



1 HESS Opinions: Improving the evaluation of
2 groundwater representation in continental to
3 global scale models

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Abstract

36 Continental- to global-scale hydrologic and land surface models increasingly include representations of
37 the groundwater system, driven by crucial Earth science and sustainability problems. These models are
38 essential for examining, communicating, and understanding the dynamic interactions between the Earth
39 System above and below the land surface as well as the opportunities and limits of groundwater
40 resources. A key question for this nascent and rapidly developing field is how to evaluate the realism
41 and performance of such large-scale groundwater models given limitations in data availability and
42 commensurability. Our objective is to provide clear recommendations for improving the evaluation of
43 groundwater representation in continental- to global-scale models. We identify three evaluation
44 approaches, including comparing model outputs with available observations of groundwater levels or
45 other state or flux variables (observation-based evaluation); comparing several models with each other
46 with or without reference to actual observations (model-based evaluation); and comparing model
47 behavior with expert expectations of hydrologic behaviors that we expect to see in particular regions or
48 at particular times (expert-based evaluation). Based on current and evolving practices in model
49 evaluation as well as innovations in observations, machine learning and expert elicitation, we argue that
50 combining observation-, model-, and expert-based model evaluation approaches may significantly
51 improve the realism of groundwater representation in large-scale models, and thus our quantification,
52 understanding, and prediction of crucial Earth science and sustainability problems. We encourage
53 greater community-level communication and cooperation on these challenges, including among global
54 hydrology and land surface modelers, local to regional hydrogeologists, and hydrologists focused on
55 model development and evaluation.

56 1. WHY AND HOW IS GROUNDWATER MODELED AT CONTINENTAL TO GLOBAL SCALES?

57 Groundwater is the largest human- and ecosystem-accessible freshwater storage component of the
58 hydrologic cycle (UNESCO, 1978; Margat & Van der Gun, 2013; Gleeson et al., 2016). Therefore, better
59 understanding of groundwater dynamics is critical at a time when the ‘great acceleration’ (Steffen et al.,
60 2015) of many human-induced processes is increasing stress on water resources (Wagner et al., 2010;
61 Montanari et al., 2013; Sivapalan et al., 2014; van Loon et al., 2016), especially in regions with limited
62 data availability and analytical capacity. Groundwater is often considered to be an inherently regional
63 rather than global resource or system. This is partially reasonable because local to regional peculiarities
64 of hydrology, politics and culture are paramount to groundwater resource management (Foster et al.
65 2013) and groundwater dynamics in different continents are less directly connected and coupled than
66 atmospheric dynamics. Regional groundwater analysis is a mature, well-established field (Hill &
67 Tiedeman, 2007; Kresic, 2009; Zhou & Li, 2011; Hiscock & Bense, 2014; Anderson et al. 2015a) and
68 regional approaches may be preferable for some issues and objectives; yet, important global aspects of
69 groundwater both as a resource and as part of the Earth System are emerging (Gleeson et al. 2020).
70 First, our increasingly globalized world trades virtual groundwater and other groundwater-dependent
71 resources in the food-energy-water nexus, and groundwater often crosses borders in transboundary
72 aquifers. A solely regional approach can be insufficient to analysing and managing these complex global



73 interlinkages. Second, from an Earth system perspective, groundwater is part of the hydrological cycle
74 and connected to the atmosphere, oceans and the deeper lithosphere. A solely regional approach is
75 insufficient to uncover and understand the complex interactions and teleconnections of groundwater
76 within the Earth System. For example, to assess the impact of groundwater depletion on sea level rise,
77 groundwater storage loss rate on all continents of the Earth **must be aggregated**. Thus, we argue that
78 groundwater is simultaneously a local, regional, and increasingly global resource and system and that
79 examining groundwater problems, solutions, and interactions at all scales is crucial. As a consequence,
80 we urgently require predictive understanding about how groundwater, used by humans and connected
81 with other components of the Earth System, operates at a variety of scales.

82

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

86 (1) To understand and quantify interactions between groundwater and past, present and future
87 climate. Groundwater systems can have far-reaching effects on climate affecting modulation of
88 surface energy and water partitioning with a long-term memory (Anyah et al., 2008; Maxwell and
89 Kollet, 2008; Koirala et al. 2013; Krakauer et al., 2014; Maxwell et al., 2016; Taylor, et al., 2013;
90 Meixner et al., 2018; Wang et al., 2018; Keune et al., 2018). While there have been significant
91 advances in understanding the role of lateral groundwater flow on evapotranspiration (Maxwell &
92 Condon, 2016; Bresciani et al., 2016), the interactions between climate and groundwater over
93 longer time scales (Cuthbert et al., 2019) as well as between irrigation, groundwater, and climate
94 (Condon and Maxwell, 2019; Condon et al. 2020) remain largely unresolved. Additionally, it is well
95 established that old groundwater with slow turnover times are common at depth (Befus et al.
96 2017; Jasechko et al. 2017), but the relationship between groundwater and climate (and how that
97 potentially impacts current water resources) in the Holocene and Pleistocene is also largely
98 unresolved.

