Groundwater representation in continental to global hydrologic models: a call for open and holistic evaluation, conceptualization and classification

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Key points

- As groundwater is increasingly being included in large-scale models, we seek to improve transparency in model formulation and evaluation
- Integration of data-, model-, and expert-driven model evaluation approaches can reduce evaluation limitations due to data scarcity
- Holistic evaluation, transparent conceptualization and systematic classification may significantly improve groundwater representation in large-scale models

Abstract

Continental- to global-scale hydrologic models increasingly include representations of the Earth's groundwater system. A key question is how to evaluate the realism and performance quality of such large-scale groundwater models given limitations in data availability. We argue for a transparent approach to system conceptualization, which would enable distinguishing differences in model behavior that are caused by system conceptualization from those that are caused by differences in the implementation of physical processes in models. In addition, we argue for systematic model classification to distinguish the impacts of choices in model implementation. Evaluation options include comparing model outputs with available observations of groundwater levels or other state or flux variables (data-driven evaluation); comparing several models with each other with or without reference to actual observations (model-driven evaluation); or relying on experts to propose hydrologic behaviors that we expect to see in particular regions or at particular times (expert-driven evaluation). We discuss the strengths and weaknesses of these three evaluation strategies as well as how they might be integrated to achieve a more holistic approach. We call on various scientific communities to join us in our effort to improve the representation of groundwater in continental to global models using the recommendations discussed here.

Plain language summary

Groundwater is increasingly being included in large-scale (continental to global) land surface and hydrologic simulations. However, it is challenging to evaluate these simulations because groundwater is "hidden" underground and thus hard to measure. Here, we make recommendations to improve the incorporation of groundwater in large-scale models. These include: more clearly describing our mental models of how groundwater flows and interacts with other processes ('model conceptualization'); classifying different approaches to including groundwater in models, and choosing an approach based on its suitability to the goals of a study ('model classification'); and using multiple complementary strategies to assess the performance of a model ('model evaluation'). As large-scale land surface and hydrologic models "move down" into the subsurface, modeling strategies from the hydrogeology community need to "move up" towards the surface and be combined with improved model evaluation strategies.

WHY AND HOW MODEL GROUNDWATER AT CONTINENTAL TO GLOBAL SCALES?

Groundwater is the largest human- and ecosystem-accessible freshwater storage component of the hydrologic cycle (Gleeson et al., 2016; UNESCO, 1978). Therefore, better understanding of groundwater dynamics is critical at a time when the 'great acceleration' (Steffen et al., 2015) of many human-induced processes is increasing stress on water resources (Wagener et al., 2010), especially in regions with limited data availability and analytical capacity. We urgently require predictive understanding about how groundwater, used by humans and connected with other components of the Earth System, operates at a variety of scales. The goals of representing groundwater in continental to global models include:

(1) Understanding and quantifying interactions between groundwater and past, present and future climate. Groundwater systems can have far-reaching effects on climate affecting modulation of

surface energy and water partitioning with a long-term memory (Anyah et al., 2008; Maxwell and Kollet, 2008; Krakauer et al., 2014; Maxwell et al., 2016; Taylor, et al., 2013; Meixner et et, 2018; Wang et al., 2018; Keune et al., 2018). For example, while there have been significant advances in understanding the role of lateral groundwater flow on evapotranspiration (Maxwell & Condon, 2016; Bresciani et al, 2016), the broader time and space scales of the interactions between climate and groundwater remain incompletely resolved (Cuthbert et al., 2019).

(2) Understanding and quantifying two-way interactions between groundwater and the rest of the hydrologic cycle, as well as the broader Earth System. As the main storage component of the freshwater hydrologic cycle, groundwater systems impact the sea level (Döll et al., 2014; Wada, 2016; Wada et al. 2016); freshwater and solute inputs to the ocean (Moore, 2010; Sawyer et al., 2016); agricultural productivity and other ecosystem services in both irrigated and rainfed systems (Scanlon et al., 2012; Qiu et al., 2019; Visser, 1959; Zipper et al., 2015, 2017); and streamflows and groundwater-dependent ecosystems (Batelaan et al., 2003; Boulton & Hancock, 2006; Kløve et al., 2011).

(3) Informing water decisions and policy for large, and often transboundary, groundwater systems in an increasingly globalized world (Wada & Heinrich, 2013). For example, global trade in virtual water causing aquifer stress in disparate regions (Dalin et al., 2017) shows the value of large-scale models in groundwater policy. Another example is sub-Saharan Africa, where groundwater recharge from large-scale models has been used to quantify groundwater resources, even though large-scale models do not yet include all recharge processes that are important in this region (Taylor et al., 2013).

(4) Offering the opportunity to create visualizations and interactive opportunities that engender local and global populations to understand and appreciate what is happening in the large time and space scales of environmental systems.

