conditions: Citizen-based observations could provide helpful additional information for low and medium streamflow conditions, while the added value was low for high flows or in snow periods due to the difficulties in taking reliable measurements considering higher risk. Weeser et al. (2019) highlighted that crowd-sourced water level monitoring can shed light in process understanding of ungauged basins.

2.2. Challenges of Modeling Under Our Feet - Subsurface Hydrology

This special issue received several contributions on linking the surface and subsurface water fluxes. Demasking this interaction is a key to our understanding for sustainable water management. These papers are generally asking for more rigorous investigation of surface water - ground water interactions, while calling for careful evaluation of often accepted assumptions and conceptualizations.

Barclay et al. (2020) investigated the impact of various subsurface conceptualizations on model performance. Various models, if "well calibrated", can result in similar performance metrics while they exhibit different spatial properties. This finding emphasizes the need for new approaches to observe and evaluate groundwater flow at relevant scales. Hong et al. (2020) have developed a bidirectional exchange scheme applied to the Brazos River in Texas, USA, for studying the interaction of subsurface water and streamflow, which allows for a more rigorous representation of interactions of subsurface flow, the saturated zone, and the stream. The impact of root exudation on subsurface processes was considered in Roque-Malo et al. (2020) with a biogeochemical view on the nutrient cycle in the soil. Schuler et al. (2020) investigated the modeling of a karstic basin in Ireland with springs and a pipe model conceptualization. They evaluated their model result with spring discharge values, while accounting for different types of noise in the data. A theoretical contribution highlighted the importance of spatial sampling of groundwater observations, which can affect the inference of the subsurface flow (Naderi & Gupta, 2020).

The special issue also received contributions on the coupling of surface and subsurface flow at larger scale and under various climate conditions and scenarios. Ghasemizade et al. (2019) evaluated recharge strategies for the agricultural managed aquifer of the southern Central Valley in California. They quantified the risks and benefits of various recharge scenarios on the agriculture activity itself. The authors, based on the model, predicted that agricultural land cover mismanagement can result in depletion or increase in groundwater level affecting the agricultural activities in a feedback process. In another study, water storage to support irrigation in dry phases was analyzed for Ethiopian hilllands by developing a parsimonious hillslope model (Alemie et al., 2019). Taie Semiromi and Koch (2020) evaluated subsurface water conditions in the Garasou River Basin in Iran considering the impact of climatic and human intervention through pumping. They showed that eliminating human intervention in the future may not be enough to maintain the current status of the natural system and water levels, as climate change will become a dominant factor. Rajib et al. (2020) analyzed the importance of prairie potholes in surface hydrology and the impact they can have on water yield, model performance with regards to streamflow, and simulated soil moisture in comparison with satellite observations. They concluded that inclusion of potholes processes, in the employed SWAT model, improved streamflow simulation accuracy and also altered the spatial patterns and magnitudes of water yields across the upper Mississippi River basin.

Adding more processes explicitly in models calls for a number of considerations. Perhaps inclusion of certain [unconventional] processes or structures are essential to properly answer the research question at a given specific location. On the other hand, it is challenging to identify processes that are not only relevant in very specific cases, but are of general importance (at least under certain physio-geographical conditions) and are therefore worth to be generally included in models. Furthermore, one should evaluate if implementing a novel (sub-)process warrants the added complexity [with use of additional data sources].

2.3. Evapotranspiration Rattling the Gates of Hydrological Modeling

While distributed observations of precipitation are becoming the standard, and streamflow is by definition a catchment integrator, observations of evapotranspiration at catchment or large scale are still particularly challenging and uncertain, despite increasing availability of process-based models and remote sensing products. Accurate estimates of evapotranspiration and its spatio-temporal variability are however fundamental for an accurate characterization of the hydrological budget. This is likely the reason why several contributions for the special issue provide insights on the evapotranspiration process.

Looking at the physics of bare-soil evaporation, Novak (2019) employed a process based model to test the validity of the equilibrium approximation assumption for evaporation of water in the soil, For example, whether soil pore liquid and water vapor can be considered in thermodynamic equilibrium. Nonequlibrium effects are indeed demonstrated to be negligible for cumulative evaporation for most practical cases.

