

1 GMD Perspective: the quest to improve the  
2 evaluation of groundwater representation in  
3 continental to global scale models

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## Abstract

47 Continental- to global-scale hydrologic and land surface models increasingly include  
48 representations of the groundwater system. Such large-scale models are essential for

49 examining, communicating, and understanding the dynamic interactions between the Earth  
50 System above and below the land surface as well as the opportunities and limits of  
51 groundwater resources. We argue that both large-scale and regional-scale groundwater models  
52 have utility, strengths and limitations so continued modeling at both scales is essential and  
53 mutually beneficial. A crucial quest is how to evaluate the realism, capabilities and performance  
54 of large-scale groundwater models given their modeling purpose of addressing large-scale  
55 science or sustainability questions as well as limitations in data availability and  
56 commensurability. Evaluation should identify if, when or where large-scale models achieve  
57 their purpose or where opportunities for improvements exist so that such models better  
58 achieve their purpose. We suggest that reproducing the spatio-temporal details of regional-  
59 scale models and matching local data is not a relevant goal. Instead, it is important to decide on  
60 reasonable model expectations regarding when a large scale model is performing 'well enough'  
61 in the context of its specific purpose. The decision of reasonable expectations is necessarily  
62 subjective even if the evaluation criteria are quantitative. Our objective is to provide  
63 recommendations for improving the evaluation of groundwater representation in continental-  
64 to global-scale models. We describe current modeling strategies and evaluation practices, and  
65 subsequently discuss the value of three evaluation strategies: 1) comparing model outputs with  
66 available observations of groundwater levels or other state or flux variables (observation-based  
67 evaluation); 2) comparing several models with each other with or without reference to actual  
68 observations (model-based evaluation); and 3) comparing model behavior with expert  
69 expectations of hydrologic behaviors in particular regions or at particular times (expert-based  
70 evaluation). Based on evolving practices in model evaluation as well as innovations in

71 observations, machine learning and expert elicitation, we argue that combining observation-,  
72 model-, and expert-based model evaluation approaches, while accounting for  
73 commensurability issues, may significantly improve the realism of groundwater representation  
74 in large-scale models. Thus advancing our ability for quantification, understanding, and  
75 prediction of crucial Earth science and sustainability problems. We encourage greater  
76 community-level communication and cooperation on this quest, including among global  
77 hydrology and land surface modelers, local to regional hydrogeologists, and hydrologists  
78 focused on model development and evaluation.

79 **1. INTRODUCTION: why and how is groundwater modeled at continental to global scales?**

80 Groundwater is the largest human- and ecosystem-accessible freshwater storage component of  
81 the hydrologic cycle (UNESCO, 1978; Margat & Van der Gun, 2013; Gleeson et al., 2016).

82 Therefore, better understanding of groundwater dynamics is critical at a time when the ‘great  
83 acceleration’ (Steffen et al., 2015) of many human-induced processes is increasing stress on  
84 water resources (Wagner et al., 2010; Montanari et al., 2013; Sivapalan et al., 2014; van Loon  
85 et al., 2016), especially in regions with limited data availability and analytical capacity.

86 Groundwater is often considered to be an inherently regional rather than global resource or  
87 system. This is partially reasonable because local to regional peculiarities of hydrology, politics  
88 and culture are paramount to groundwater resource management (Foster et al. 2013) and  
89 groundwater dynamics in different continents are less directly connected and coupled than  
90 atmospheric dynamics. Regional-scale analysis and models are essential for addressing local to  
91 regional groundwater issues. Generally, regional scale modeling is a mature, well-established

92 field (Hill & Tiedeman, 2007; Kresic, 2009; Zhou & Li, 2011; Hiscock & Bense, 2014; Anderson et  
93 al. 2015a) with clear and robust model evaluation guidelines (e.g. ASTM, 2016; Barnett et al.,  
94 2012). Regional models have been developed around the world; for example, Rossman &  
95 Zlotnik (2014) and Vergnes et al. (2020) synthesize regional-scale groundwater models across  
96 the western United States and Europe, respectively.

97

98 Yet, important global aspects of groundwater both as a resource and as part of the Earth  
99 System are emerging (Gleeson et al. 2020). First, our increasingly globalized world trades virtual  
100 groundwater and other groundwater-dependent resources in the food-energy-water nexus,  
101 and groundwater often crosses borders in transboundary aquifers. A solely regional approach  
102 can be insufficient to analysing and managing these complex global interlinkages. Second, from  
103 an Earth system perspective, groundwater is part of the hydrological cycle and connected to  
104 the atmosphere, oceans and the deeper lithosphere. A solely regional approach is insufficient  
105 to uncover and understand the complex interactions of groundwater within the Earth System  
106 and teleconnections, which are groundwater levels or flows in one region linked to  
107 geographically separated regions via physical or socio-economic processes. Regional  
108 approaches generally focus on important aquifers which underlie only a portion of the world's  
109 land mass or population and do not include many other parts of the land surface that may be  
110 important for processes like surface water-groundwater exchange flows and  
111 evapotranspiration. A global approach is also essential to assess the impact of groundwater  
112 depletion on sea level rise, since groundwater storage loss rate on all continents of the Earth

113 must be aggregated. Thus, we argue that groundwater is simultaneously a local, regional, and  
114 increasingly global resource and system and that examining groundwater problems, solutions,  
115 and interactions at all scales is crucial. As a consequence, we urgently require predictive  
116 understanding about how groundwater, used by humans and connected with other  
117 components of the Earth System, operates at a variety of scales.

118

119 Based on the arguments above for considering global perspectives on groundwater, we see four  
120 specific purposes of representing groundwater in continental- to global-scale hydrological or  
121 land surface models and their climate modeling frameworks:

122 (1) To understand and quantify interactions between groundwater and past, present and  
123 future climate. Groundwater systems can have far-reaching effects on climate affecting  
124 modulation of surface energy and water partitioning with a long-term memory (Anyah  
125 et al., 2008; Maxwell and Kollet, 2008; Koirala et al. 2013; Krakauer et al., 2014;  
126 Maxwell et al., 2016; Taylor, et al., 2013a; Meixner et et, 2018; Wang et al., 2018;  
127 Keune et al., 2018). While there have been significant advances in understanding the  
128 role of lateral groundwater flow on evapotranspiration (Maxwell & Condon, 2016;  
129 Bresciani et al, 2016), the interactions between climate and groundwater over longer  
130 time scales (Cuthbert et al., 2019) as well as between irrigation, groundwater, and  
131 climate (Condon and Maxwell, 2019; Condon et al 2020) remain largely unresolved.  
132 Additionally, it is well established that old groundwater with slow turnover times are  
133 common at depth (Befus et al. 2017; Jasechko et al. 2017). Groundwater connections to

134 the atmosphere are well documented in modeling studies (e.g. Forrester and Maxwell,  
135 2020). Previous studies have demonstrated connections between the atmospheric  
136 boundary layer and water table depth (e.g. Maxwell et al 2007; Rahman et al, 2015),  
137 under land cover disturbance (e.g. Forrester et al 2018), under extremes (e.g. Kuene et  
138 al 2016) and due to groundwater pumping (Gilbert et al 2017). While a number of  
139 open source platforms have been developed to study these connections (e.g. Maxwell  
140 et al 2011; Shrestha et al 2014; Sulis, 2017), these platforms are regional to continental  
141 in extent. Recent work has shown global impacts of groundwater on atmospheric  
142 circulation (Wang et al 2018), but groundwater is still quite simplified in this study.

143 (2) To understand and quantify two-way interactions between groundwater, the rest of  
144 the hydrologic cycle, and the broader Earth System. As the main storage component of  
145 the freshwater hydrologic cycle, groundwater systems support baseflow levels in  
146 streams and rivers, and thereby ecosystems and agricultural productivity and other  
147 ecosystem services in both irrigated and rainfed systems (Scanlon et al., 2012; Qiu et  
148 al., 2019; Visser, 1959; Zipper et al., 2015, 2017). When pumped groundwater is  
149 transferred to oceans (Konikow 2011; Wada et al., 2012; Döll et al., 2014a; Wada,  
150 2016; Caceres et al., 2020; Luijendijk et al. 2020), resulting sea-level rise can impact  
151 salinity levels in coastal aquifers, and freshwater and solute inputs to the ocean  
152 (Moore, 2010; Sawyer et al., 2016). Difficulties are complicated by international trade  
153 of virtual groundwater which causes aquifer stress in disparate regions (Dalin et al.,  
154 2017)

155 (3) To inform water decisions and policy for large, often transboundary groundwater  
156 systems in an increasingly globalized world (Wada & Heinrich, 2013; Herbert & Döll,  
157 2019). For instance, groundwater recharge from large-scale models has been used to  
158 quantify groundwater resources in Africa, even though large-scale models do not yet  
159 include all recharge processes that are important in this region (Taylor et al., 2013b;  
160 Jasechko et al. 2014; Cuthbert et al., 2019; Hartmann et al., 2017).

161 (4) To create visualizations and interactive opportunities that inform citizens and  
162 consumers, whose decisions have global-scale impacts, about the state of groundwater  
163 all around the world such as the World Resources Institute's Aqueduct website  
164 (<https://www.wri.org/aqueduct>), a decision-support tool to identify and evaluate  
165 global water risks.

166 The first two purposes are science-focused while the latter two are sustainability-focused. In  
167 sum, continental- to global-scale hydrologic models incorporating groundwater offer a coherent  
168 scientific framework to examine the dynamic interactions between the Earth System above and  
169 below the land surface, and are compelling tools for conveying the opportunities and limits of  
170 groundwater resources to people so that they can better manage the regions they live in, and  
171 better understand the world around them. We consider both large-scale and regional-scale  
172 models to be useful practices that should both continue to be conducted rather than one  
173 replacing another. Ideally large-scale and regional-scale models should benefit from the other  
174 since each has strengths and weaknesses and together the two practices enrich our  
175 understanding and support the management of groundwater across scales (Section 2).