In sum, continental- to global-scale hydrologic models incorporating groundwater offer a coherent scientific framework to examine the dynamic interactions between the Earth System above and below the land surface, and are compelling tools for conveying the opportunities and limits of water resources to people so that they can better manage the regions they live in, and better understand the world around them.

Numerous land surface models, global hydrological and water resource models, and Earth System models (herein we refer to all these types of continental to global models as 'large-scale models') have incorporated or intend to incorporate groundwater to varying levels of complexity depending on the model provenance, users, and purposes. Historically, large-scale hydrological models were intended for simulating streamflow, with groundwater only included to define baseflow or for its influence on land surface processes, like evapotranspiration and runoff production, via soil moisture / groundwater fluxes. As a result, groundwater was not explicitly represented or represented in simple ways such that lateral subsurface flow only occurs to the draining river in each grid cell, and it is often described by a linear reservoir (Alcamo et al., 2003; Gascoin et al., 2009; Ngo-Duc et al., 2007), or using subgrid scale approaches based on the topographic index (Famiglietti & Wood, 1994; Koster et al., 2000; Niu et al., 2003; Takata et al 2003.). More recently, more rigorous approaches have been developed to explicitly simulate lateral groundwater flows between all model grid cells or elements for large-scale models (Fan et al, 2013; Lemieux et al 2008; de Graaf et al., 2017; Kollet et al., 2017; Maxwell et al., 2016; Reinecke et al., 2018; Vergnes & Decharme, 2012). It is important to note that herein 'large-scale models' refer to models that are laterally extensive across multiple regions (hundreds of kilometers), rather than specific to regional aquifers and focus on the shallow subsurface (upper hundreds of meters). We acknowledge and build upon well-established modeling strategies for regional aquifer systems (Anderson & Woessner, 1992; Rossman & Zlotnik, 2013), deeper groundwater flow (Garven, 1995; Person et al., 1996), regional groundwater flow (Tóth, 1963, Freeze and Witherspoon, 1966). The simulation of groundwater in large-scale models is a nascent and rapidly developing field with significant computational and parameterization challenges which has led to significant and important efforts to develop and evaluate individual models. Now that a number of models are developed and developing, it is equally important that we advance how we evaluate and test such models.

The goal of this commentary is to advocate and provide recommendations for the transparent conceptualization, systematic classification, and robust evaluation of the groundwater component of large-scale models in order to improve the representation of groundwater, and thus promote better understanding of global water science and sustainability. We bring together somewhat disparate scientific communities as a step towards greater community-level cooperation on these issues, including global hydrology and land surface modelers, local to regional hydrogeologists, and hydrologists focused on model development and evaluation. Our main focus is model evaluation because this is the heart of model trust and reproducibility (Hutton et al., 2016). We start however with a discussion on model conceptualization and classification which we believe are integral to the evaluation process as discussed below. We develop a holistic framework for evaluating global groundwater models (that could be extended to other elements of hydrological models) that includes and extends current efforts to compare large-scale hydrologic models (Scanlon et al., 2018) or evaluate large-scale groundwater models and schemes (e.g. Döll et al., 2014; Maxwell and Condon 2016; de Graaf et al., 2017; Koirala et al., 2019). In each section we conclude with goals and possible actions meant to invigorate the scientific community. Since groundwater is being integrated into a diverse range of models, we expect multiple Earth Science communities to be interested and impacted by these tangible steps towards improved representation of groundwater in large-scale models.

SYSTEM CONCEPTUALIZATION

Local to regional groundwater models conventionally start with clearly drawn and described conceptual models, which are often seen as a hypothesis or a combination of hypotheses for the aspects of the groundwater system that are relevant to the model objective (Enemark et al., 2019); this is such an important part of local to regional groundwater models that it has been codified into standard practice (e.g. ASTM standards). We define 'conceptual models' (following Anderson & Woessner, 1992; Enemark et al., 2019) as pictorial, qualitative descriptions of the hydrologic system in terms of its salient subsurface geometry and properties as well as surface water and land surface processes and geometry (similar to perceptual models in hydrologic modeling; Beven, 2001). This type of conceptual model is slightly different than other conceptual models representing hydrologic processes (e.g. Salvucci & Entekhabi, 1995 Figure 4; Kollet & Maxwell, 2008 Figure 1; Fan, 2015 Figures 2 and 4, Sutanudjaja et al., 2018 Figure 1) that generally do not include subsurface geometry and properties. It is important to differentiate conceptual models from 'computer models' which are any analytical or numerical procedures that simulate the behavior of an environmental system.