Process based modeling is also used to show that the spatial discretization of near-surface meteorological forcing data can be averaged without losing accuracy in the estimate of the total evaporative water loss, given that soil conditions are well characterized (Trautz et al., 2019). This implies that effort should be dedicated to estimate soil textural observations accurately, rather than to detailed reconstruction of above surface meteorological profiles. Estimates of bare-soil evaporation were also the objective of Or and Lehmann (2019), who developed a novel method to compute soil evaporation based only on considerations of soil hydraulic properties and meteorological forcing, but without specific assumptions that are typical for classic formulations such as the Penman-Monteith equation. They defined an active surface evaporative capacitor depth based on the characteristic length of evaporation which depends on soil textural properties. This relatively simple model allows to spatially resolve bare-soil evaporation at the global scale with estimates that are in reasonable agreement with previous global products, but also challenge some of the current assumptions in computing bare-soil evaporation at large scales.

Beyond bare soil evaporation, there has been a recent raising interest in estimating the ratio between transpiration T and evapotranspiration ET. Along these lines, Cui et al. (2020) used a high-frequency laser spectroscopy to analyze water vapor isotopes and constraining estimates of T/ET for an alpine meadow ecosystem in the Tibetan Plateau. They found a strong seasonal variability of T/ET from 0.15 to 0.73, mostly controlled by near surface soil water content and only in a minor fraction by LAI. Using isotopes for ecohydrological separation, Evaristo et al. (2019) showed that different plant species use water of different ages in an experimental study run in the controlled experimental facility of Biosphere-2. Most importantly, soil water is significantly older than the mobile water that rapidly recharge the groundwater through preferential flow pathways. The conclusion is that there are more complex mechanisms at play than simply considering water in the soil as well-mixed and trees roots as preferential pumps for water uptake.

From a model perspective, Wei et al. (2020) refined estimates of evapotranspiration using the Shuttleworth-Wallace model and Bayesian model evaluation to scrutinize multiple hypotheses about alternative representations of energy exchange, specifically how to account for the energy imbalance in flux observations and energy interaction between the canopy and the surface. Finally, evapotranspiration estimates at 1 km^2 resolution were also used to constrain irrigation amounts applied in the Haihe River Basin. This is achieved by comparing remotely sensed land surface temperature combined with the Priestly-Taylor Jet Propulsion Laboratory model to estimate actual ET and a simulation with mHM (mesoscale Hydrologic Model) that does not include irrigation (Koch et al., 2020). The difference of these two ET estimates was used to infer actual irrigation. Results show that irrigation areas have increased between 2002 and 2016 in the North China Plains and this was accompanied by an increase in crop water use efficiency.

In summary, the studies in this special section range from a pure physical description of the bare soil evaporation process (Novak, 2019; Trautz et al., 2019) to estimates of evaporation and evapotranspiration at the field (Cui et al., 2020; Wei et al., 2020), catchment (Koch et al., 2020), and global scale (Or & Lehmann, 2019). While diverse in methodology and scope, all the studies highlight how evapotranspiration remains central to the hydrological discussion and how important it is to separate the abiotic evaporation from the biotic transpiration flux as well as to link ET with water sources in the soil column. In order to understand the ET process, an interdisciplinary approach linking hydrology and ecology is required. A better accuracy in space and time of evapotranspiration fluxes is increasingly demanded by the community to both understand fundamental processes related to water transport as well as to answer practical water management questions.

2.4. Top Down and Bottom Up Both Needed in Model Structure Analysis

Scientific progress is a constant interaction between new observations and new theories. New observations can lead to the development of new theories, which can again stimulate new ways of observing. In the context of the development of hydrological models, we recognize the same interaction between observations and model formulations in the contributions to this special issue. Model improvement can come from studying and measuring a specific phenomenon in very much detail. The obtained understanding should eventually be translated into a model concept at different scales. This is what we call a *bottom up* approach: moving from specific data to general model formulations. The special issue, however, also received many contributions where the model was the starting point. Scrutinizing the model behavior could lead to new understanding of system functioning. This should eventually be translated to specific (novel) measurements to validate this new understanding. Starting from the modeling concept is what we call a *top down* approach: starting from general model formulations, one moves to specific observations to test these formulations. Both approaches reinforce one another, together forming the cycle that stimulates scientific progress.