176 The challenge of incorporating groundwater processes into continental- or global-scale models  
177 is formidable and sometimes controversial. Some of the controversy stems from unanswered  
178 questions about how best to represent groundwater in the models whereas some comes from  
179 skepticism about the feasibility of modelling groundwater at non-traditional scales. We  
180 advocate for the representation of groundwater stores and fluxes in continental to global  
181 models for the four reasons described above. We do not claim to have all the answers on how  
182 best to meet this challenge. We contend, however, that the hydrologic community needs to  
183 work deliberately and constructively towards effective representations of groundwater in  
184 global models.

185

186 Driven by the increasing recognition of the purpose of representing groundwater in  
187 continental- to global-scale models, many global hydrological models and land surface models  
188 have incorporated groundwater to varying levels of complexity depending on the model  
189 provenance and purpose. Different from regional-scale groundwater models that generally  
190 focus on subsurface dynamics, the focus of these models is on estimating either runoff and  
191 streamflow (hydrological models) or land-atmosphere water and energy exchange (land surface  
192 models). Simulation of groundwater storages and hydraulic heads mainly serve to quantify  
193 baseflow that affects streamflow during low flow periods or capillary rise that increases  
194 evapotranspiration. Some land-surface models use approaches based on the topographic index  
195 to simulate fast surface and slow subsurface runoff based on the fraction of saturated area in  
196 the grid cell (Clark et al., 2015; Fan et al., 2019); groundwater in these models does not

197 explicitly have water storage or hydraulic heads (Famiglietti & Wood, 1994; Koster et al., 2000;  
198 Niu et al., 2003; Takata et al., 2003). In many hydrological models, groundwater is represented  
199 as a linear reservoir that is fed by groundwater recharge and drains to a river in the same grid  
200 cell (Müller Schmied et al., 2014; Gascoin et al., 2009; Ngo-Duc et al., 2007). Time series of  
201 groundwater storage but not hydraulic heads are computed. This prevents simulation of lateral  
202 groundwater flow between grid cells, capillary rise and two-way exchange flows between  
203 surface water bodies and groundwater (Döll et al., 2016). However, representing groundwater  
204 as a water storage compartment that is connected to soil and surface water bodies by  
205 groundwater recharge and baseflow and is affected by groundwater abstractions and returns,  
206 enables global-scale assessment of groundwater resources and stress (Herbert and Döll, 2019)  
207 and groundwater depletion (Döll et al., 2014a; Wada et al., 2014; de Graaf et al., 2014). In some  
208 land surface models, the location of the groundwater table with respect to the land surface is  
209 simulated within each grid cell to enable simulation of capillary rise (Niu et al., 2007) but, as in  
210 the case of simulating groundwater as a linear reservoir, lateral groundwater transport or two-  
211 way surface water-groundwater exchange cannot be simulated with this approach.

212

213 Increasingly, models for simulating groundwater flows between all model grid cells in entire  
214 countries or globally have been developed, either as stand-alone models or as part of  
215 hydrological models (Vergnes & Decharme, 2012; Fan et al., 2013; Lemieux et al. 2008; de Graaf  
216 et al., 2017; Kollet et al., 2017; Maxwell et al., 2015; Reinecke et al., 2018, de Graaf et al 2019).  
217 The simulation of groundwater in large-scale models is a nascent and rapidly developing field

218 with significant computational and parameterization challenges which have led to significant  
219 and important efforts to develop and evaluate individual models. It is important to note that  
220 herein 'large-scale models' refer to models that are laterally extensive across multiple regions  
221 (hundreds to thousands of kilometers) and generally include the upper tens to hundreds of  
222 meters of subsurface and have resolutions sometimes as small as ~1 km. In contrast, 'regional-  
223 scale' models (tens to hundreds of kilometers) have long been developed for a specific region  
224 or aquifer and can include greater depths and resolutions, more complex hydrostratigraphy and  
225 are often developed from conceptual models with significant regional knowledge. Regional-  
226 scale models include a diverse range of approaches from stand-alone groundwater models (i.e.,  
227 representing surface water and vadose zone processes using boundary conditions such as  
228 recharge) to fully integrated groundwater-surface water models. In the future, large-scale  
229 models could be developed in a number of different directions which we only briefly introduce  
230 here to maintain our primary focus on model evaluation. One important direction is clearer  
231 representation of three-dimensional geology and heterogeneity including karst (Condon et al.  
232 in review) which should be considered as part of conceptual model development prior to  
233 numerical model implementation.

234

235 Now that a number of models that represent groundwater at continental to global scales have  
236 been developed and will continue evolving, it is equally important that we advance how we  
237 evaluate these models. To date, large-scale model evaluation has largely focused on individual  
238 models, with inconsistent practices between models and little community-level discussion or

239 cooperation, that lack the rigor of regional-scale model evaluation. Overall, we have only a  
240 partial and piecemeal understanding of the capabilities and limitations of different approaches  
241 to representing groundwater in large-scale models. Our objective is to provide clear  
242 recommendations for evaluating groundwater representation in continental and global models.  
243 We focus on model evaluation because this is the heart of model trust and reproducibility  
244 (Hutton et al., 2016) and improved model evaluation will guide how and where it is most  
245 important to focus future model development. We describe current model evaluation practices  
246 (Section 2) and consider diverse and uncertain sources of information, including observations,  
247 models, and experts to holistically evaluate the simulation of groundwater-related fluxes,  
248 stores and hydraulic heads (Section 3). We stress the need for an iterative and open-ended  
249 process of model improvement through continuous model evaluation against the different  
250 sources of information. We explicitly contrast the terminology used herein of ‘evaluation’ and  
251 ‘comparison’ against terminology such as ‘calibration’ or ‘validation’ or ‘benchmarking’, which  
252 suggests a modelling process that is at some point complete. We extend previous  
253 commentaries advocating improved hydrologic process representation and evaluation in large-  
254 scale hydrologic models (Clark et al. 2015; Melsen et al. 2016) by adding expert-elicitation and  
255 machine learning for more holistic evaluation. We also consider model objective and model  
256 evaluation across the diverse hydrologic landscapes which can both uncover blindspots in  
257 model development. It is important to note that we do not consider water quality or  
258 contamination, even though water quality or contamination is important for water resources,  
259 management and sustainability, since large-scale water quality models are in their infancy (van  
260 Vliet et al., 2019)

261

262 We bring together somewhat disparate scientific communities as a step towards greater  
263 community-level cooperation on these challenges, including global hydrology and land surface  
264 modelers, local to regional hydrogeologists, and hydrologists focused on model development  
265 and evaluation. We see three audiences beyond those currently directly involved in large-scale  
266 groundwater modeling that we seek to engage to accelerate model evaluation: 1) regional  
267 hydrogeologists who could be reticent about global models, and yet have crucial knowledge  
268 and data that would improve evaluation; 2) data scientists with expertise in machine learning,  
269 artificial intelligence etc. whose methods could be useful in a myriad of ways; and 3) the  
270 multiple Earth Science communities that are currently working towards integrating  
271 groundwater into a diverse range of models so that improved evaluation approaches are built  
272 directly into model development.

## 273 **2. CURRENT MODEL EVALUATION PRACTICES**

274 Here we provide a brief overview of current large-scale groundwater models, the synergies and  
275 differences between regional-scale and large-scale model evaluation and development as well  
276 as the imitations of current evaluation practices for large-scale models.

### 277 **2.1 Brief overview of current large-scale groundwater models**

278 Various large-scale models exist along a spectrum of model complexity, which can make it  
279 difficult to determine the most appropriate model for a specific application. We developed a  
280 simple but systematic classification of current large-scale groundwater models (Table 1) to

281 summarize the main characteristics of existing models for the interdisciplinary audience of  
282 GMD. This classification builds on other reviews (Bierkens 2015; Condon et al., in review) and is  
283 not exhaustive, nor is it the only way to classify large-scale groundwater models. It is meant to  
284 be a first classification attempt that should evolve with time. We suggest that groundwater in  
285 current large-scale models can be classified functionally by two aspects that are crucial to how  
286 groundwater impacts water, energy, and nutrient budgets. First, whether lateral subsurface  
287 flow to a river is simulated within each cell independently of other cells, as 2D lateral  
288 groundwater flow between all cells or as 3D groundwater flow. Second, we distinguish two  
289 types of coupling between groundwater and related compartments (variably saturated soil  
290 zone, surface water, atmospheric processes): ‘one-way’ coupling (for example, recharge is  
291 imposed from the surface with no feedback from capillary rise or vegetation uptake, or  
292 groundwater flow to the surface does not depend on surface head) from ‘two-way’ coupling  
293 involves feedback loops. We also note atmospheric coupling which involves coupling a  
294 groundwater-surface model with an atmospheric model to propagate the influence of  
295 groundwater from the surface to the atmosphere, and the resulting feedback onto the surface  
296 and groundwater. This classification scheme (which could also be called a model typology) is  
297 based on a number of model characteristics such as the fluxes, stores and other features (Table  
298 1).

299

## 300 **2.2 Synergies between regional-scale and large-scales**

301 Regional-scale and large-scale groundwater models are both governed by the same physical  
302 equations and share many of the same challenges. Like large-scale models, some regional-scale  
303 models have challenges with representing important regional hydrologic processes such as  
304 mountain block recharge (Markovich et al. 2019), and data availability challenges (such as the  
305 lack of reliable subsurface parameterization and hydrologic monitoring data) are common. We  
306 propose there are largely untapped potential synergies between regional-scale and large-scale  
307 models based on these commonalities and the inherent strengths and limitations of each scale  
308 (Section 1).

309

310 Much can be learned from regional-scale models to inform the development and evaluation of  
311 large-scale groundwater models. Regional-scale models are evaluated using a variety of data  
312 types, some of which are available and already used at the global scale and some of which are  
313 not. In general, the most common data types used for regional-scale groundwater model  
314 evaluation match global-scale groundwater models: hydraulic head and either total streamflow  
315 or baseflow estimated using hydrograph separation approaches (eg. RRCA, 2003; Woolfenden  
316 and Nishikawa, 2014; Tolley et al., 2019). However, numerous data sources unavailable or not  
317 currently used at the global scale have also been applied in regional-scale models, such as  
318 elevation of surface water features (Hay et al., 2018), existing maps of the potentiometric  
319 surface (Meriano and Eyles, 2003), and dendrochronology (Schilling et al., 2014) and stable and  
320 radiogenic isotopes for determining water sources and residence times (Sanford, 2011). These  
321 and other ‘non-classical’ observations (Schilling et al. 2019) could be the inspiration for model

322 evaluation of large-scale models in the future but are beyond our scope to discuss. Further,  
323 given the smaller domain size of regional-scale models, expert knowledge and local ancillary  
324 data sources can be more directly integrated and automated parameter estimation approaches  
325 such as PEST are tractable (Leaf et al., 2015; Hunt et al., 2013). We directly build upon this  
326 practice of integration of expert knowledge below in Section 3.3.