Conceptual models form the basis of computer models and allow for multiple, competing conceptualizations and hypotheses, which is healthy for scientific progress (Enemark et al., 2019), and valuable for communication within scientific circles and with stakeholders (Mahmoud et al., 2009). However, conceptual models for large-scale models have generally not been published or received the attention they deserve. Figure 1 is in fact one of these conceptual models, in the mind of one of the developers of the global hydrologic model PCR-GLOBWB (M. Bierkens), but never before published. Not publishing, discussing, or debating conceptual models impedes rapid and clear understanding of the assumptions on which models rely, and does not communicate how the modeller sees the hydrologic system under study.

Conceptual models likely have to differ between local- and large-scale models; at the local-scale actual geology and surface water features can be included in a pictorial drawing of the model domain, which is not (yet) possible in the conceptual models for large-scale computer models. We argue that conceptual models are crucial for developing better computer models of groundwater systems, as well as for presenting and deriving hypotheses that could be used in evaluation, as described below. In fact, the hydrologic modelling community has argued for some time that consistency between the conceptual model and the resulting expected behavior is at least as important as some optimal statistical fits to observations (Wagener & Gupta, 2005; Hrachowitz et al., 2014). For the sake of brevity, drawing and describing possible conceptual models for large-scale models is beyond the scope of this commentary and will be the focus on a future related commentary. **We recommend that large-scale model development always includes open and published conceptual models and descriptions that capture the modelers' understanding of the hydrologic system, without being limited to the capabilities of computer models.**

MODEL CLASSIFICATION

Computer models are used to translate qualitative conceptual models into quantitative information about hydrologic systems. Various large-scale models exist along a spectrum of model complexity so it can be difficult to determine the most appropriate model for a specific problem. To facilitate model selection and comparison, we developed a simple but systematic classification for groundwater in large-scale models (Table S1). We argue that groundwater in current large-scale models can be classified functionally by two aspects that are crucial to how groundwater impacts water, energy, and nutrient budgets. First, whether lateral subsurface flow is simulated to a river within a cell, as 2D lateral groundwater flow between all cells or as 3D groundwater flow. Second, we distinguish two types of coupling between groundwater and related compartments (variably saturated soil zone, surface water, atmospheric processes in terrestrial and aquatic settings): ‘one-way’ coupling (recharge is imposed from the surface, with no feedback from capillary rise; groundwater flow to the surface does not depend on surface head) from ‘two-way’ coupling involves feedback loops. We also note atmospheric coupling which involves coupling a groundwater-surface model with an atmospheric model, to propagate the influence of groundwater from the surface to the atmosphere, and the resulting feedback onto the surface and groundwater. This classification scheme (which could also be called a model typology) is based on a number of model characteristics such as the fluxes, stores and other features (Table S1). We suggest use of this process-based classification scheme rather than grouping models by model purpose because many models are used for multiple purposes.

The spectrum of model complexity is significant, so an important question is ‘what level of complexity is appropriate?’ This question depends primarily on the model purpose (i.e. the question to be answered), the alignment of the computer model with the appropriate conceptual model, and the computer model’s performance. All models have an inherent purpose (even if not clearly stated) and the principle of parsimony suggests that models should only be as complex as appropriate for their purpose (Young et al., 1996), though researcher and stakeholder familiarity with a model are also common and important considerations (Addor & Melsen, 2019). For example, a model with no 2D lateral flow between cells may be appropriate for the purpose of basin-scale water balance estimation in certain regions over large time scales. But the same model would be clearly inappropriate for assessing the role of regional groundwater flow because lateral flow between basins is not considered. **We thus recommend that the purpose of any groundwater implementation in large-scale models should be clearly stated and salient model characteristics are comprehensively considered and described (using Table S1 as a guide).**

MODEL EVALUATION

We suggest that a holistic framework is needed for evaluating global groundwater models that requires at least three dimensions (Figure 2): data-, model- and expert-based evaluation that are potentially mutually beneficial because each strategy has strengths and weaknesses.