99 (2) To understand and quantify two-way interactions between groundwater, the rest of the
100 hydrologic cycle, and the broader Earth System. Groundwater connections to the atmosphere are
101 well documented in modeling studies (e.g. Forrester and Maxwell, 2020). Previous studies have
102 demonstrated connections between the atmospheric boundary layer and water table depth (e.g.
103 Maxwell et al. 2007; Rahman et al., 2015), under land cover disturbance (e.g. Forrester et al. 2018),
104 under extremes (e.g. Kuene et al. 2016) and due to groundwater pumping (Gilbert et al. 2017).
105 While a number of open source platforms have been developed to study these connections (e.g.
106 Maxwell et al. 2011; Shrestha et al. 2014; Sulis, 2017) these platforms are regional to continental in
107 extent. Recent work has shown global impacts of groundwater on atmospheric circulation (Wang
108 et al. 2018), groundwater is still quite simplified. As the main storage component of the
109 freshwater hydrologic cycle, groundwater systems support baseflow levels in streams and rivers,
110 and thereby ecosystems and agricultural productivity and other ecosystem services in both
111 irrigated and rainfed systems (Scanlon et al., 2012; Qiu et al., 2019; Visser, 1959; Zipper et al.,
112 2015, 2017). When pumped groundwater is transferred to oceans (Konikow 2011; Wada et al.,
113 2012; Döll et al., 2014a; Wada, 2016; Caceres et al., 2020; Luijendijk et al. 2020), resulting sea-
114 level rise can impact salinity levels in coastal aquifers, and freshwater and solute inputs to the



- 115 ocean (Moore, 2010; Sawyer et al., 2016). Difficulties are complicated by international trade of
116 virtual groundwater which causes aquifer stress in disparate regions (Dalin et al., 2017)
- 117 (3) To inform water decisions and policy for large, often transboundary groundwater systems in an
118 increasingly globalized world (Wada & Heinrich, 2013; Herbert & Döll, 2019). For instance,
119 groundwater recharge from large-scale models has been used to quantify groundwater resources
120 in Africa, even though large-scale models do not yet include all recharge processes that are
121 important in this region (Taylor et al., 2013; Jasechko et al. 2014; Cuthbert et al., 2019; Hartmann
122 et al., 2017).
- 123 (4) To create visualizations and interactive opportunities that inform citizens and consumers, whose
124 decisions have global-scale impacts, about the state of groundwater all around the world such as
125 the World Resources Institute's Aqueduct website (<https://www.wri.org/aqueduct>), a decision-
126 support tool to identify and evaluate global water risks.

127 The first two purposes are science-focused while the latter two are sustainability-focused. In sum,
128 continental- to global-scale hydrologic models incorporating groundwater offer a coherent scientific
129 framework to examine the dynamic interactions between the Earth System above and below the land
130 surface, and are compelling tools for conveying the opportunities and limits of groundwater resources
131 to people so that they can better manage the regions they live in, and better understand the world
132 around them.

133

134 As a result, many global hydrological models and land surface models have incorporated groundwater to
135 varying levels of complexity depending on the model provenance and purpose. Different from regional-
136 scale groundwater models that generally focus on subsurface dynamics, the focus of these models is on
137 estimating either runoff and streamflow (hydrological models) or land-atmosphere water and energy
138 exchange (land surface models). Simulation of groundwater storages and hydraulic heads mainly serve
139 to quantify baseflow that affects streamflow during low flow periods or capillary rise that increases
140 evapotranspiration. Some land-surface models use approaches based on the topographic index to
141 simulate fast surface and slow subsurface runoff based on the fraction of saturated area in the grid cell
142 (Clark et al., 2015; Fan et al., 2019); groundwater in these models does not have water storage nor by
143 hydraulic heads (Famiglietti & Wood, 1994; Koster et al., 2000; Niu et al., 2003; Takata et al., 2003). In
144 some global hydrological models, groundwater is still represented as a linear reservoir that is fed by
145 groundwater recharge and drains to a river in each grid cell (Müller Schmied et al., 2014; Gascoin et al.,
146 2009; Ngo-Duc et al., 2007). Time series of groundwater storage but not hydraulic heads are computed.
147 This prevents simulation of lateral groundwater flow between grid cells, capillary rise and two-way
148 exchange flows between surface water bodies and groundwater (Döll et al., 2016). However,
149 representing groundwater as a water storage compartment that is connected to soil and surface water
150 bodies by groundwater recharge and baseflow and is affected by groundwater abstractions and returns
151 enables global-scale assessment of groundwater resources and stress (Herbert and Döll, 2019) and
152 groundwater depletion (Döll et al., 2014a; Wada et al., 2014; de Graaf et al., 2014). In some land surface
153 models, the location of the groundwater table with respect to the land surface is simulated within each
154 grid cell to enable simulation of capillary rise (Niu et al., 2007) but, as in the case of simulating
155 groundwater as a linear reservoir, lateral groundwater transport or two-way surface water-groundwater
156 exchange cannot be simulated with this approach.



157

158 Increasingly, models for simulating groundwater flows **between all model grid cells in entire countries** or
159 globally have been developed, either as stand-alone models or as part of hydrological models (Vergnes
160 & Decharme, 2012; Fan et al., 2013; Lemieux et al. 2008; de Graaf et al., 2017; Kollet et al., 2017;
161 Maxwell et al., 2015; Reinecke et al., 2018, de Graaf et al 2019). The simulation of groundwater in large-
162 scale models is a nascent and rapidly developing field with significant computational and
163 parameterization challenges which has led to significant and important efforts to develop and evaluate
164 individual models. It is important to note that **herein ‘large-scale models’ refer to models that are**
165 **laterally extensive across multiple regions** (hundreds to thousands of kilometers) and generally include
166 the upper tens to hundreds of meters of subsurface and have resolutions sometimes as small as ~1 km.
167 In contrast, ‘regional-scale’ models (tens to hundreds of kilometers) have long been developed for a
168 specific region or aquifer and can include greater depths and resolutions, more complex
169 hydrostratigraphy and are often developed from conceptual models with significant regional knowledge.
170 Regional-scale models include a diverse range of approaches from stand-alone groundwater models
171 (i.e., representing surface water and vadose zone processes using boundary conditions such as recharge)
172 to fully integrated groundwater-surface water models. We consider both large-scale and regional-scale
173 models to be useful practices that should both continue to be conducted rather than one replacing
174 another; ideally both should benefit from the other since each has strengths and weaknesses and
175 together the two practices enrich our understanding and support the management of groundwater
176 across scales.