327

328 We propose that there may also be potential benefits of large-scale models for the  
329 development of regional-scale models. For instance, the boundary conditions of some regional-  
330 scale models could be improved with large-scale model results. The boundary conditions of  
331 regional-scale models are often assumed, calibrated or derived from other models or data. In a  
332 regional-scale model, increasing the model domain (moving the boundary conditions away  
333 from region of interests) or incorporating more hydrologic processes (for example, moving the  
334 boundary condition from recharge to the land surface incorporating evapotranspiration and  
335 infiltration) both can reduce the impact of boundary conditions on the region and problem of  
336 interest. Another potential benefit of large-scale models for regional-scale models is fuller  
337 inclusion of large-scale hydrologic and human processes that could further enhance the ability  
338 of regional-scale models to address both the science-focused and sustainability-focused  
339 purposes described in Section 1. For example, the stronger representation of large-scale  
340 atmospheric processes means that the downwind impact of groundwater irrigation on  
341 evapotranspiration on precipitation and streamflow can be assessed (DeAngelis et al., 2010;  
342 Kustu et al., 2011). Or, the effects of climate change and increased water use that affect the



343 inflow of rivers into the regional modelling domain can be taken from global scale analyses  
344 (Wada and Bierkens, 2014 ). Also, regional groundwater depletion might be largely driven by  
345 virtual water trade which can be better represented in global analysis and models than  
346 regional-scale models (Dalin et al. 2017). Therefore the processes and results of large-scale  
347 models could be used to make regional-scale models even more robust and better address key  
348 science and sustainability questions.

349

350 Given the strengths of regional models, a potential alternative to development of large-scale  
351 groundwater models would be combining or aggregating multiple regional models in a  
352 patchwork approach (as in Zell and Sanford, 2020) to provide global coverage. This would have  
353 the advantage of better respecting regional differences but potentially create additional  
354 challenges because the regional models would have different conceptual models, governing  
355 equations, boundary conditions etc. in different regions. Some challenges of this patchwork  
356 approach include 1) the required collaboration of a large number of experts from all over the  
357 world over a long period of time; 2) regional groundwater flow models alone are not sufficient,  
358 they need to be integrated into a hydrological model so that groundwater-soil water and the  
359 surface water-groundwater interactions can be simulated; 3) the extent of regional aquifers  
360 does not necessarily coincide with the extent of river basins; and 4) the bias of regional  
361 groundwater models towards important aquifers which as described above, underlie only a  
362 portion of the world's land mass or population and may bias estimates of fluxes such as surface  
363 water-groundwater exchange or evapotranspiration. Given these challenges, we argue that a

364 patchwork approach of integrating multiple regional models is a compelling idea but likely  
365 insufficient to achieve the purposes of large-scale groundwater modeling described in Section  
366 1. Although this nascent idea of aggregating regional models is beyond the scope of this  
367 manuscript, we consider this an important future research avenue, and encourage further  
368 exploration and improvement of regional-scale model integration from the groundwater  
369 modeling community.

370

### 371 **2.3 Differences between regional-scale and large-scales**

372 Although there are important similarities and potential synergies across scales, it is important  
373 to consider how or if large-scale models are fundamentally different to regional-scale models,  
374 especially in ways that could impact evaluation. The primary differences between large-scale  
375 and regional-scale models are that large-scale models (by definition) cover larger areas and, as  
376 a result, typically include more data-poor areas and are generally built at coarser resolution.

377 These differences impact evaluations in at least five relevant ways:

378 1) Commensurability errors (also called 'representativeness' errors) occur either when  
379 modelled grid values are interpolated and compared to an observation 'point' or when  
380 aggregation of observed 'point' values are compared to a modelled grid value (Beven,  
381 2005; Tustison et al., 2001; Beven, 2016; Pappenberger et al., 2009; Rajabi et al., 2018).

382 For groundwater models in particular, commensurability error will depend on the number  
383 and locations of observation points, the variability structure of the variables being

384 compared such as hydraulic head and the interpolation or aggregation scheme applied  
385 (Tustison et al., 2001; Pappenberger et al., 2009; Reinecke et al., 2020). Commensurability  
386 is a problem for most scales of modelling, but likely more significant the coarser the  
387 model. Regional-scale groundwater models typically have fewer (though not insignificant)  
388 commensurability issues due to smaller grid cell sizes compared to large-scale models.

389 2) Specificity to region, objective and model evaluation criteria because regional-scale  
390 models are developed specifically for a certain region and modeling or management  
391 objective whereas large-scale models are often more general and include different  
392 regions. As a result, large-scale models often have greater heterogeneity of processes and  
393 parameters, may not adopt the same calibration targets and variables, and are not subject  
394 to the policy or litigation that sometimes drives model evaluation of regional-scale  
395 models.

396 3) Computational requirements can be immense for large-scale models which leads to  
397 challenges with uncertainty and sensitivity analysis. While some regional-scale models  
398 also have large computational demands, large-scale models cover larger domains and are  
399 therefore more vulnerable to this potential constraint.

400 4) Data availability for large-scale models can be limited because they typically include data-  
401 poor areas, which leads to challenges when only using observations for model evaluation.  
402 While data availability also affects regional-scale models, they are often developed for  
403 regions with known hydrological challenges based on existing data and/or modeling  
404 efforts are preceded by significant regional data collection from detailed sources (such as

405 local geological reports) that are not often included in continental to global datasets used  
406 for large-scale model parameterization.

407 5) Subsurface detail in regional-scale models routinely include heterogeneous and  
408 anisotropic parameterizations which could be improved in future large-scale models. For  
409 example, intense vertical anisotropy routinely induces vertical flow dynamics from vertical  
410 head gradients that are tens to thousands of times greater than horizontal gradients  
411 which profoundly alter the meaning of the deep and shallow groundwater levels, with  
412 only the latter remotely resembling the actual water table. In contrast, currently most  
413 large-scale models use a single vertically homogeneous value for each grid cell, or at best  
414 have two layers (de Graaf et al., 2017)

415

#### 416 **2.4 Limitations of current evaluation practices for large-scale models**

417 Evaluation of large-scale models has often focused on streamflow or evapotranspiration  
418 observations but joint evaluation together with groundwater-specific variables is appropriate  
419 and necessary (e.g. Maxwell et al. 2015; Maxwell and Condon, 2016). Groundwater-specific  
420 variables useful for evaluating the groundwater component of large-scale models include: a)  
421 hydraulic head or water table depth; b) groundwater storage and groundwater storage changes  
422 which refer to long-term, negative or positive trends in groundwater storage where long-term,  
423 negative trends are called groundwater depletion; c) groundwater recharge; d) flows between  
424 groundwater and surface water bodies; and e) human groundwater abstractions and return

425 flows to groundwater. It is important to note that groundwater and surface water hydrology  
426 communities often have slightly different definitions of terms like recharge and baseflow  
427 (Barthel, 2014); we therefore suggest trying to precisely define the meanings of such words  
428 using the actual hydrologic fluxes which we do below. Table 2 shows the availability of  
429 observational data for these variables but does not evaluate the quality and robustness of  
430 observations. Overall there are significant inherent challenges of commensurability and  
431 measurability of groundwater observations in the evaluation of large-scale models. We  
432 describe the current model evaluation practices for each of these variables here:

433

434 a) Simulated hydraulic heads or water table depth in large scale models are  
435 frequently compared to well observations, which are often considered the crucial  
436 data for groundwater model evaluation. Hydraulic head observations from a large  
437 number groundwater wells (>1 million) have been used to evaluate the spatial  
438 distribution of steady-state heads (Fan et al., 2013, de Graaf et al., 2015; Maxwell et  
439 al., 2015; Reinecke et al., 2019a, 2020). Transient hydraulic heads with seasonal  
440 amplitudes (de Graaf et al. 2017), declining heads in aquifers with groundwater  
441 depletion (de Graaf et al. 2019) and daily transient heads (Tran et al 2020) have also  
442 been compared to well observations. All evaluation with well observations is  
443 severely hampered by the incommensurability of point values of observed head with  
444 simulated heads that represent averages over cells of a size of tens to hundreds  
445 square kilometers; within such a large cell, land surface elevation, which strongly

446 governs hydraulic head, may vary a few hundred meters, and average observed  
447 head strongly depends on the number and location of well within the cell (Reinecke  
448 et al., 2020). Additional concerns with head observations are the 1) strong sampling  
449 bias of wells towards accessible locations, low elevations, shallow water tables, and  
450 more transmissive aquifers in wealthy, generally temperate countries (Fan et al.,  
451 2019); 2) the impacts of pumping which may or may not be well known; 3)  
452 observational errors and uncertainty (Post and von Asmuth, 2013; Fan et al., 2019);  
453 and 4) that heads can reflect the poro-elastic effects of mass loading and unloading  
454 rather than necessarily aquifer recharge and drainage (Burgess et al, 2017). To date,  
455 simulated hydraulic heads have more often been compared to observed heads  
456 (rather than water table depth) which results in lower relative errors (Reinecke et  
457 al., 2020) because the range of heads (10s to 1000s m head) is much larger than the  
458 range of water table depths (<1 m to 100s m).