Data-driven model evaluation is the focus of most current efforts and is important because we want models to be consistent with real-world observations, though what we mean by consistent might vary as discussed below. Data-driven model evaluation could use data at site, basin/regional, and global scales, and is thus dependent on the quality, distribution, and availability of data (Table 1). Unfortunately, there are significant inherent challenges with regard to groundwater data because groundwater fluxes and stores are largely unmeasurable: groundwater recharge is not directly measurable except for meter-scale lysimeters (Scanlon et al., 2002); change in groundwater storage can be indirectly estimated from satellite gravimetry (GRACE: Gravity Recovery And Climate Experiment) but only after model-based subtraction of water storage changes in glaciers, snow, soil and surface water bodies (Lo et al., 2016; Rodell et al., 2009; Wada, 2016); baseflow from groundwater to surface water bodies is only derived using a baseflow separation algorithms or tracers (Genereux, 1998; Tallaksen, 1995) but this is only possible if there are not significant surface water bodies upstream; and the groundwater contributions to evapotranspiration in groundwater-dependent ecosystems can be estimated using water table fluctuations (Loheide et al., 2005), but this is rarely done and also requires specific yield estimates which are often highly uncertain. Even hydraulic head data from well observations, often considered the crucial data for groundwater model evaluation, have limitations for use in large-scale model evaluation such as (1) observational errors and uncertainty (Post and von Asmuth, 2013); (2) groundwater storage variation can only be derived using estimated storage coefficients; (3) heads can reflect the poro-elastic effects of mass loading and unloading rather than necessarily aquifer recharge and drainage (Burgess et al, 2017); (4) heads can be directly used to evaluate models that compute head and not only storage variations, and (5) even if models compute heads, there is a scale problem (point observation vs. simulated grid cell average). To date, models have been compared to observed heads rather than depths to water table, which would show greater discrepancy but are more meaningful descriptors of system dynamics. For all data, there is a significant commensurability problem (scale difference between observation and modelled variable or state) (Beven and Cloke, 2012). In sum, much of the data sometimes called 'observations' are modeled or derived quantities, and often at the wrong scale for evaluating large-scale models, which means modelers have to ask themselves what level of agreement is reasonable to aim for given these data limitations.

Despite these challenges, we foresee significant opportunities for data-driven model evaluation and do not see data availability as a reason to exclude groundwater in Earth System models or to avoid evaluating these models. So far, all efforts to our best knowledge have only used GRACE, hydraulic head data, or baseflow (Lo et al., 2008; Döll et al., 2014; Maxwell and Condon, 2016; de Graaf et al., 2017; Scanlon et al., 2018) but there are significant possibilities for new data sources (see Table 1 for strengths, limitations and availability of each data source). Large-scale models could be more holistically evaluated with existing data such as the spatial distribution of perennial streams and baseflow data. In some cases, observed evapotranspiration from global networks (e.g., FLUXNET) and novel soil moisture technologies (e.g., COSMOS; Rosolem et al., 2014) may also help to constrain groundwater recharge estimates (Hartmann et al., 2015). We might also be able to utilize existing datasets in new ways; for example, Hartmann et al. (2017) used recharge studies of 38 separate karst systems across Europe to assess the variability of recharge modelled in their large-scale model across this domain. The use of various datasets derived from or for large-scale models, such as evapotranspiration, vegetation indices and surface water inundation, could be refined to evaluate groundwater models, as recently attempted in the Ouémé basin (Benin) by Rashid et al. (2019) to evaluate three land surface models with groundwater against multiple observations. Such datasets are not listed in Table 1 as methods to use them globally have not yet been developed, but recent advances to constrain distributed estimations of the global water cycle by Earth observation products including GRACE (Pan et al., 2012; Pellet et al., 2019) are particularly promising. Some of them have also been explicitly compared with residence time and tracer data (Maxwell et al., 2016) which have also been recently compiled globally (Gleeson et al., 2016; Jasechko et al., 2017). This could be an important evaluation tool for large-scale models that are capable of simulating flow paths, or can be modified to do so. In the future, additional new datasets could be derived using meta-analysis and/or, geospatial analysis of gaining or losing stream reaches (e.g., from interpolated head measurements close to the streams), springs and groundwater-dependent surface water bodies, evapotranspiration from groundwater and piezometric lysimetry; each of these new data sources could in principle be developed using methods already applied at regional-scales. **We recommend evaluating models with a broader range of currently available data sources (with explicit consideration of data uncertainty) while also simultaneously working to derive new data sets.** However, data distribution and commensurability issues will likely still be present, which underscores the importance of the two following strategies.