Studies with a clear *bottom up* perspective in our definition, are Zhou et al. (2020) and Dudunake et al. (2020). Zhou et al. (2020) conducted controlled measurements on freezing and thawing of soil, and formulated a unified model based on these experimental data. Dudunake et al. (2020) investigated the role of boulder-induced morphological change on hyporheic exchange. With a combination of controlled observations and computational modeling, they demonstrated that there is a relation between hyporheic flow and the geomorphic responses of the river bed. Both studies uncovered relevant processes currently not represented in most hydrological models. A next challenge is to translate these, usually, local concepts into regional scale models and investigate the general relevance of this process (as discussed in Section 2.2).

Imhoff et al. (2020) argued that better availability of data with high spatial coverage facilitate the model development from *bottom up*. They parametrized the hydrological model wflow_sbm based on point-scale pedo-transfer functions, from there upscaling the model parameters to different model resolutions. In estimating parameter values at the relevant scale, it is aimed to obtain more realistic process representation. Hereby, Imhoff et al. (2020) investigated model scalability as well as flux matching. Also analyzing across different scales, Saksena et al. (2020) emphasized the requirement of a more precise implementation of urban water infrastructure for flood modeling at large scales, and a more physically-based coupling of hydrology and hydrodynamics.

Baroni et al. (2019) provided a clear example of the *top down* approach. Based on a comprehensive model intercomparison, they identified which data are needed to further assess and improve hydrological models. They highlighted that process adequacy in models depends on the way the models are structured and how data availability fits to the study goal. Also Pilz et al. (2020) took the model as a starting point to formulate new hypotheses of system functioning. In their framework, they conducted an automatic identification of a flexible process-based hydrological model. They demonstrated how to identify uncertainties in the representation of different processes using flexible model structures. Thoroughly testing different hypotheses is helpful to identify accurate ways of implementing processes in the model structure. Issues with model identifiability relate to data requirements, hence providing directions for data needs to further constrain hydrological models.

Both the bottom up and the top down approach can improve our understanding of the hydrological system, and improve the way we represent this system in models.

3. Concluding Remarks

We would like to conclude this editorial by reflecting on our observations on the special issue contributions:

- The diversity of methodological approaches and topics presented in this special issue was higher than our initial expectations. Despite this diversity, general trends could be identified as summarized in the four topics discussed in Section 2.
- The special issue contributions have illustrated that the use of additional and novel data sources (e.g., remote sensing products or isotopes) concurrently challenges our process understanding. To better achieve the linkage between data and models, scientific and technical efforts are required to enable the assimilation of new data sources into models. Based on the contributions of the special issue, there exists a significant potential in the exploitation of novel data in model setup, evaluation, and assessment.
- Several studies have shown that explicitly including a specific (sub-)process leads to improved model behavior, at the scale of interest. Additionally, some contributions of the special issue focus on evapotranspiration and provide ideas and concepts for better process representation, such as separating abiotic evaporation and biotic transpiration. However, the overarching challenge of how to meaningfully and reliably transfer the obtained process knowledge across models and scale remains. Integration of bottom-up and top-down perspectives is an essential element of scientific progress and model improvement that emerges also from this special issue.
- Based on the received contributions, the potential for better process representation in models relies upon the diversity and quality of data sources rather than on model optimization or the use of machine learning approaches. Investigation of causality relationships remains the main focus of process-based hydrological modeling that can be supported by refined hydrological hypotheses.

We believe, as it was the merit of the conference sessions and workshops that resulted in this section, more discussions among modelers and experimentalists on the modeling efforts are needed to better bridge the gaps of process modeling and understanding across scales, and observations of these processes (see Seibert and McDonnell, 2002). This editorial serves as a snapshot of such ongoing activities.

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