459

460 b) Simulated groundwater storage trends or anomalies in large-scale hydrological  
461 models have been evaluated using observations of groundwater well levels  
462 combined with estimates of storage parameters, such as specific yield; local-scale  
463 groundwater modeling; and translation of regional total water storage trends and  
464 anomalies from satellite gravimetry (GRACE: Gravity Recovery And Climate  
465 Experiment) to groundwater storage changes by estimating changes in other  
466 hydrological storages (Döll et al., 2012; 2014a). Groundwater storage changes

467 volumes and rates have been calculated for numerous aquifers, primarily in the  
468 United States, using calibrated groundwater models, analytical approaches, or  
469 volumetric budget analyses (Konikow, 2010). Regional-scale models have also been  
470 used to simulate groundwater storage trends untangling the impacts of water  
471 management during drought (Thatch et al. 2020). Satellite gravimetry (GRACE) is  
472 important but has limitations (Alley and Konikow, 2015). First, monthly time series  
473 of very coarse-resolution groundwater storage are indirectly estimated from  
474 observations of total water storage anomalies by satellite gravimetry (GRACE) but  
475 only after model- or observation-based subtraction of water storage changes in  
476 glaciers, snow, soil and surface water bodies (Lo et al., 2016; Rodell et al., 2009;  
477 Wada, 2016). As soil moisture, river or snow dynamics often dominate total water  
478 storage dynamics, the derived groundwater storage dynamics can be so uncertain  
479 that severe groundwater drought cannot be detected in this way (Van Loon et al.,  
480 2017). Second, GRACE cannot detect the impact of groundwater abstractions on  
481 groundwater storage unless groundwater depletion occurs (Döll et al., 2014a,b).  
482 Third, the very coarse resolution can lead to incommensurability but in the opposite  
483 direction of well observations. It is important to note that the focus is on storage  
484 trends or anomalies since total groundwater storage to a specific depth (Gleeson et  
485 al., 2016) or in an aquifer (Konikow, 2010) can be estimated but the total  
486 groundwater storage in a specific region or cell cannot be simulated or observed  
487 unless the depth of interest is specified (Condon et al., 2020).

488

489 c) Simulated large-scale groundwater recharge (vertical flux across the water table)  
490 has been evaluated using compilations of point estimates of groundwater recharge,  
491 results of regional-scale models, baseflow indices, and expert opinion (Döll and  
492 Fiedler, 2008; Hartmann et al., 2015) or compared between models (e.g. Wada et al.  
493 2010). In general, groundwater recharge is not directly measurable except by meter-  
494 scale lysimeters (Scanlon et al., 2002), and many groundwater recharge methods  
495 such as water table fluctuations and chloride mass balance also suffer from similar  
496 commensurability issues as water table depth data. Although sometimes an input or  
497 boundary condition to regional-scale models, recharge in many large-scale  
498 groundwater models is simulated and thus can be evaluated.

499  
500 d) The flows between groundwater and surface water bodies (rivers, lakes, wetlands)  
501 are simulated by many models but are generally not evaluated directly against  
502 observations of such flows since they are very rare and challenging. Baseflow (the  
503 slowly varying portion of streamflow originating from groundwater or other delayed  
504 sources) or streamflow 'low flows' (when groundwater or other delayed sources  
505 predominate), generally cannot be used to directly quantify the flows between  
506 groundwater and surface water bodies at large scales. Groundwater discharge to  
507 rivers can be estimated from streamflow observations only in the very dense gauge  
508 network and/or if streamflow during low flow periods is mainly caused by  
509 groundwater discharge and not by water storage in upstream lakes, reservoirs or



510 wetlands. These conditions are rarely met in case of streamflow gauges with large  
511 upstream areas that can be used for comparison to large-scale model output. de  
512 Graaf et al. (2019) compared the simulated timing of changes in groundwater  
513 discharge to observations and regional-scale models, but only compared the fluxes  
514 directly between the global- and regional-scale models. Due to the challenges of  
515 directly observing the flows between groundwater and surface water bodies at large  
516 scales, this is not included in the available data in Table 2; instead in Section 3 we  
517 highlight the potential for using baseflow or the spatial distribution of perennial,  
518 intermittent and ephemeral streams in the future.

519

520 e) Groundwater abstractions have been evaluated by comparison to national, state  
521 and county scale statistics in the U.S. (Wada et al. 2010, Döll et al., 2012, 2014a, de  
522 Graaf et al. 2014). Irrigation is the dominant groundwater use sector in many  
523 regions; however, irrigation pumpage is generally estimated from crop water  
524 demand and rarely metered. GRACE and other remote sensing data have been used  
525 to estimate the irrigation water abstractions (Anderson et al. 2015b). The lack of  
526 records or observations of abstraction introduces significant uncertainties into large-  
527 scale models and is simulated and thus can be evaluated. Human groundwater  
528 abstractions and return flows as well as groundwater recharge and the flows  
529 between groundwater and surface water bodies are necessary to simulate storage  
530 trends (described above). But each of these are considered separate observations

531 since they each have different data sources and assumptions. Groundwater  
532 abstraction data at the well scale are severely hampered by the incommensurability  
533 like hydraulic head and recharge described above.

### 534 **3. HOW TO IMPROVE THE EVALUATION OF LARGE-SCALE GROUNDWATER MODELS**

535 Based on Section 2, we argue that the current model evaluation practices are insufficient to  
536 robustly evaluate large-scale models. We therefore propose evaluating large-scale models using  
537 at least three strategies (pie-shapes in Figure 1): observation-, model-, and expert-driven  
538 evaluation which are potentially mutually beneficial because each strategy has its strengths and  
539 weaknesses. We are not proposing a brand new evaluation method here but rather separating  
540 strategies to consider the problem of large-scale model evaluation from different but highly  
541 interconnected perspectives. All three strategies work together for the common goal of  
542 'improved model large-scale model evaluation' which is what is the centre of Figure 1.

543

544 When evaluating large-scale models, it is necessary to first consider reasonable expectations or  
545 how to know a model is 'well enough'. Reasonable expectations should be based on the  
546 modeling purpose, hydrologic process understanding and the plausibly achievable degree of  
547 model realism. First, model evaluation should be clearly linked to the four science- or  
548 sustainability-focused purposes of representing groundwater in large-scale models (Section 1)  
549 and second, to our understanding of relevant hydrologic processes. The objective of large-scale  
550 models cannot be to reproduce the spatio-temporal details that regional-scale models can

551 reproduce. Determining the reasonable expectations is necessarily subjective, but can be  
552 approached using observation-, model-, and expert-driven evaluation. As a simple first step in  
553 setting realistic expectations, we propose that three physical variables can be used to form  
554 more convincing arguments that a large-scale model is well enough: change in groundwater  
555 storage, water table depth, and regional fluxes between groundwater and surface water. Below  
556 we explore in more detail additional variables and approaches that can support this simple  
557 approach.

558

559 Across all three model evaluation strategies of observation-, model-, and expert-driven  
560 evaluation, we advocate three principles underpinning model evaluation (base of Figure 1),  
561 none of which we are the first to suggest but we highlight here as a reminder: 1) model  
562 objectives, such as the groundwater science or groundwater sustainability objective  
563 summarised in Section 1, are important to model evaluation because they provide the context  
564 through which relevance of the evaluation outcome is set; 2) all sources of information  
565 (observations, models and experts) are uncertain and this uncertainty needs to be quantified  
566 for robust evaluation; and 3) regional differences are likely important for large-scale model  
567 evaluation - understanding these differences is crucial for the transferability of evaluation  
568 outcomes to other places or times.

569

570 We stress that we see the consideration and quantification of uncertainty as an essential need  
571 across all three types of model evaluation we describe below, so we discuss it here rather than  
572 with model-driven model evaluation (Section 3.2) where uncertainty analysis more narrowly  
573 defined would often be discussed. We further note that large-scale models have only been  
574 assessed to a very limited degree with respect to understanding, quantifying, and attributing  
575 relevant uncertainties. Expanding computing power, developing computationally frugal  
576 methods for sensitivity and uncertainty analysis, and potentially employing surrogate models  
577 can enable more robust sensitivity and uncertainty analysis such as used in regional-scale  
578 models (Habets et al., 2013; Hill, 2006; Hill & Tiedeman, 2007; Reinecke et al., 2019b). For now,  
579 we suggest applying computationally frugal methods such as the elementary effect test or local  
580 sensitivity analysis (Hill, 2006; Morris, 1991; Saltelli et al., 2000). Such sensitivity and  
581 uncertainty analyses should be applied not only to model parameters and forcings but also to  
582 model structural properties (e.g. boundary conditions, grid resolution, process simplification,  
583 etc.) (Wagener and Pianosi, 2019). This implies that the (independent) quantification of  
584 uncertainty in all model elements (observations, parameters, states, etc.) needs to be improved  
585 and better captured in available metadata.

586

587 We advocate for considering regional differences more explicitly in model evaluation since  
588 likely no single model will perform consistently across the diverse hydrologic landscapes of the  
589 world (Van Werkhoven et al., 2008). Considering regional differences in large-scale model  
590 evaluation is motivated by recent model evaluation results and is already starting to be

591 practiced. Two recent sensitivity analyses of large-scale models reveal how sensitivities to input  
592 parameters vary in different regions for both hydraulic heads and flows between groundwater  
593 and surface water (de Graaf et al. 2019; Reinecke et al., 2020). In mountain regions, large-scale  
594 models tend to underestimate steady-state hydraulic head, possibly due to over-estimated  
595 hydraulic conductivity in these regions, which highlights that model performance varies in  
596 different hydrologic landscapes. (de Graaf et al., 2015; Reinecke et al. 2019b). Additionally,  
597 there are significant regional differences in performance with low flows for a number of large-  
598 scale models (Zaherpour et al. 2018) likely because of diverse implementations of groundwater  
599 and baseflow schemes. Large-scale model evaluation practice is starting to shift towards  
600 highlighting regional differences as exemplified by two different studies that explicitly mapped  
601 hydrologic landscapes to enable clearer understanding of regional differences. Reinecke et al.  
602 (2019b) identified global hydrological response units which highlighted the spatially distributed  
603 parameter sensitivities in a computationally expensive model, whereas Hartmann et al. (2017)  
604 developed and evaluated models for karst aquifers in different hydrologic landscapes based on  
605 different a priori system conceptualizations. Considering regional differences in model  
606 evaluation suggests that global models could in the future consider a patchwork approach of  
607 different conceptual models, governing equations, boundary conditions etc. in different  
608 regions. Although beyond the scope of this manuscript, we consider this an important future  
609 research avenue.