Model-driven model evaluation which includes model intercomparison projects (MIP) and model sensitivity and uncertainty analysis can be done with or without explicitly using observed data for comparison. The original MIP concept offers a framework to consistently evaluate and compare models, and associated model input, structural, and parameter uncertainty under different objectives (e.g., climate change, model performance, human impacts and developments). Since the Project for the Intercomparison of Land-Surface Parameterization Schemes (PILPS; Sellers et al., 1993), the first model intercomparison project (MIP), LSM community has exploited MIPs to deepen understanding of land physical processes and to improve their numerical implementations to be represented in various scales from regional (e.g., Rhône-aggregation project; Boone et al., 2004) to global (e.g., Global Soil Wetness Project; Dirmeyer, 2011). Two examples of recent model intercomparison efforts, including some models of Table S1, illustrate the general MIP objectives and practice. First, ISIMIP (Schewe et al., 2014; Warszawski et al., 2014) assessed water scarcity at different levels of global warming. Second, IH-MIP2 (Kollet et al., 2017) used both synthetic domains and an actual watershed to assess fully-integrated hydrologic models because these cannot be validated easily by comparison with analytical solutions and uncertainty remains in the attribution of hydrologic responses to model structural errors. Model comparisons have revealed differences, but it is often unclear whether these stem from differences in the model structures, differences in how the parameters were estimated, or from different other modelling choices (Duan et al., 2006). Attempts for modular modelling frameworks to enable comparisons (e.g. Clark et al., 2015) or at least shared explicit modelling protocols and boundary conditions (Ceola et al., 2015; Warszawski et al., 2014) have been proposed to reduce these problems. Inter-scale model comparison - for example, comparing a global model to a regional model - is a potentially useful approach which is emerging for surface hydrology models (Hattermann et al., 2017; Huang et al., 2017) and could be applied to large-scale groundwater models. Combining inter-model and inter-scale comparisons could leverage the strengths of each of the methods. For example, attempts to document and compare flow path and transit time distributions, currently limited to the small scale (Thomas et al., 2016), could be extended to larger scales. Finally, we note that large-scale groundwater models have only been assessed to a very limited degree with respect to understanding, quantifying, and attributing relevant uncertainties. Expanding computing power, along with the improvement of conceptualization and classification that we call for above, will all enable more robust sensitivity and uncertainty analysis such as used in regional-scale groundwater models (Habets et al., 2013; Hill, 2006; Hill & Tiedeman, 2007). For now, we suggest applying computationally frugal methods such as the elementary effect test or local sensitivity analysis (Hill, 2006; Morris, 1991; Saltelli et al., 2000). Such sensitivity and uncertainty analyses should be applied not only to model parameters and forcings but also to model structural properties (e.g. boundary conditions, grid resolution, process simplification, etc.) (Pianosi et al., 2016). **We thus recommend significant expansion of groundwater focused model inter-comparison projects (both inter-model and inter-scale) as well as more sensitivity and uncertainty analyses.**

A path much less traveled is **expert-driven model evaluation** which would develop hypotheses of phenomena (and related behaviors or signatures) we expect to emerge from large-scale groundwater systems based on our expert knowledge, intuition, or experience. The recent discussion by Fan et al. (2019) shows how hypotheses about large-scale behavior might be derived from expert knowledge gained from studying smaller scale systems such as critical zone observatories. Large-scale models could then be evaluated against these hypotheses, providing a general opportunity to advance how we connect hydrologic understanding with large-scale modeling - a strategy that could potentially reduce epistemic uncertainty which may be especially useful for groundwater systems given the data limitations described above. Choosing appropriate and effective hypotheses is crucial and should likely focus on large-scale controlling factors or relationships between controlling factors and output in different parts of the model domain; hypotheses that are too specific may only be able to be tested by certain model complexities. To illustrate the type of hypotheses we are suggesting, we list some examples of hypotheses drawn from current literature:

- water table depth and lateral flow strongly affect transpiration partitioning (Famiglietti and Wood, 1994; Salvucci and Entekhabi, 1995; Maxwell & Condon, 2016);
- the percentage of inter-basinal regional groundwater flow increases with aridity or decreases in frequency of perennial streams (Gleeson & Manning, 2008; Goderniaux et al, 2013); or

- human water use systematically redistributes water resources at the continental scale via non-local atmospheric feedbacks (Al-Yaari et al., 2019; Keune et al., 2018).

Alternatively, hypotheses could be drawn from hydrologic intuition and form the basis of model experiments, potentially including extreme model experiments (far from the natural conditions). For example, an experiment that artificially lowers the water table by decreasing precipitation (or recharge directly) could hypothesize that 'the drainage flux will increase and evaporation flux will decrease as the water table is lowered'. These hypotheses are meant only for illustrative purposes and we hope future community debate will clarify the most appropriate and effective hypotheses. There is a close link between this approach and the need for open system conceptualizations in which this knowledge could be captured.

Moving such expert-driven approaches forward should include more formal approaches to elicit expert-knowledge in a structured manner (Aspinall, 2010; Cooke, 1991), preferably including the uncertainty in this knowledge. In the groundwater modelling community, the term *expert knowledge* is often used to describe the constraints on parameter values that are provided prior to calibration or uncertainty analysis (Ross et al., 2009; Doherty and Christensen, 2011; Brunner et al., 2012; Knowling and Werner, 2016; Rajabi and Ataie-Ashtiani, 2016). The term expert opinion is sometimes alternatively used (Ross et al., 2009; Rajabi and Ataie-Ashtiani, 2016). The latter term may be preferable because it emphasizes a preliminary state of knowledge (Krueger et al., 2012). Expert knowledge/opinion is also implicitly used at higher levels when defining the model structure (i.e., all the way from conceptualization down to mathematical solution) (Krueger et al., 2012; Rajabi et al., 2018).