177

178 Now that a number of models that represent groundwater at continental to global scales have been
179 developed and are being developed, it is equally important that we advance how we evaluate these
180 models. To date, large-scale model evaluation has largely focused on individual models and lacked the
181 **rigor of regional-scale model evaluation**, with inconsistent practices between models and little
182 community-level discussion or cooperation. Our objective is to provide clear recommendations for
183 evaluating groundwater representation in large-scale (continental and global) models. We focus on
184 model evaluation because this is the heart of model trust and reproducibility (Hutton et al., 2016). We
185 describe current model evaluation practices (Section 2) and consider diverse and uncertain sources of
186 information, including observations, models and experts to holistically evaluate the simulation of
187 groundwater-related fluxes, stores and hydraulic heads (Section 3). We stress the need for an iterative
188 and open-ended process of model improvement through continuous model evaluation against the
189 different sources of information. We explicitly contrast the terminology used herein of ‘evaluation’ and
190 ‘comparison’ against terminology such as ‘calibration’ or ‘validation’ or ‘benchmarking’, which suggests
191 a modelling process that is at some point complete. We extend previous commentaries advocating
192 improved hydrologic process representation and evaluation in large-scale hydrologic models (Clark et al.
193 2015; Melsen et al. 2016) by adding expert-elicitation and machine learning for more holistic evaluation.
194 We also consider model objective and model evaluation across the diverse hydrologic landscapes which
195 can both uncover blindspots in model development.

196

197 We bring together somewhat disparate scientific communities as a step towards greater community-
198 level cooperation on these challenges, including global hydrology and land surface modelers, **local to**



199 regional hydrogeologists, and hydrologists focused on model development and evaluation. We see three
200 audiences beyond those currently directly involved in large-scale groundwater modeling that we seek to
201 engage to accelerate model evaluation: 1) regional hydrogeologists who could be reticent about global
202 models, and yet have crucial knowledge and data that would improve evaluation; 2) data scientists with
203 expertise in machine learning, artificial intelligence etc. whose methods could be useful in a myriad of
204 ways; and 3) the multiple Earth Science communities that are currently working towards integrating
205 groundwater into a diverse range of models so that improved evaluation approaches are built directly
206 into model development.

207 2. CURRENT MODEL EVALUATION PRACTICES

208 Here we provide a brief overview of evaluation of both large-scale hydrological models as well as
209 regional-scale models to highlight some of the evaluation differences and opportunities at different
210 scales. It is important to consider how or if large-scale models are fundamentally different to regional-
211 scale models, especially in ways that could impact evaluation. As defined above, large-scale models
212 cover larger areas, often including data-poor areas and generally at coarser resolution compared to
213 regional-scale models. These differences impact evaluations in at least five relevant ways:

- 214 a) commensurability errors (also called ‘representativeness’ errors) occur either when modelled grid
215 values are interpolated and compared to an observation ‘point’ or when aggregation of observed
216 ‘point’ values are compared to a modelled grid value (Beven, 2005; Tustison et al., 2001; Beven,
217 2016; Pappenberger et al., 2009; Rajabi et al., 2018). For groundwater models in particular,
218 commensurability error will depend on the number and locations of observation points, the
219 variability structure of the variables being compared such as hydraulic head and the interpolation or
220 aggregation scheme applied (Tustison et al., 2001; Pappenberger et al., 2009; Reinecke et al., 2020).
221 Commensurability is a problem for most scales of modelling, but likely more significant the coarser
222 the model;
- 223 b) specificity to region and objective because regional-scale models are developed specifically for a
224 certain region and modeling or management objective whereas large-scale models are often more
225 general and include different regions leading to greater heterogeneity of processes and parameters;
- 226 c) large-scale models have immense computational requirements which leads to challenges with
227 uncertainty and sensitivity analysis, while it is important to note that some regional-scale models
228 also face computational demands;
- 229 d) including data-poor areas in large-scale models leads to challenges when only using observations
230 for model evaluation; and
- 231 e) regional-scale models routinely include heterogeneous and anisotropic parameterizations which
232 could be improved in future large-scale models. For example, intense vertical anisotropy routinely
233 induces vertical flow dynamics from vertical head gradients that are tens to thousands of times
234 greater than horizontal gradients which profoundly alter the meaning of the deep and shallow
235 groundwater levels, with only the latter remotely resembling the actual water table.

236 Despite differences between model evaluation at different scales, we suggest that well-established
237 modeling strategies at regional scales, that we describe more below, can be adapted and built upon to
238 improve large-scale model evaluation.