### 610 **3.1 Observation-based model evaluation**

611 Observation-based model evaluation is the focus of most current efforts and is important  
612 because we want models to be consistent with real-world observations. Section 2 and Table 2  
613 highlight both the strengths and limitations of current practices using observations. Despite  
614 existing challenges, we foresee significant opportunities for observation-based model  
615 evaluation and do not see data scarcity as a reason to exclude groundwater in large-scale  
616 models or to avoid evaluating these models. It is important to note that most so-called  
617 'observations' are modeled or derived quantities, and often at the wrong scale for evaluating  
618 large-scale models (Table 2; Beven, 2019). Given the inherent challenges of direct  
619 measurement of groundwater fluxes and stores especially at large scales, herein we consider  
620 the word 'observation' loosely as any measurements of physical stores or fluxes that are  
621 combined with or filtered through models for an output. For example, GRACE gravity  
622 measurements are combined with model-based estimates of water storage changes in glaciers,  
623 snow, soil and surface water for 'groundwater storage change observations' or streamflow  
624 measurements are filtered through baseflow separation algorithms for 'baseflow observations'.  
625 The strengths and limitations as well as the data availability and spatial and temporal attributes  
626 of different observations are summarized in Table 2 which we hope will spur more systematic  
627 and comprehensive use of observations.

628

629 Here we highlight nine important future priorities for improving evaluation using available  
630 observations. The first five priorities focus on current observations (Table 2) whereas the latter  
631 four focus on new methods or approaches:

632 1) Focus on transient observations of the water table depth rather than  
633 hydraulic head observations that are long-term averages or individual times  
634 (often following well drilling). Water table depth are likely more robust  
635 evaluation metrics than hydraulic head because water table depth reveals  
636 great discrepancies and is a complex function of the relationship between  
637 hydraulic head and topography that is crucial to predicting system fluxes  
638 (including evapotranspiration and baseflow). Comparing transient  
639 observations and simulations instead of long-term averages or individual  
640 times incorporates more system dynamics of storage and boundary  
641 conditions as temporal patterns are more important than absolute values  
642 (Heudorfer et al. 2019). For regions with significant groundwater depletion,  
643 comparing to declining water tables is a useful strategy (de Graaf et al. 2019),  
644 whereas in aquifers without groundwater depletion, seasonally varying  
645 water table depths are likely more useful observations (de Graaf et al. 2017).

646 2) Use baseflow, the slowly varying portion of streamflow originating from  
647 groundwater or other delayed sources. Döll and Fiedler (2008) included the  
648 baseflow index in evaluating recharge and baseflow has been used to  
649 calibrate the groundwater component of a land surface model (Lo et al.  
650 2008, 2010). But the baseflow index (BFI), linear and nonlinear baseflow  
651 recession behavior or baseflow fraction (Gnann et al., 2019) have not been  
652 used to evaluate any large-scale model that simulates groundwater flows  
653 between all model grid cells. There are limitations of using BFI and baseflow

654 recession characteristics to evaluate large-scale models (Table 2). Using  
655 baseflow only makes sense when the baseflow separation algorithm is better  
656 than the large-scale model itself, which may not be the case for some large-  
657 scale models and only in time periods that can be assumed to be dominated  
658 by groundwater discharge. Similarly, using recession characteristics is  
659 dependent on an appropriate choice of recession extraction methods. But  
660 this remains available and obvious data derived from streamflow or spring  
661 flow observations that has been under-used to date.

662 3) Use the spatial distribution of perennial, intermittent, and ephemeral  
663 streams as an observation, which to our best knowledge has not been done  
664 by any large-scale model evaluation. The transition between perennial and  
665 ephemeral streams is an important system characteristic in groundwater-  
666 surface water interactions (Winter et al. 1998), so we suggest that this might  
667 be a revealing evaluation criteria although there are similar limitations to  
668 using baseflow. The results of both quantifying baseflow and mapping  
669 perennial streams depend on the methods applied, they are not useful for  
670 quantifying groundwater-surface water interactions when there is upstream  
671 surface water storage, and they do not directly provide information about  
672 fluxes between groundwater and surface water.

673 4) Use data on land subsidence to infer head declines or aquifer properties for  
674 regions where groundwater depletion is the main cause of compaction



675 (Bierkens and Wada, 2019). Lately, remote sensing methods such as GPS,  
676 airborne and space borne radar and lidar are frequently used to infer land  
677 subsidence rates (Erban et al., 2014). Also, a number of studies combine  
678 geomechanical modelling (Ortega-Guerrero et al 1999; Minderhoud et al  
679 2017) and geodetic data to explain the main drivers of land subsidence. A  
680 few papers (e.g. Zhang and Burbey 2016) use a geomechanical model  
681 together with a withdrawal data and geodetic observations to estimate  
682 hydraulic and geomechanical subsoil properties.

683 5) Consider using socio-economic data for improving model input. For  
684 example, reported crop yields in areas with predominant groundwater  
685 irrigation could be used to evaluate groundwater abstraction rates. Or using  
686 well depth data (Perrone and Jasechko, 2019) to assess minimum aquifer  
687 depths or in coastal regions and deltas, the presence of deeper fresh  
688 groundwater under semi-confining layers.

689 6) Derive additional new datasets using meta-analysis and/or geospatial  
690 analysis such as gaining or losing stream reaches (e.g., from interpolated  
691 head measurements close to the streams), springs and groundwater-  
692 dependent surface water bodies, or tracers. Each of these new data sources  
693 could in principle be developed from available data using methods already  
694 applied at regional scales but do not currently have an 'off the shelf' global  
695 dataset. For example, some large-scale models have been explicitly

696 compared with residence time and tracer data (Maxwell et al., 2016) which  
697 have also been recently compiled globally (Gleeson et al., 2016; Jasechko et  
698 al., 2017). This could be an important evaluation tool for large-scale models  
699 that are capable of simulating flow paths, or can be modified to do, though a  
700 challenge of this approach is the conservativity of tracers. Future meta-  
701 analyses data compilations should report on the quality of the data and  
702 include possible uncertainty ranges as well as the mean estimates.

703 7) Use machine learning to identify process representations (e.g. Beven, 2020)  
704 or spatiotemporal patterns, for example of perennial streams, water table  
705 depths or baseflow fluxes, which might not be obvious in multi-dimensional  
706 datasets and could be useful in evaluation. For example, Yang et al. (2019)  
707 predicted the state of losing and gaining streams in New Zealand using  
708 Random Forest algorithms. A staggering variety of machine learning tools are  
709 available and their use is nascent yet rapidly expanding in geoscience and  
710 hydrology (Reichstein et al., 2019; Shen, 2018; Shen et al., 2018; Wagener et  
711 al., 2020). While large-scale groundwater models are often considered 'data-  
712 poor', it may seem strange to propose using data-intensive machine learning  
713 methods to improve model evaluation. But some of the data sources are  
714 large (e.g over 2 million water level measurements in Fan et al. 2013  
715 although biased in distribution) whereas other observations such as  
716 evapotranspiration (Jung et al., 2011) and baseflow (Beck et al. 2013) are  
717 already interpolated and extrapolated using machine learning. Moving

718 forwards, it is important to consider commensurability while applying  
719 machine learning in this context.

720 8) Consider comparing models against hydrologic signatures - indices that  
721 provide insight into the functional behavior of the system under study  
722 (Wagener et al., 2007; McMilan, 2020). The direct comparison of simulated  
723 and observed variables through statistical error metrics has at least two  
724 downsides. One, the above mentioned unresolved problem of  
725 commensurability, and two, the issue that such error metrics are rather  
726 uninformative in a diagnostic sense - simply knowing the size of an error does  
727 not tell the modeller how the model needs to be improved, only that it does  
728 (Yilmaz et al., 2009). One way to overcome these issues, is to derive  
729 hydrologically meaningful signatures from the original data, such as the  
730 signatures derived from transient groundwater levels by Heudorfer et al.  
731 (2019). For example, recharge ratio (defined as the ratio of groundwater  
732 recharge to precipitation) might be hydrologically more informative than  
733 recharge alone (Jasechko et al., 2014) or the water table ratio and  
734 groundwater response time (Cuthbert et al. 2019; Opie et al., 2020) which  
735 are spatially-distributed signatures of groundwater systems dynamics. Such  
736 signatures might be used to assess model consistency (Wagener & Gupta,  
737 2005; Hrachowitz et al.2014) by looking at the similarity of patterns or spatial  
738 trends rather than the size of the aggregated error, thus reducing the  
739 commensurability problem.

740 9) Understand and quantify commensurability error issues better so that a  
741 fairer comparison can be made across scales using existing data. As described  
742 above, commensurability errors will depend on the number and locations of  
743 observation points, the variability structure of the variables being compared  
744 such as hydraulic head and the interpolation or aggregation scheme applied.  
745 While to some extent we may appreciate how each of these factors affect  
746 commensurability error in theory, in practice their combined effects are  
747 poorly understood and methods to quantify and reduce commensurability  
748 errors for groundwater model purposes remain largely undeveloped. As  
749 such, quantification of commensurability error in (large-scale) groundwater  
750 studies is regularly overlooked as a source of uncertainty because it cannot  
751 be satisfactorily evaluated (Tregoning et al., 2012). Currently, evaluation of  
752 simulated groundwater heads is plagued by, as yet, poorly quantified  
753 uncertainties stemming from commensurability errors and we therefore  
754 recommend future studies focus on developing solutions to this problem. An  
755 additional, subtle but important and unresolved commensurability issue can  
756 stem from conceptual models. Different hydrogeologists examining different  
757 scales, data or interpreting geology differently can produce quite different  
758 conceptual models of the same region (Troldborg et al. 2007).

759 We recommend evaluating models with a broader range of currently available data sources  
760 (with explicit consideration of data uncertainty and regional differences) while also  
761 simultaneously working to derive new data sets. Using data (such as baseflow, land subsidence,

762 or the spatial distribution of perennial, intermittent, and ephemeral streams) that is more  
763 consistent with the scale modelled grid resolution will hopefully reduce the commensurability  
764 challenges. However, data distribution and commensurability issues will likely still be present,  
765 which underscores the importance of the two following strategies.