Hence, it can be seen that expert knowledge/opinion is commonly used to directly inform the model structure and parameters. In contrast, it seems that the use of expert knowledge/opinion about *system behavior* is less common. Yet, it is intuitive that information about system behavior can help in evaluating the plausibility of model outputs (and thus of the model itself). This is what we call expert-driven evaluation herein. **We recommend the community uses expert elicitation to develop effective hypotheses that directly link to the relevant large-scale hydrologic processes of interest.**

Ideally, all three strategies (data-driven, model-driven, expert-driven) should be pursued simultaneously because the strengths of one strategy might further improve others. For example, expert- or model-driven evaluation may highlight and motivate the need for new data in certain regions or at new resolutions. Or data-driven model evaluation could highlight and motivate further model development or lead to refined or additional hypotheses. **We thus recommend the community significantly strengthens efforts to evaluate large-scale models using all three strategies.** Implementing these three model evaluation strategies may require a significant effort from the scientific community, so we therefore conclude with a perspective on how this might be achievable. For example, in ISIMIP (Warszawski et al., 2014), modelling protocols have been developed with an international network of climate-impact modellers across different sectors (e.g. water, agriculture, energy, forestry, marine ecosystems) and spatial scales. Originally, ISIMIP started with multi-model comparison, i.e. ***model-driven model evaluation***, with a focus on understanding how model projections vary across different sectors and different climate change scenarios (ISIMIP Fast Track). However, more rigorous model evaluation came to attention more recently with ISIMIP2a, and various observation data, such as river discharge (Global Runoff Data Center), terrestrial water storage (GRACE), and water use (national statistics), have been used to evaluate historical model simulation (***data-driven model evaluation***). To better understand model differences and to quantify the associated uncertainty sources, ISIMIP2b includes evaluating scenarios (land use, groundwater use, human impacts, etc) and key assumptions (no explicit groundwater representation, groundwater availability for the future, water allocation between surface water and groundwater) which may be useful as a basis for ***expert-driven model evaluation***. While there has been a significant amount of research and publications on MIPs including surface water availability, limited multi-model assessments for large-scale groundwater studies exist. Important aspects of MIPs in general could facilitate all three model evaluation strategies: community-building and cooperation with various scientific communities and research groups, and making the model output publicly available in a standardized format. **We therefore suggest that current MIPs could be modified and expanded to explicitly consider these three model evaluation strategies which would leverage the value and effort of ongoing MIPs to more comprehensively evaluate large-scale groundwater models while offering more opportunities for experimental hydrologists to be involved in model assessment studies across scales.**

TOWARDS IMPROVED GROUNDWATER REPRESENTATION IN LARGE-SCALE MODELS

Land surface, large-scale hydrologic and Earth System models increasingly represent groundwater, which we envision will lead to a better understanding of large-scale water systems and to more sustainable water resource use. We call on various scientific communities to join us in this effort to improve the representation of groundwater in continental to global models using the specific recommendations we make for **transparent conceptualization, systematic classification, and holistic evaluation**. As described by examples above, we have already started this journey using open science (data, models, publishing and collaboration) and more holistic approaches (meaning holistic representation of hydrologic processes as well as more holistic model evaluation). We hope this will lead to better outcomes especially for the goals of including groundwater in large-scale models that we started with above: improving our understanding of Earth system processes through more robust conceptualization and evaluation; and informing water decisions and policy by enhancing the trust of stakeholders through increased transparency. Together we can better understand what has always been beneath our feet, but often forgotten or neglected.

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Table 1. Current and future observational data that could be used to evaluate large-scale models, categorized by current availability and generally arranged from globally distributed to local scale within each category. Data included here are directly linked to groundwater variables (recharge, storage, or discharge). In the future, other data such as evapotranspiration and or soil moisture could also be considered as useful constraints on groundwater fluxes and stores.

Data type	Strengths	Limitations	Spatial Attributes	Availability
Existing Data Sources				
GRACE total water storage anomalies	Globally available	Groundwater changes are model remainder; coarse resolution and limited period	Gridded and spatially continuous	Rodell et al. (2018)
Perennial stream map	Globally available and could be compared to streamflow observations	Not all perennial streams reaches are groundwater-influenced; does not provide information about magnitude of inflows/outflows.	Spatially continuous along stream networks	Schneider et al. (2017) Cuthbert et al. (2019)
Baseflow	Constrains direction and magnitude of fluxes at groundwater system boundaries.	Derived from streamflow observations; limited to basins with observations. Relevant processes occur at sub-grid-cell resolution.	Point observations at measurement locations	Beck et al. (2013).
Water table depth or fluctuations	Can provide information on performance away from model boundary conditions.	Water table fluctuations available at few locations and water table depth observations biased towards North America and Europe	Point measurements at existing wells	Water table depth from Fan et al. (2013)
Potential Future Data Sources				
Gaining or losing stream reaches	Multiple techniques for measurement (interpolated head measurements, streamflow data, water chemistry). Constrains direction of fluxes at groundwater system boundaries	Relevant processes occur at sub-grid-cell resolution.	Spatially continuous along stream networks	Not globally available but see Bresciani et al. (2018) for a regional example
Springs and groundwater-dependent surface water bodies	Constrains direction of fluxes at groundwater system boundaries	Relevant processes occur at sub-grid-cell resolution.	Point measurements at water feature locations	Springs available for various regions (e.g. Springer, & Stevens, 2009) but not globally
Tracers (heat, isotopes or other geochemical)	Provides information about temporal aspects of groundwater systems (e.g. residence time)	No large-scale models simulate transport processes (Table S1)	Point measurements at existing wells or surface water features	Isotopic data compiled (Gleeson et al., 2016; Jasechko et al., 2017) but no global data for heat or other chemistry