239
240 Evaluation of large-scale models has often focused on streamflow or evapotranspiration observations
241 but joint evaluation together with groundwater-specific variables is appropriate and necessary (e.g.
242 Maxwell et al. 2015; Maxwell and Condon, 2016). Groundwater-specific variables useful for evaluating
243 the groundwater component of large-scale models include a) hydraulic head or water table depth; b)
244 groundwater storage and groundwater storage changes which refer to long-term, negative or positive
245 trends in groundwater storage where long-term, negative trends are called groundwater depletion; c)
246 groundwater recharge; d) flows between groundwater and surface water bodies; and e) human
247 groundwater abstractions and return flows to groundwater. It is important to note that groundwater
248 and surface water hydrology communities often have slightly different definitions of terms like recharge
249 and baseflow (Barthel, 2014); we therefore suggest trying to precisely define the meanings of such
250 words using the actual hydrologic fluxes which we do below. Table 1 shows the availability of
251 observational data for these variables but does not evaluate the quality and robustness of observations.
252 Overall there are significant inherent challenges of commensurability and measurability of groundwater
253 observations in the evaluation of large-scale models. We describe the current model evaluation
254 practices for each of these variables here:

- 255
- 256 a) Simulated hydraulic heads or water table depth in large scale models are frequently compared
257 to well observations, which are often considered the crucial data for groundwater model
258 evaluation. Hydraulic head observations from a large number groundwater wells (>1 million)
259 have been used to evaluate the spatial distribution of steady-state heads (Fan et al., 2013, de
260 Graaf et al., 2015; Maxwell et al., 2015; Reinecke et al., 2019a, 2020). Transient hydraulic heads
261 with seasonal amplitudes (de Graaf et al. 2017), declining heads in aquifers with groundwater
262 depletion (de Graaf et al. 2019) and daily transient heads (Tran et al 2020) have also been
263 compared to well observations. All evaluation with well observations is severely hampered by
264 the incommensurability of point values of observed head with simulated heads that represent
265 averages over cells of a size of tens to hundreds square kilometers; within such a large cell, land
266 surface elevation, which strongly governs hydraulic head, may vary a few hundred meters, and
267 average observed head strongly depends on the number and location of well within the cell
268 (Reinecke et al., 2020). Additional concerns with head observations are the 1) strong sampling
269 bias of wells towards accessible locations, low elevations, shallow water tables, and more
270 transmissive aquifers in wealthy, generally temperate countries (Fan et al., 2019); 2) the impacts
271 of pumping which may or may not be well known; 3) observational errors and uncertainty (Post
272 and von Asmuth, 2013; Fan et al., 2019); and 4) that heads can reflect the poro-elastic effects of
273 mass loading and unloading rather than necessarily aquifer recharge and drainage (Burgess et al,
274 2017). To date, simulated hydraulic heads have more often been compared to observed heads
275 (rather than water table depth) which results in lower relative errors (Reinecke et al., 2020)
276 because the range of heads (10s to 1000s m head) is much larger than the range of water table
277 depths (<1 m to 100s m).
- 278
- 279 b) Simulated groundwater storage trends or anomalies in large-scale hydrological models have
280 been evaluated using observations of groundwater well levels combined with estimates of



281 storage parameters, such as specific yield; local-scale groundwater modeling; and translation of
282 regional total water storage trends and anomalies from satellite gravimetry (GRACE: Gravity
283 Recovery And Climate Experiment) to groundwater storage changes by estimating changes in
284 other hydrological storages (Döll et al., 2012; 2014a). Groundwater storage changes volumes
285 and rates have been calculated for numerous aquifers, primarily in the United States, using
286 calibrated groundwater models, analytical approaches, or volumetric budget analyses (Konikow,
287 2010). Regional-scale models have also been used to simulate groundwater storage trends
288 untangling the impacts of water management during drought (Thatch et al. 2020). Satellite
289 gravimetry (GRACE) is important but has limitations (Alley and Konikow, 2015). First, monthly
290 time series of very coarse-resolution groundwater storage are indirectly estimated from
291 observations of total water storage anomalies by satellite gravimetry (GRACE) but only after
292 model- or observation-based subtraction of water storage changes in glaciers, snow, soil and
293 surface water bodies (Lo et al., 2016; Rodell et al., 2009; Wada, 2016). As soil moisture, river or
294 snow dynamics often dominate total water storage dynamics, the derived groundwater storage
295 dynamics can be so uncertain that severe groundwater drought cannot be detected in this way
296 (Van Loon et al., 2017). Second, GRACE cannot detect the impact of groundwater abstractions
297 on groundwater storage unless groundwater depletion occurs (Döll et al., 2014a,b). Third, the
298 very coarse resolution can lead to incommensurability but in the opposite direction of well
299 observations. It is important to note that the focus is on storage trends or anomalies since total
300 groundwater storage to a specific depth (Gleeson et al., 2016) or in an aquifer (Konikow, 2010)
301 can be estimated but the total groundwater storage in a specific region or cell cannot be
302 simulated or observed unless the **depth of interest is specified** (Condon et al., 2020).
303

304 c) Simulated large-scale groundwater recharge (vertical flux across the water table) has been
305 evaluated using compilations of point estimates of groundwater recharge, results of regional-
306 scale models, baseflow indices, and expert opinion (Döll and Fiedler, 2008; Hartmann et al.,
307 2015) or compared between models (e.g. Wada et al. 2010). In general, groundwater recharge is
308 not directly measurable except **by meter-scale lysimeters** (Scanlon et al., 2002), and many
309 groundwater recharge methods such as water table fluctuations and chloride mass balance also
310 suffer from similar commensurability issues as water table depth data. Although sometimes an
311 input or boundary condition to regional-scale models, recharge in many large-scale groundwater
312 models is simulated and thus can be evaluated.
313

314 d) The flows between groundwater and surface water bodies (rivers, lakes, wetlands) are
315 simulated by many models but are generally not evaluated directly against observations of such
316 flows since they are very rare and challenging. Baseflow (the slowly varying portion of
317 streamflow originating from groundwater or other delayed sources) or streamflow ‘low flows’
318 (when groundwater or other delayed sources predominate), generally cannot be used to directly
319 quantify the flows between groundwater and surface water bodies at large scales. Groundwater
320 discharge to rivers can be estimated from streamflow observations only in the very dense gauge
321 network and/or if streamflow during low flow periods is mainly caused by groundwater
322 discharge and not by water storage in upstream lakes, reservoirs or wetlands. These conditions