### 766 **3.2. Model-based model evaluation**

767 Model-based model evaluation, which includes model intercomparison projects (MIP) and  
768 model sensitivity and uncertainty analysis, can be done with or without explicitly using  
769 observations. We describe both inter-model and inter-scale comparisons which could be  
770 leveraged to maximize the strengths of each of these approaches.

771

772 The original MIP concept offers a framework to consistently evaluate and compare models, and  
773 associated model input, structural, and parameter uncertainty under different objectives (e.g.,  
774 climate change, model performance, human impacts and developments). Early model  
775 intercomparisons of groundwater models focused on nuclear waste disposal (SKI, 1984). Since  
776 the Project for the Intercomparison of Land-Surface Parameterization Schemes (PILPS; Sellers et  
777 al., 1993), the first large-scale MIP, the land surface modeling community has used MIPs to  
778 deepen understanding of land physical processes and to improve their numerical  
779 implementations at various scales from regional (e.g., Rhône-aggregation project; Boone et al.,  
780 2004) to global (e.g., Global Soil Wetness Project; Dirmeyer, 2011). Two examples of recent  
781 model intercomparison efforts illustrate the general MIP objectives and practice. First, ISIMIP  
782 (Schewe et al., 2014; Warszawski et al., 2014) assessed water scarcity at different levels of

783 global warming. Second, IH-MIP2 (Kollet et al., 2017) used both synthetic domains and an  
784 actual watershed to assess fully-integrated hydrologic models because these cannot be  
785 validated easily by comparison with analytical solutions and uncertainty remains in the  
786 attribution of hydrologic responses to model structural errors. Model comparisons have  
787 revealed differences, but it is often unclear whether these stem from differences in the model  
788 structures, differences in how the parameters were estimated, or from other modelling choices  
789 (Duan et al., 2006). Attempts for modular modelling frameworks to enable comparisons  
790 (Wagener et al., 2001; Leavesley et al., 2002; Clark et al., 2008; Fenicia et al., 2011; Clark et al.,  
791 2015) or at least shared explicit modelling protocols and boundary conditions (Refsgaard et al.,  
792 2007; Ceola et al., 2015; Warszawski et al., 2014) have been proposed to reduce these  
793 problems.

794

795 Inter-scale model comparison - for example, comparing a global model to a regional-scale  
796 model - is a potentially useful approach which is emerging for surface hydrology models  
797 (Hattermann et al., 2017; Huang et al., 2017) and could be applied to large-scale models with  
798 groundwater representation. For example, declining heads and decreasing groundwater  
799 discharge have been compared between a calibrated regional-scale model (RRCA, 2003) and a  
800 global model (de Graaf et al., 2019). A challenge to inter-scale comparisons is that regional-  
801 scale models often have more spatially complex subsurface parameterizations because they  
802 have access to local data which can complicate model inter-comparison. Another approach  
803 which may be useful is running large-scale models over smaller (regional) domains at a higher

804 spatial resolution (same as a regional-scale model) so that model structure influences the  
805 comparison less. In the future, various variables that are hard to directly observe at large scales  
806 but routinely simulated in regional-scale models such as baseflow or recharge could be used to  
807 evaluate large-scale models, although these flux estimates can contain large uncertainty. In this  
808 way, the output fluxes and intermediate spatial scale of regional models provide a bridge across  
809 the “river of incommensurability” between highly location-specific data such as well  
810 observations and the coarse resolution of large-scale models. In such an evaluation, the  
811 uncertainty of flux estimates and scale of aggregation are both important to consider. It is  
812 important to consider that regional-scale models are not necessarily or inherently more  
813 accurate than large-scale models since problems may arise from conceptualization,  
814 groundwater-surface water interactions, scaling issues, parameterization etc.

815

816 In order for a regional-scale model to provide a useful evaluation of a large-scale model, there  
817 are several important documentation and quality characteristics it should meet. At a bare  
818 minimum, the regional-scale model must be accessible and therefore meet basic replicability  
819 requirements including open and transparent input and output data and model code to allow  
820 large-scale modelers to run the model and interpret its output. Documentation through peer  
821 review, either through a scientific journal or agency such as the US Geological Survey, would be  
822 ideal. It is particularly important that the documentation discusses limitations, assumptions and  
823 uncertainties in the regional-scale model so that a large-scale modeler can be aware of  
824 potential weaknesses and guide their comparison accordingly. Second, the boundary conditions

825 and/or parameters being evaluated need to be reasonably comparable between the regional-  
826 and large-scale models. For example, if the regional-scale model includes human impacts  
827 through groundwater pumping while the large-scale model does not, a comparison of baseflow  
828 between the two models may not be appropriate. Similarly, there needs to be consistency in  
829 the time period simulated between the two models. Finally, as with data-driven model  
830 evaluation, the purpose of the large-scale model needs to be consistent with the model-based  
831 evaluation; matching the hydraulic head of a regional-scale model, for instance, does not  
832 indicate that estimates of stream-aquifer exchange are valid. Ideally, we recommend  
833 developing a community database of regional-scale models that meet this criteria. It is  
834 important to note that Rossman & Zlotnik (2014) review 88 regional-scale models while a good  
835 example of such a repository is the California Groundwater Model Archive  
836 ([https://ca.water.usgs.gov/sustainable-groundwater-management/california-groundwater-  
837 modeling.html](https://ca.water.usgs.gov/sustainable-groundwater-management/california-groundwater-modeling.html)).

838

839 In addition to evaluating whether models are similar in terms of their outputs, e.g. whether  
840 they simulate similar groundwater head dynamics, it is also relevant to understand whether the  
841 influence of controlling parameters are similar across models. This type of analysis provides  
842 insights into process controls as well as dominant uncertainties. Sensitivity analysis provides  
843 the mathematical tools to perform this type of model evaluation (Saltelli et al., 2008; Pianosi et  
844 al., 2016; Borgonovo et al., 2017). Recent applications of sensitivity analysis to understand  
845 modelled controls on groundwater related processes include the study by Reinecke et al.



846 (2019b) trying to understand parametric controls on groundwater heads and flows within a  
847 global groundwater model. Maples et al. (2020) demonstrated that parametric controls on  
848 groundwater recharge can be assessed for complex models, though over a smaller domain. As  
849 highlighted by both of these studies, more work is needed to understand how to best use  
850 sensitivity analysis methods to assess computationally expensive, spatially distributed and  
851 complex groundwater models across large domains (Hill et al., 2016). In the future, it would be  
852 useful to go beyond parameter uncertainty analysis (e.g. Reinecke et al. 2019b) to begin to look  
853 at all of the modelling decisions holistically such as the forcing data (Weiland et al., 2015) and  
854 digital elevation models (Hawker et al., 2018). Addressing this problem requires advancements  
855 in statistics (more efficient sensitivity analysis methods), computing (more effective model  
856 execution), and access to large-scale models codes (Hutton et al. 2016), but also better  
857 utilization of process understanding, for example to create process-based groups of parameters  
858 which reduces the complexity of the sensitivity analysis study (e.g. Hartmann et al., 2015;  
859 Reinecke et al., 2019b).

### 860 **3.3 Expert-based model evaluation**

861 A path much less traveled is expert-based model evaluation which would develop hypotheses  
862 of phenomena (and related behaviors, patterns or signatures) we expect to emerge from large-  
863 scale groundwater systems based on expert knowledge, intuition, or experience. In essence,  
864 this model evaluation approach flips the traditional scientific method around by using  
865 hypotheses to test the simulation of emergent processes from large-scale models, rather than  
866 using large-scale models to test our hypotheses about environmental phenomena. This might

867 be an important path forward for regions where available data is very sparse or unreliable. The  
868 recent discussion by Fan et al. (2019) shows how hypotheses about large-scale behavior might  
869 be derived from expert knowledge gained through the study of smaller scale systems such as  
870 critical zone observatories. While there has been much effort to improve our ability to make  
871 hydrologic predictions in ungauged locations through the regionalization of hydrologic variables  
872 or of model parameters (Bloeschl et al., 2013), there has been much less effort to directly  
873 derive expectations of hydrologic behavior based on our perception of the systems under  
874 study.

875

876 Large-scale models could then be evaluated against such hypotheses, thus providing a general  
877 opportunity to advance how we connect hydrologic understanding with large-scale modeling - a  
878 strategy that could also potentially reduce epistemic uncertainty (Beven et al., 2019), and which  
879 may be especially useful for groundwater systems given the data limitations described above.

880 Developing appropriate and effective hypotheses is crucial and should likely focus on large-  
881 scale controlling factors or relationships between controlling factors and output in different  
882 parts of the model domain; hypotheses that are too specific may only be able to be tested by  
883 certain model complexities or in certain regions. To illustrate the type of hypotheses we are  
884 suggesting, we list some examples of hypotheses drawn from current literature:

- 885 • water table depth and lateral flow strongly affect transpiration partitioning  
886 (Famiglietti and Wood, 1994; Salvucci and Entekhabi, 1995; Maxwell & Condon,  
887 2016);

888           • the percentage of inter-basinal regional groundwater flow increases with aridity or  
889           decreases with frequency of perennial streams (Gleeson & Manning, 2008;  
890           Goderniaux et al, 2013; Schaller and Fan, 2008); or

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

893   Alternatively, it might be helpful to also include hypotheses that have been shown to be  
894   incorrect since models should also not show relationships that have been shown to not exist in  
895   nature. For example of a hypotheses that has recently been shown to be incorrect is that the  
896   baseflow fraction (baseflow volume/precipitation volume) follows the Budyko curve (Gnann et  
897   al. 2019) . As yet another alternative, hydrologic intuition could form the basis of model  
898   experiments, potentially including extreme model experiments (far from the natural  
899   conditions). For example, an experiment that artificially lowers the water table by decreasing  
900   precipitation (or recharge directly) could hypothesize the spatial variability across a domain  
901   regarding how ‘the drainage flux will increase and evaporation flux will decrease as the water  
902   table is lowered’. These hypotheses are meant only for illustrative purposes and we hope  
903   future community debate will clarify the most appropriate and effective hypotheses. We  
904   believe that the debate around these hypotheses alone will lead to advance our understanding,  
905   or, at least highlight differences in opinion.