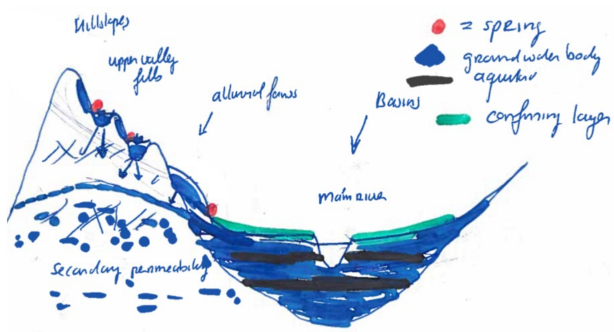

Figure 1: The conceptual model underlying some of the development of PCR-GLOBWB coupled with MODFLOW (De Graaf et al. 2017), which has never been previously published. Ideally conceptual models should also explicitly include recharge, flow and discharge patterns.

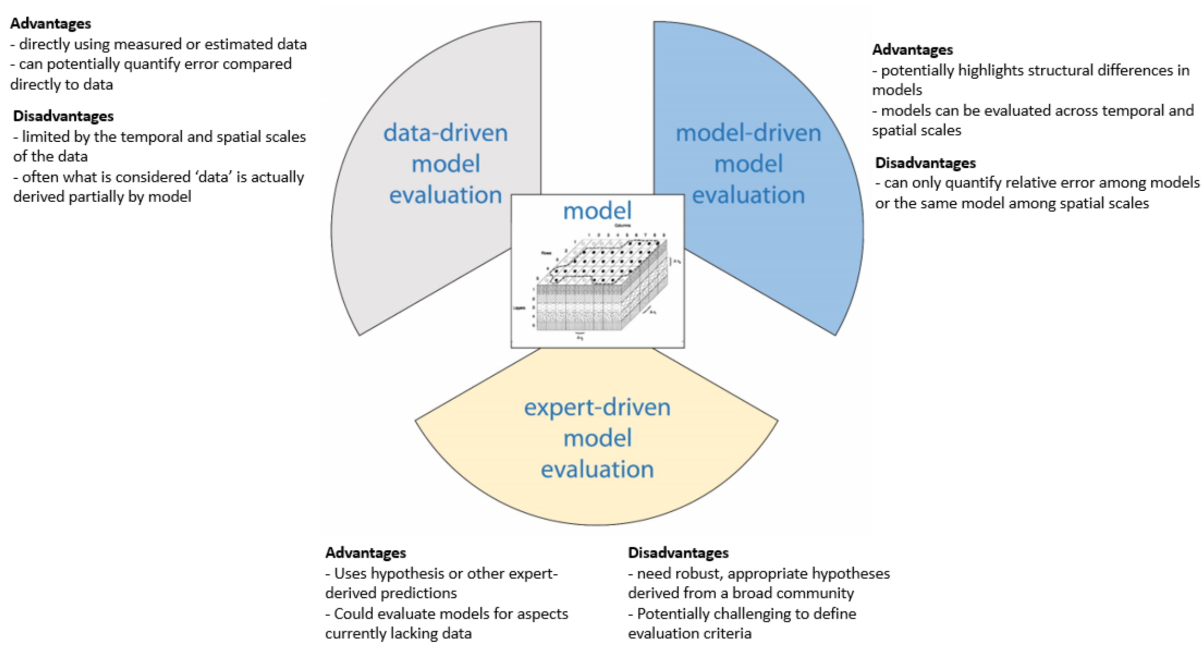

Figure 2: A framework for evaluating groundwater in large-scale models, with the large-scale model being in the centre of the framework surrounded by the three strategies. Strategies include data-, model-, and expert-driven model evaluation, each which have advantages and disadvantages.