323 are rarely met in case of streamflow gauges with large upstream areas that can be used for
324 comparison to large-scale model output. de Graaf et al. (2019) compared the simulated timing
325 of changes in groundwater discharge to observations and regional-scale models, but only
326 compared the fluxes directly between the global- and regional-scale models. Due to the
327 challenges of directly observing the flows between groundwater and surface water bodies at
328 large scales, this is not included in the available data in Table 1; instead in Section 3 we highlight
329 the potential for using baseflow or the spatial distribution of perennial, intermittent and
330 ephemeral streams in the future.

331
332 e) Groundwater abstractions have been evaluated by comparison to national, state and county
333 scale statistics in the U.S. (Wada et al. 2010, Döll et al., 2012, 2014a, de Graaf et al. 2014).
334 Irrigation is the dominant groundwater use sector in many regions; however, irrigation pumpage
335 is generally estimated from crop water demand and rarely metered although GRACE and other
336 remote sensing data have been used to estimate the irrigation water demand (Anderson et al.
337 2015b). Groundwater abstraction uncertainties introduce significant uncertainties into large-
338 scale models and is simulated and thus can be evaluated. Human groundwater abstractions and
339 return flows as well as groundwater recharge and the flows between groundwater and surface
340 water bodies are necessary to simulate storage trends (described above). But each of these are
341 considered separate observations since they each have different data sources and assumptions.
342 Groundwater abstraction data at the well scale are severely hampered by the
343 incommensurability like hydraulic head and recharge described above.

344
345 Regional-scale groundwater models typically have fewer (though not insignificant) commensurability
346 issues due to smaller grid cell sizes compared to global-scale models, and may have different challenges
347 related to data availability, such as the lack of reliable hydrologic monitoring data in many regions.
348 Regional-scale models are evaluated using a variety of data types, some of which are available and
349 already used at the global scale and some of which are not. In general, the most common data types
350 used for regional-scale groundwater model evaluation match global-scale groundwater models:
351 hydraulic head and either total streamflow or baseflow estimated using hydrograph separation
352 approaches (eg. RRCA, 2003; Woolfenden and Nishikawa, 2014; Tolley et al., 2019). However, numerous
353 data sources unavailable or not currently used at the global scale have also been applied in regional-
354 scale models, such as elevation of surface water features (Hay et al., 2018), existing maps of the
355 potentiometric surface (Meriano and Eyles, 2003), and dendrochronology (Schilling et al., 2014) - these
356 and other 'non-classical' observations (Schilling et al. 2019) could be inspiration for model evaluation of
357 large-scale models in the future but are beyond our scope to discuss. Further, given the smaller domain
358 size of regional-scale models, expert knowledge and local ancillary data sources can be more directly
359 integrated and automated parameter estimation approaches such as PEST are tractable (Leaf et al.,
360 2015; Hunt et al., 2013). We directly build upon this practice of integration of expert knowledge below
361 in Section 3.3.



362 3. HOW TO IMPROVE THE EVALUATION OF LARGE-SCALE GROUNDWATER MODELS

363

364 Based on Section 2, we argue that the current model evaluation practices are insufficient to robustly
365 evaluate large-scale models. We therefore propose evaluating large-scale models using at least three
366 strategies (pillars of Figure 1): observation-, model-, and expert-driven evaluation which are potentially
367 mutually beneficial because each strategy has its strengths and weaknesses. Across all three model
368 evaluation strategies, we advocate three principles underpinning model evaluation (base of Figure 1),
369 none of which we are the first to suggest but we highlight here as a reminder: 1) model objectives, such
370 as the groundwater science or groundwater sustainability objective summarised in Section 1, are
371 important to model evaluation because they provide the context through which relevance of the
372 evaluation outcome is set; 2) all sources of information (observations, models and experts) are
373 uncertain and this uncertainty needs to be quantified for robust evaluation; and 3) regional differences
374 are likely important for large-scale model evaluation - understanding these differences is crucial for the
375 transferability of evaluation outcomes to other places or times. For example, in assessing climate change
376 impacts on groundwater **the objective is relatively clear**, uncertainty is an integral part of the evaluation,
377 and regional differences are common.

378

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

394

395 We advocate for considering regional differences more explicitly in model evaluation since likely no
396 single model will perform consistently across the diverse hydrologic landscapes of the world (Van
397 Werkhoven et al., 2008). Considering regional differences in large-scale model evaluation is motivated
398 by recent model evaluation results and is already starting to be practiced. Two recent sensitivity
399 analyses of large-scale models reveal how sensitivities to input parameters vary in different regions for
400 both hydraulic heads and flows between groundwater and surface water (de Graaf et al. 2019; Reinecke
401 et al., 2020). In mountain regions, large-scale models tend to underestimate steady-state hydraulic
402 head, possibly due to over-estimated hydraulic conductivity in these regions, which highlights that