906

907 Formal approaches are available to gather the opinions of experts and to integrate them into a  
908 joint result, often called expert elicitation (Aspinall, 2010; Cooke, 1991; O'Hagan, 2019). Expert  
909 elicitation strategies have been used widely to describe the expected behavior of  
910 environmental or man-made systems for which we have insufficient data or knowledge to build  
911 models directly. Examples include aspects of future sea-level rise (Bamber and Aspinall, 2013),  
912 tipping points in the Earth system (Lenton et al., 2018), or the vulnerability of bridges to scour  
913 due to flooding (Lamb et al., 2017). In the groundwater community, expert opinion is already  
914 widely used to develop system conceptualizations and related model structures (Krueger et al.,  
915 2012; Rajabi et al., 2018; Refsgaard et al., 2007), or to define parameter priors (Ross et al.,  
916 2009; Doherty and Christensen, 2011; Brunner et al., 2012; Knowling and Werner, 2016; Rajabi  
917 and Ataie-Ashtiani, 2016). The term expert opinion may be preferable to the term expert  
918 knowledge because it emphasizes a preliminary state of knowledge (Krueger et al., 2012).

919

920 A critical benefit of expert elicitation is the opportunity to bring together researchers who have  
921 experienced very different groundwater systems around the world. It is infeasible to expect  
922 that a single person could have gained in-depth experience in modelling groundwater in semi-  
923 arid regions, in cold regions, in tropical regions etc. Being able to bring together different  
924 experts who have studied one or a few of these systems to form a group would certainly create  
925 a whole that is bigger than the sum of its parts. If captured, it would be a tremendous source of  
926 knowledge for the evaluation of large-scale groundwater models. Expert elicitation also has a  
927 number of challenges including: 1) formalizing this knowledge in such a way that it is still usable

928 by third parties that did not attend the expert workshop itself; and 2) perceived or real  
929 differences in perspectives, priorities and backgrounds between regional-scale and large-scale  
930 modelers.

931

932 So, while expert opinion and judgment play a role in any scientific investigation (O'Hagan,  
933 2019), including that of groundwater systems, we rarely use formal strategies to elicit this  
934 opinion. It is also less common to use expert opinion to develop hypotheses about the dynamic  
935 behavior of groundwater systems, rather than just priors on its physical characteristics. Yet, it is  
936 intuitive that information about system behavior can help in evaluating the plausibility of model  
937 outputs (and thus of the model itself). This is what we call expert-based evaluation herein.

938 Expert elicitation is typically done in workshops with groups of a dozen or so experts (e.g. Lamb  
939 et al., 2018). Upscaling such expert elicitation in support of global modeling would require some  
940 web-based strategy and a formalized protocol to engage a sufficiently large number of people.

941 Contributors could potentially be incentivized to contribute to the web platform by publishing a  
942 data paper with all contributors as co-authors and a secondary analysis paper with just the core  
943 team as coauthors. We recommend the community develop expert elicitation strategies to  
944 identify effective hypotheses that directly link to the relevant large-scale hydrologic processes  
945 of interest.

946 **4. CONCLUSIONS: towards a holistic evaluation of groundwater representation in large-scale models**

947 Ideally, all three strategies (observation-based, model-based, expert-based) should be pursued  
948 simultaneously because the strengths of one strategy might further improve others. For  
949 example, expert- or model-based evaluation may highlight and motivate the need for new  
950 observations in certain regions or at new resolutions. Or observation-based model evaluation  
951 could highlight and motivate further model development or lead to refined or additional  
952 hypotheses. We thus recommend the community significantly strengthens efforts to evaluate  
953 large-scale models using all three strategies. Implementing these three model evaluation  
954 strategies may require a significant effort from the scientific community, so we therefore  
955 conclude with two tangible community-level initiatives that would be excellent first steps that  
956 can be pursued simultaneously with efforts by individual research groups or collaborations of  
957 multiple research groups.

958

959 First, we need to develop a 'Groundwater Modeling Data Portal' that would both facilitate and  
960 accelerate the evaluation of groundwater representation in continental to global scale models  
961 (Bierkens, 2015). Existing initiatives such as IGRAC's Global Groundwater Monitoring Network  
962 (<https://www.un-igrac.org/special-project/ggmn-global-groundwater-monitoring-network>) and  
963 HydroFrame ([www.hydroframe.org](http://www.hydroframe.org)), are an important first step but were not designed to  
964 improve the evaluation of large-scale models and the synthesized data remains very  
965 heterogeneous - unfortunately, even groundwater level time series data often remains either  
966 hidden or inaccessible for various reasons. This open and well documented data portal should  
967 include:

- 968 a) observations for evaluation (Table 2) as well as derived signatures (Section 3.1);
- 969 b) regional-scale models that meet the standards described above and could facilitate
- 970 inter-scale comparison (Section 3.2) and be a first step towards linking regional
- 971 models (Section 2.2);
- 972 c) Schematizations, conceptual or perceptual models of large-scale models since
- 973 these are the basis of computational models; and
- 974 d) Hypothesis and other results derived from expert elicitation (Section 3.3).

975 Meta-data documentation, data tagging, aggregation and services as well as consistent data

976 structures using well-known formats (netCDF, .csv, .txt) will be critical to developing a useful,

977 dynamic and evolving community resource. The data portal should be directly linked to

978 harmonized input data such as forcings (climate, land and water use etc.) and parameters

979 (topography, subsurface parameters etc.), model codes, and harmonized output data. Where

980 possible, the portal should follow established protocols, such as the Dublin Core Standards for

981 metadata (<https://dublincore.org>) and ISIMIP protocols for harmonizing data and modeling

982 approach, and would ideally be linked to or contained within an existing disciplinary repository

983 such as HydroShare (<https://www.hydroshare.org/>) to facilitate discovery, maintenance, and

984 long-term support. Additionally, an emphasis on model objective, uncertainty and regional

985 differences as highlighted (Section 3) will be important in developing the data portal. Like

986 expert-elicitation, contribution to the data portal could be incentivized through co-authorship

987 in data papers and by providing digital object identifiers (DOIs) to submitted data and models

988 so that they are citable. By synthesizing and sharing groundwater observations, models, and  
989 hypotheses, this portal would be broadly useful to the hydrogeological community beyond just  
990 improving global model evaluation.

991

992 Second, we suggest ISIMIP, or a similar model intercomparison project, could be harnessed as a  
993 platform to improve the evaluation of groundwater representation in continental to global  
994 scale models. For example, in ISIMIP (Warszawski et al., 2014), modelling protocols have been  
995 developed with an international network of climate-impact modellers across different sectors  
996 (e.g. water, agriculture, energy, forestry, marine ecosystems) and spatial scales. Originally,  
997 ISIMIP started with multi-model comparison (model-based model evaluation), with a focus on  
998 understanding how model projections vary across different sectors and different climate  
999 change scenarios (ISIMIP Fast Track). However, more rigorous model evaluation came to  
1000 attention more recently with ISIMIP2a, and various observation data, such as river discharge  
1001 (Global Runoff Data Center), terrestrial water storage (GRACE), and water use (national  
1002 statistics), have been used to evaluate historical model simulation (observation-based model  
1003 evaluation). To better understand model differences and to quantify the associated uncertainty  
1004 sources, ISIMIP2b includes evaluating scenarios (land use, groundwater use, human impacts,  
1005 etc) and key assumptions (no explicit groundwater representation, groundwater availability for  
1006 the future, water allocation between surface water and groundwater), highlighting that  
1007 different types of hypothesis derived as part of the expert-based model evaluation could  
1008 possibly be simulated as part of the ISIMIP process in the future. While there has been a



1009 significant amount of research and publications on MIPs including surface water availability,  
1010 limited multi-model assessments for large-scale groundwater studies exist. Important aspects  
1011 of MIPs in general could facilitate all three model evaluation strategies: community-building  
1012 and cooperation with various scientific communities and research groups, and making the  
1013 model input and output publicly available in a standardized format.

1014

1015 Large-scale hydrologic and land surface models increasingly represent groundwater, which we  
1016 envision will lead to a better understanding of large-scale water systems and to more  
1017 sustainable water resource use. We call on various scientific communities to join us in this  
1018 effort to improve the evaluation of groundwater in continental to global models. As described  
1019 by examples above, we have already started this journey and we hope this will lead to better  
1020 outcomes especially for the goals of including groundwater in large-scale models that we  
1021 started with above: improving our understanding of Earth system processes; and informing  
1022 water decisions and policy. Along with the community currently directly involved in large-scale  
1023 groundwater modeling, above we have made pointers to other communities who we hope will  
1024 engage to accelerate model evaluation: 1) regional hydrogeologists, who would be useful  
1025 especially in expert-based model evaluation (Section 3.3); 2) data scientists with expertise in  
1026 machine learning, artificial intelligence etc. whose methods could be useful especially for  
1027 observation- and model-based model evaluation (Sections 3.1 and 3.2); and 3) the multiple  
1028 Earth Science communities that are currently working towards integrating groundwater into a  
1029 diverse range of models so that improved evaluation approaches are built directly into model

1030 development. Together we can better understand what has always been beneath our feet, but  
1031 often forgotten or neglected.

1032

1033

1034

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1036

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1045

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1047 author contributions) conceptualization and writing original draft: TG, TW and PD; writing -

1048 review and editing; all co-authors. Authors are ordered by contribution for the first three  
 1049 coauthors (TG, TW and PD) and then ordered in reverse alphabetical order for all remaining  
 1050 coauthors.

1051  
 1052 **Code and data availability:** This Perspective paper does not present any computational results.  
 1053 There is therefore no code or data associated with this paper.