Supplementary Information

Table S1. Model classification based on three models classes and various model characteristics; see link to <u>google doc</u> to view easier or edit (google doc will be migrated to a community github page)

Table 1. Model classification for large-scale models representing groundwater (1)													
groundwater flow	No GW flow	lateral groundwater flow to a river within a cell						2D lateral groundwater flow between all cells				3D groundwater flow	
groundwater-surface coupling (2)		one-way		two-way				one-way			two-way		
surface-atmosphere coupling	yes							no					
example model (3)	JULES	ORCHIDEE	LM3	VIC-ground	CLM5	TOPLATS	Catchment	WaterGAP2-G3M	LEAF hydro	PCRGLOB-WB - MODFLOW	ISBA-TRIP	HydroGeoSphere	ParFlow
groundwater recharge (diffuse)	Free-drainage	Recharge = P-R-ET	Recharge = P-R-ET	Recharge depends on WT head and capillary fluxes	Recharge depends on WT head and capillary fluxes	Recharge depends on WT head and capillary fluxes	Recharge depends on WT head and capillary fluxes	currently uncoupled	recharge derived from WGM	Recharge depends on WT head and capillary fluxes	Recharge depends on WT head and capillary fluxes	directly represented	directly represented
focused recharge (4)	not represented	optional (via enhanced infiltration in ponds)	not represented	not represented	not represented	not represented	not represented	represented after coupling	not represented	represented from lakes and perenial rivers?	not represented	not represented	not represented
surface water boundary condition or coupling	not represented	not represented	not reresented	not represented	not represented	not represented	not represented	currently uncoupled with boundary condition using conductance	no head-based interactions with surface water	one-way coupling with three boundary conditions including drainage from linear reservoir	directly represented	directly represented	directly represented
variably saturated or partially saturated (5)	1D Richards' in soil layers	1D Richards' in soil layers	1D Richards' in soil layers	1D Richards' in soil layers	1D Richards' in soil layers	1D Richards' in soil layers	Lumped 3D Richards	partially saturated	partially saturated	Vertical fluxes in soils depend ing on soil saturation and GW level	1D Richards' in soil layers	variably saturated using 3D Richard's equation	variably saturated using 3D Richard's equation
water table and hydraulic head	Optional WT diagnostic based on TOPMODEL	not represented	represented, parameterised	directly represented	First layer from bedrock where soil moisture < 0.9	represented following TOPMODEL	represented following TOPMODEL	directly represented	directly represented	directly represented	directly represented	directly represented	directly represented
groundwater storage	not represented	represented as linear reservoir	represented	represented	represented	represented	represented	directly represented	represented	directly represented	directly represented	directly represented	directly represented
lateral flow	not represented	represented	represented through lateral flow divergence	parametrized following Francini and Pacciani (2001)	parameterised, calibration parameter related to baseflow	represented following TOPMODEL	represented following TOPMODEL	directly represented but not along flowlines	directly represented	directly represented	directly represented	directly represented	directly represented
groundwater bottom boundary conditon	gravity drainage from soil	function of reservior	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux
groundwater use	not represented	not represented	not represented	not represented	not represented	not represented	not represented	to be included in future	not represented	represented	not represented	not represented	not represented
preferential flow	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented
groundwater temperature	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented
groundwater quality	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented
groundwater density	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented
confined conditions	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	represented	not represented	not represented	not represented
coupling with ocean (and ocean models)	no	no	no	no	no	no	no	no	ocean boundary condition	ocean boundary condition	???	ocean boundary condition	possible
isotope-enabled	no	no	no	no	no	no	no	no	no	no	no	no	no
Included in current assimilation schemes	yes	???	no	no	yes	???	no	no	no	no	no	no	no
paleo groundwater	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented
Reference	Best et al. (2011)	Guimberteau et al. (:	Milly et al (2014)	Liang et al. (2003	Andre et al. (2018	Famiglietti & Wood (	Koster et al. (2000)	Reinecke et al. (201	Fan et al. (2013	de Graaf et al. (2017	Vergnes et al. (2014)	Brunner and Simmo	Maxwell et al (2017)

Notes:

(1) Only the most RECENT version of models with published results at continental to global scales are included. Analytical solutions (including the water table ratio or groundwater response times) are not described here.

(2) one-way coupling means that SM => recharge => GW => stream flow, but no reverse influence; in this case, the GW model is dependent on surface simulations to provide recharge. two-way coupling means there is a fully coupling of surf

(3) Other models exist with similar features

(4) Focused recharge refers to any recharge that occurs beneath water bodies such as streams or lakes; whereas preferential flow to mean recharge that bypasses the soil matrix during diffuse recharge through fractures or other macropores

(5) Variably saturated means that the saturation, and related constituative relations can vary continiously, while partially saturated means that saturation can only discretely vary between fully saturated and unsaturated.