403 model performance varies in different hydrologic landscapes. (de Graaf et al., 2015; Reinecke et al.
404 2019b). Additionally, there are significant regional differences in performance with low flows for a
405 number of large-scale models (Zaherpour et al. 2018) likely because of diverse implementations of
406 groundwater and baseflow schemes. Large-scale model evaluation practice is starting to shift towards
407 highlighting regional differences as exemplified by two different studies that explicitly mapped
408 hydrologic landscapes to enable clearer understanding of regional differences. Reinecke et al. (2019b)
409 identified global hydrological response units which highlighted the spatially distributed parameter
410 sensitivities in a computationally expensive model, whereas Hartmann et al. (2017) developed and
411 evaluated models for karst aquifers in different hydrologic landscapes based on different a priori system
412 conceptualizations. Considering regional differences in model evaluation suggests that global models
413 could in the future consider a patchwork approach of different conceptual models, governing equations,
414 boundary conditions etc. in different regions. Although beyond the scope of this manuscript, we
415 consider this an important future research avenue.
416

417 3.1 Observation-based model evaluation

418 Observation-based model evaluation is the focus of most current efforts and is important because we
419 want models to be consistent with real-world observations. Section 2 and Table 1 highlight both the
420 strengths and limitations of current practices using observations. Despite existing challenges, we foresee
421 significant opportunities for observation-based model evaluation and do not see data scarcity as a
422 reason to exclude groundwater in large-scale models or to avoid evaluating these models. It is important
423 to note that most so-called ‘observations’ are modeled or derived quantities, and often at the wrong
424 scale for evaluating large-scale models (Table 1; Beven, 2019). Given the inherent challenges of direct
425 measurement of groundwater fluxes and stores especially at large scales, herein we consider the word
426 ‘observation’ loosely as any measurements of physical stores or fluxes that are combined with or filtered
427 through models for an output. For example, GRACE gravity measurements are combined with model-
428 based estimates of water storage changes in glaciers, snow, soil and surface water for ‘groundwater
429 storage change observations’ or streamflow measurements are filtered through baseflow separation
430 algorithms for ‘baseflow observations’. The strengths and limitations as well as the data availability and
431 spatial and temporal attributes of different observations are summarized in Table 1 which we hope will
432 spur more systematic and comprehensive use of observations.
433

434 Here we highlight nine important future priorities for improving evaluation using available observations.
435 The first five priorities focus on current observations (Table 1) whereas the latter four focus on new
436 methods or approaches:

- 437 1) Focus on transient observations of the water table depth rather than hydraulic head
438 observations that are long-term averages or individual times (often following well
439 drilling). Water table depth are likely more robust evaluation metrics than hydraulic
440 head because water table depth reveals great discrepancies and is a complex function of
441 the relationship between hydraulic head and topography that is crucial to predicting
442 system fluxes (including evapotranspiration and baseflow). Comparing transient



443 observations and simulations instead of long-term averages or individual times
444 incorporates more system dynamics of storage and boundary conditions as temporal
445 patterns are more important than absolute values (Heudorfer et al. 2019). For regions
446 with significant groundwater depletion, comparing to declining water tables is a useful
447 strategy (de Graaf et al. 2019), whereas in aquifers without groundwater depletion,
448 seasonally varying water table depths are likely more useful observations (de Graaf et
449 al. 2017).

450 2) Use baseflow, the slowly varying portion of streamflow originating from groundwater or
451 other delayed sources. Döll and Fiedler (2008) included the baseflow index in evaluating
452 recharge and baseflow has been used to calibrate the groundwater component of a land
453 surface model (Lo et al. 2008, 2010). But the baseflow index (BFI), baseflow recession (k)
454 or baseflow fraction (Gnann et al., 2019) have not been used to evaluate any large-scale
455 model that simulates groundwater flows between all model grid cells. There are
456 limitations of using BFI and baseflow recession (k) to evaluate large-scale models (Table
457 1) and this only makes sense when the baseflow separation algorithm is better than the
458 large-scale model itself, which may not be the case for some large-scale models. But this
459 remains available and obvious data derived from streamflow observations that has been
460 under-used to date.

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

471 4) Use data on land subsidence to infer head declines or aquifer properties for regions
472 where groundwater depletion is the main cause of compaction (Bierkens and Wada,
473 2019). Lately, remote sensing methods such as GPS, airborne and space borne radar and
474 lidar are frequently used to infer land subsidence rates (Erban et al., 2014). Also, a
475 number of studies combine geomechanical modelling (Ortega-Guerrero et al 1999;
476 Minderhoud et al 2017) and geodetic data to explain the main drivers of land
477 subsidence. A few papers (e.g. Zhang and Burbey 2016) use a geomechanical model
478 together with a withdrawal data and geodetic observations to estimate hydraulic and
479 geomechanical subsoil properties.