1054  
 1055 **Table 1. A possible model classification based on three model classes and various model characteristics; see link**  
 1056 **to google doc to view easier (google doc will be migrated to a community github page if article accepted)**

1057

Table 1. Model classification for large-scale models representing groundwater [1]	lateral groundwater flow to a river within a cell										3D lateral groundwater flow between all cells				3D groundwater flow	
	No GW flow		one-way				two-way				one-way		two-way			
	yes										no		no			
example model [3]	RULES	ORCHDEE	LMS	VIC-ground	CLMS	TOPLATS	Catchment	WaterGAP2-G3-M	LEAF hydro	FOR2DLO-WS-MOOFLOW	ISBA-TRIP	HydroGeoSphere	ParFlow			
groundwater flow [30/31]	free drainage	recharge + P-E-T	recharge + P-E-T	recharge depends on soil head and capillary fluxes	recharge depends on soil head and capillary fluxes	recharge depends on soil head and capillary fluxes	recharge depends on soil head and capillary fluxes	currently uncoupled	recharge derived from water	recharge depends on soil head and capillary fluxes	recharge depends on soil head and capillary fluxes	directly represented	directly represented			
focused recharge [4]	not represented	optional (via enhanced infiltration in points)	not represented	not represented	not represented	not represented	not represented	represented after drapling	not represented	represented from, lake and perennial rivers?	not represented	not represented	not represented			
surface water boundary condition or coupling	not represented	not represented	not represented	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 [2]	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	1D Richards' in soil layers	partially saturated	partially saturated	vertical fluxes in soils depending on soil saturation and GW level	1D Richards' in soil layers	variably saturated using TO-Richard's equation	variably saturated using TO-Richard's equation			
water table and hydraulic head	Optional soil diagnostic based on TOPMODEL	not represented	represented, parameterized	directly represented	First layer from bedrock where soil moisture < 0.3	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	parameterized following Francini and Pizzani (2005)	parameterized, calibration	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 condition	gravity drainage from soil	function of reservoir	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	no	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	yes	???	no	no	no	no	no	no	no			
public 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	Beet et al. (2012)	Sumbereau et al. (2014)	Liang et al. (2003)	Andre et al. (2018)	Fangliang & Wood (2008)	Koster et al. (2006)	Hacke et al. (2011)	Fin et al. (2013)	de Groot et al. (2017)	regnier et al. (2014)	Bruner and Simoh-Marwell 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 time) are not described here.  
 (2) one-way coupling means that S.W. => 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. & gw.  
 (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 constitutive relations can vary continuously, while partially saturated means that saturation can only discretely vary between fully saturated and unsaturated.

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**Table 1. Model classification for large-scale models representing groundwater (1)**

groundwater flow	lateral groundwater flow to a river within a cell											lateral groundwater flow between all cells			
	No GW flow		one-way				two-way					one-way		two-way	
	yes	no	yes	no	yes	no	yes	no	yes	no	yes	no	yes	no	
groundwater recharge (efflux)	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	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	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
focused recharge (5)	not represented	optional (via enhanced infiltration in ponds)	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
surface water boundary condition or coupling	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	currently uncoupled	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 (6)	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	1D Richards' in soil layers	partially saturated	partially saturated	partially saturated	Vertical fluxes in soils depending on soil saturation and CWC level	1D Richards' in soil layers	variably saturated using 3D Richards' equation	variably saturated using 3D Richards' equation
water table and hydraulic head	Optional WT diagnostic based on TOPMODEL	not represented	represented, parameterised	represented	First layer from bedrock where soil moisture < 0.5	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL
groundwater storage	not represented	represented as linear storage	represented	represented	represented	represented	represented	represented	represented	represented	represented	represented	represented	represented	represented
lateral flow	not represented	represented	represented through lateral flow-dispersance	parameterised following Francis and Pecunia (2011)	parameterised, calibration parameter related to bedrock	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL	represented following TOPMODEL
groundwater bottom boundary condition	gravity drainage from soil	function of reservoir	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux	no flux
groundwater use (7)	not represented	not represented	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	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	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	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	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	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	not represented	not represented
confined conditions	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	not represented	represented	not represented	potentially represented	potentially represented
coupling with ocean (and ocean models)	no	no	no	no	no	no	no	no	no	no	ocean boundary condition	ocean boundary condition	unclear	ocean boundary condition	possible
isotope-enabled	no	no	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	no	no
open 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	not represented	not represented
Reference	Beet et al. (2011)	Guarnieri et al. (2014)	Milly et al. (2014)	Lang et al. (2008)	Goode et al. (2008)	Songpratt & Wood (2008)	Koster et al. (2009)	Takaue et al. (2009)	Renwick et al. (2009)	Lee et al. (2011)	de Gooijer et al. (2011)	Beegun et al. (2014)	Burner and Simons (2011)	Beegun et al. (2014)	Burner and Simons (2011)

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 soil moisture ↔ recharge ↔ groundwater system ↔ stream flow, but no reverse influence; in this case, the groundwater model is dependent on surface simulations to provide recharge. two-way coupling means there is a full coupling of surface and groundwater.  
 (3) surface-atmosphere coupling means that the groundwater component can be coupled with atmospheric or weather models.  
 (4) Other models exist with similar features.  
 (5) 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.  
 (6) Variably saturated means that the saturation, and related constitutive relations can vary continuously, while partially saturated means that saturation can only discretely vary between fully saturated and unsaturated.  
 (7) Groundwater use means groundwater pumping rather than via evapotranspiration.

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1067 **Table 2. Available observations for evaluating the groundwater component of large-scale models**

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Data type	Strengths	Limitations	Data availability and spatial resolution
<b>Available observations already used to evaluate large-scale models</b>			
Hydraulic heads or water table depth (averages or single times)	Direct observation of groundwater levels and storage	observations biased towards North America and Europe; non-commensurable with large-scale models; mixture of observation times	<a href="#">IGRAC Global Groundwater Monitoring Network</a> ; USGS; Fan et al. (2013)  Point measurements at existing wells
Hydraulic heads or water table depth (transient)	Direct observation of changing groundwater levels and storage	As above	time-series available in a few regions, especially through USGS and <a href="#">European Groundwater Drought Initiative</a>  Point measurements at existing wells
Total water storage anomalies (GRACE)	Globally available and regionally integrated signal of water storage trends and anomalies	Groundwater changes are uncertain model remainder; very coarse spatial resolution and limited period	Various mascons gridded with resolution of ~100,000 km <sup>2</sup> which are then processed as groundwater storage change; Scanlon et al. (2016)
Storage change (regional aquifers)	Regionally integrated response of aquifer (independent estimates derived by various methods)	Bias towards North America and Europe	Konikow (2011); Döll et al. (2014a)  Regional aquifers (10,000s to 100,000s km <sup>2</sup> )
Recharge	Direct inflow of groundwater system	Challenging to measure and upscale	Döll and Fiedler (2008); Hartmann et al. (2017); Mohan et al. (2018); Moeck et al. (2020)

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			Point to small basin
Abstractions	Crucial for groundwater depletion and sustainability studies	National scale data highly variable in quality; downscaling uncertain	de Graaf et al. (2014); Döll et al. (2014a)  National-scale data down-scaled to grid
Streamflow or spring flow observations	Widely available at various scales; low flows can be related to groundwater	Challenging to quantify the flows between groundwater and surface water from streamflow	Global Runoff Data Centre (GRDC) or other <a href="#">data sources</a> ; large to small basin; Olarinoye et al. (2020)  point measurements of spring flow
Evapotranspiration	Widely available; related to groundwater recharge or discharge (for shallow water tables)	Not a direct groundwater observations	Various datasets; e.g. Miralles et al. (2016);  gridded
<b>Available observations not being used to evaluate large-scale models</b>			
Baseflow index (BFI) or (non-)linear baseflow recession behavior	Possible integrator of groundwater contribution to streamflow over a basin	BFI and k values vary with method; baseflow may be dominated by upstream surface water storage rather than groundwater inflow; can not identify losing river conditions	Beck et al. (2013)  Point observations extrapolated by machine learning

Perennial stream map	Ephemeral streams are losing streams, whereas perennial streams could be gaining (or impacted by upstream surface water storage)	Mapping perennial streams requires arbitrary streamflow and duration cutoffs; not all perennial stream reaches are groundwater-influenced; does not provide information about magnitude of inflows/outflows.	Schneider et al. (2017); Cuthbert et al. (2019);  Spatially continuous along stream networks
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.	Not globally available but see Bresciani et al. (2018) for a regional example;  Spatially continuous along stream networks
Springs and groundwater-dependent surface water bodies	Constrains direction of fluxes at groundwater system boundaries	Relevant processes occur at sub-grid-cell resolution.	Springs available for various regions but not globally; Springer, & Stevens (2009) Point measurements at water feature locations
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)	Isotopic data compiled but no global data for heat or other chemistry; Gleeson et al. (2016); Jasechko et al. (2017)  Point measurements at existing wells or surface water features
Surface elevation data (leveling, GPS, radar/lidar) and in particular land subsidence observations	Provides information about changes in surface elevation that are related to groundwater head variations or groundwater head decline	Provides indirect information and needs a geomechanical model to translate to head. Introduces additional uncertainty of geomechanical properties.	Leveling data, GPS data and lidar observations mostly limited to areas of active subsidence; Minderhoud et al. (2019,2020).  Global data on elevation change are available from the Sentinel 1 mission.



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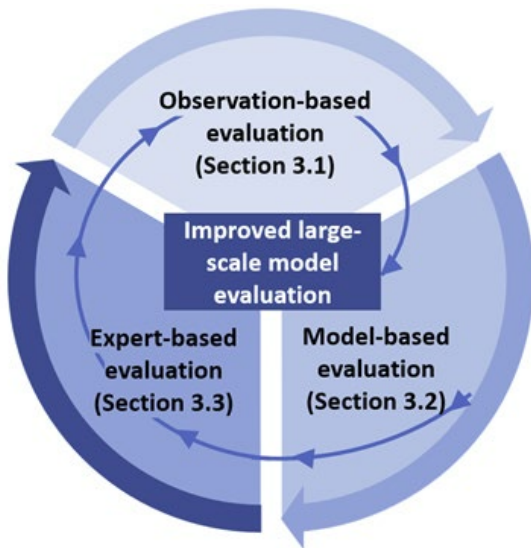
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1074 **Figure 1: Improved large-scale model evaluation rests on three pillars: observation-, model-,**  
1075 **and expert-based model evaluation. We argue that each pillar is an essential strategy so that**  
1076 **all three should be simultaneously pursued by the scientific community. The three pillars of**  
1077 **model evaluation all rest on three core principles related to 1) model objectives, 2)**  
1078 **uncertainty and 3) regional differences.**



**Improved model evaluation rests of three core principles:**

- 1) Modelling purpose or objective are paramount
- 2) All sources of information are uncertain
- 3) Regional differences are important

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1083 **References**

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