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



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- 6) Derive additional new datasets using meta-analysis and/or geospatial analysis such as gaining or losing stream reaches (e.g., from **interpolated head measurements** close to the streams), springs and groundwater-dependent surface water bodies, or tracers. Each of these new data sources could in principle be developed from available data using methods already applied at regional scales but do not currently have an ‘off the shelf’ global dataset. For example, some large-scale models have been explicitly **compared with residence time and tracer data** (Maxwell et al., 2016) which have also been recently compiled globally (Gleeson et al., 2016; Jasechko et al., 2017). This could be an important evaluation tool for large-scale models that are capable of simulating flow paths, or can be modified to do so. Future meta-analyses data compilations should report on the quality of the data and include possible uncertainty ranges as well as the mean estimates.
 - 7) **Use machine learning** to identify spatiotemporal patterns, for example of perennial streams, **depth** table depths or baseflow fluxes, which might not be obvious in multi-dimensional datasets and could be useful in evaluation. For example, Yang et al. (2019) predicted the state of losing and gaining streams in New Zealand using random forests. A staggering variety of machine learning tools are available and their use is nascent yet rapidly expanding in geoscience and hydrology (Reichstein et al., 2019; Shen, 2018; Shen et al., 2018; Wagener et al., 2020). While large-scale groundwater models are often considered ‘data-poor’, it may seem strange to propose using data-intensive machine learning methods to improve model evaluation. But some of the data sources are large (e.g over 2 million water level measurements in Fan et al. 2013 although biased in distribution) whereas other observations such as evapotranspiration (Jung et al., 2011) and baseflow (Beck et al. 2013) are already interpolated and extrapolated using machine learning.
 - 8) Consider comparing models against hydrologic signatures - indices that provide insight into the functional behavior of the system under study (Wagener et al., 2007; McMillan, 2020). The direct comparison of simulated and observed variables through statistical error metrics has at least two downsides. One, the above mentioned unresolved problem of commensurability, and two, the issue that such error metrics are rather uninformative in a diagnostic sense - simply knowing the size of an error does not tell the modeller how the model needs to be improved, only that it does (Yilmaz et al., 2009). One way to overcome these issues, is to derive hydrologically meaningful signatures from the original data, such as the signatures derived from transient groundwater levels by Heudorfer et al. (2019). For example, recharge ratio (defined as the ratio of groundwater recharge to precipitation) might be hydrologically more informative than recharge alone (Jasechko et al., 2014) or the water table ratio and groundwater response time (Cuthbert et al. 2019) which are spatially-distributed signatures of groundwater systems dynamics. **Such signatures might be used to assess model consistency** (Wagener & Gupta, 2005; Hrachowitz et al.2014) by looking at the similarity of patterns or spatial trends rather than the size of the aggregated error, thus reducing the commensurability problem.



527 9) Understand and quantify commensurability error issues better so that a fairer
528 comparison can be made across scales using existing data. As described above,
529 commensurability errors will depend on the number and locations of observation
530 points, the variability structure of the variables being compared such as hydraulic head
531 and the interpolation or aggregation scheme applied. While to some extent we may
532 appreciate how each of these factors affect commensurability error in theory, in
533 practice their combined effects are poorly understood and methods to quantify and
534 reduce commensurability errors for groundwater model purposes remain largely
535 undeveloped. As such, quantification of commensurability error in (large-scale)
536 groundwater studies is regularly overlooked as a source of uncertainty because it cannot
537 be satisfactorily evaluated (Tregoning et al., 2012). **Currently, evaluation of simulated**
538 **groundwater heads is plagued by, as yet, poorly quantified uncertainties stemming from**
539 **commensurability errors** and we therefore recommend future studies focus on
540 developing solutions to this problem.

541 We recommend evaluating models with a broader range of currently available data sources (with
542 explicit consideration of data uncertainty and regional differences) while also simultaneously working to
543 derive new data sets. However, data distribution and commensurability issues will likely still be present,
544 which underscores the importance of the two following strategies.

545 3.2. Model-based model evaluation

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

550
551 The original MIP concept offers a framework to consistently evaluate and compare models, and
552 associated model input, structural, and parameter uncertainty under different objectives (e.g., climate
553 change, model performance, human impacts and developments). Since the Project for the
554 **Intercomparison of Land-Surface Parameterization Schemes** (PILPS; Sellers et al., 1993), the first MIP,
555 the land surface modeling community has used MIPs to deepen understanding of land physical
556 processes and to improve their numerical implementations at various scales from regional (e.g., Rhône-
557 aggregation project; Boone et al., 2004) to global (e.g., Global Soil Wetness Project; Dirmeyer, 2011).
558 Two examples of recent model intercomparison efforts illustrate the general MIP objectives and
559 practice. First, ISIMIP (Schewe et al., 2014; Warszawski et al., 2014) assessed water scarcity at different
560 levels of global warming. Second, IH-MIP2 (Kollet et al., 2017) used both synthetic domains and an
561 actual watershed to assess fully-integrated hydrologic models because these cannot be validated easily
562 by comparison with analytical solutions and uncertainty remains in the attribution of hydrologic
563 responses to model structural errors. Model comparisons have revealed differences, but it is often
564 unclear whether these stem from differences in the model structures, differences in how the
565 parameters were estimated, or from other modelling choices (Duan et al., 2006). Attempts for modular
566 modelling frameworks to enable comparisons (Wagener et al., 2001; Leavesley et al., 2002; Clark et al.,



567 2008; Fenicia et al., 2011; Clark et al., 2015) or at least shared explicit modelling protocols and boundary
568 conditions (Refsgaard et al., 2007; Ceola et al., 2015; Warszawski et al., 2014) have been proposed to
569 reduce these problems.

570
571 Inter-scale model comparison - for example, comparing a global model to a regional-scale model - is a
572 potentially useful approach which is emerging for surface hydrology models (Hattermann et al., 2017;
573 Huang et al., 2017) and could be applied to large-scale models with groundwater representation. For
574 example, declining heads and decreasing groundwater discharge have been compared between a
575 calibrated regional-scale model (RRCA, 2003) and a global model (de Graaf et al., 2019). A challenge to
576 inter-scale comparisons is that regional-scale models often have more spatially complex subsurface
577 parameterizations because they have access to local data which can complicate model inter-
578 comparison. Another approach which may be useful is running large-scale models over smaller
579 (regional) domains at a higher spatial resolution (same as a regional-scale model) so that model
580 structure influences the comparison less. In the future, various variables that are hard to directly
581 observe at large scales but routinely simulated in regional-scale models such as baseflow or recharge
582 could be used to evaluate large-scale models. In this way, the output fluxes and intermediate spatial
583 scale of regional models provide a bridge across the “river of incommensurability” between highly
584 location-specific data such as well observations and the coarse resolution of large-scale models. It is
585 important to consider that regional-scale models are not necessarily or inherently more accurate than
586 large-scale models since problems may arise from conceptualization, groundwater-surface water
587 interactions, scaling issues, parameterization etc.

588
589 In order for a regional-scale model to provide a useful evaluation of a large-scale model, there are
590 several important documentation and quality characteristics it should meet. At a bare minimum, the
591 regional-scale model must be accessible and therefore meet basic replicability requirements including
592 open and transparent input and output data and model code to allow large-scale modelers to run the
593 model and interpret its output. Documentation through peer review, either through a scientific journal
594 or agency such as the US Geological Survey, would be ideal. It is particularly important that the
595 documentation discusses limitations, assumptions and uncertainties in the regional-scale model so that
596 a large-scale modeler can be aware of potential weaknesses and guide their comparison accordingly.
597 Second, the boundary conditions and/or parameters being evaluated need to be reasonably comparable
598 between the regional- and large-scale models. For example, if the regional-scale model includes human
599 impacts through groundwater pumping while the large-scale model does not, a comparison of baseflow
600 between the two models may not be appropriate. Similarly, there needs to be consistency in the time
601 period simulated between the two models. Finally, as with data-driven model evaluation, the purpose of
602 the large-scale model needs to be consistent with the model-based evaluation; matching the hydraulic
603 head of a regional-scale model, for instance, does not indicate that estimates of stream-aquifer
604 exchange are valid. Ideally, we recommend developing a community database of regional-scale models
605 that meet this criteria. It is important to note that Rossman & Zlotnik (2014) review 88 regional-scale
606 models while a good example of such a repository is the California Groundwater Model Archive
607 ([https://ca.water.usgs.gov/sustainable-groundwater-management/california-groundwater-](https://ca.water.usgs.gov/sustainable-groundwater-management/california-groundwater-modeling.html)
608 [modeling.html](https://ca.water.usgs.gov/sustainable-groundwater-management/california-groundwater-modeling.html)).



609
610 In addition to evaluating whether models are similar in terms of their outputs, e.g. whether they
611 simulate similar groundwater head dynamics, it is also relevant to understand whether the influence of
612 controlling parameters are similar across models. This type of analysis provides insights into process
613 controls as well as dominant uncertainties. Sensitivity analysis provides the mathematical tools to
614 perform this type of model evaluation (Saltelli et al., 2008; Pianosi et al., 2016; Borgonovo et al., 2017).
615 Recent applications of sensitivity analysis to understand modelled controls on groundwater related
616 processes include the study by Reinecke et al. (2019b) trying to understand parametric controls on
617 groundwater heads and flows within a global groundwater model. Maples et al. (2020) demonstrated
618 that parametric controls on groundwater recharge can be assessed for complex models, though over a
619 smaller domain. As highlighted by both of these studies, more work is needed to understand how to
620 best use sensitivity analysis methods to assess computationally expensive, spatially distributed and
621 complex groundwater models across large domains (Hill et al., 2016). In the future, it would be useful to
622 go beyond parameter uncertainty analysis (e.g. Reinecke et al. 2019b) to begin to look at all of the
623 modelling decisions holistically such as the forcing data (Weiland et al., 2015) and digital elevation
624 models (Hawker et al., 2018). Addressing this problem requires advancements in statistics (more
625 efficient sensitivity analysis methods), computing (more effective model execution), and access to large-
626 scale models codes (Hutton et al. 2016), but also better utilization of process understanding, for
627 example to create process-based groups of parameters which reduces the complexity of the sensitivity
628 analysis study (e.g. Hartmann et al., 2015; Reinecke et al., 2019b).
629

630 3.3 Expert-based model evaluation

631 A path much less traveled is expert-based model evaluation which would develop hypotheses of
632 phenomena (and related behaviors, patterns or signatures) we expect to emerge from large-scale
633 groundwater systems based on expert knowledge, intuition, or experience. In essence, this model
634 evaluation approach flips the traditional scientific method around by using hypotheses to test the
635 simulation of emergent processes from large-scale models, rather than using large-scale models to test
636 our hypotheses about environmental phenomena. This might be an important path forward for regions
637 where available data is very sparse or unreliable. The recent discussion by Fan et al. (2019) shows how
638 hypotheses about large-scale behavior might be derived from expert knowledge gained through the
639 study of smaller scale systems such as critical zone observatories. While there has been much effort to
640 improve our ability to make hydrologic predictions in ungauged locations through the regionalization of
641 hydrologic variables or of model parameters (Bloeschl et al., 2013), there has been much less effort to
642 directly derive expectations of hydrologic behavior based on our perception of the systems under study.
643
644 Large-scale models could then be evaluated against such hypotheses, thus providing a general
645 opportunity to advance how we connect hydrologic understanding with large-scale modeling - a strategy
646 that could also potentially reduce epistemic uncertainty (Beven et al., 2019), and which may be
647 especially useful for groundwater systems given the data limitations described above. Developing
648 appropriate and effective hypotheses is crucial and should likely focus on large-scale controlling factors



649 or relationships between controlling factors and output in different parts of the model domain;
650 hypotheses that are too specific may only be able to be tested by certain model complexities or in
651 certain regions. To illustrate the type of hypotheses we are suggesting, we list some examples of
652 hypotheses drawn from current literature:

- 653 • water table depth and lateral flow strongly affect transpiration partitioning (Famiglietti and
654 Wood, 1994; Salvucci and Entekhabi, 1995; Maxwell & Condon, 2016);
- 655 • the percentage of inter-basinal regional groundwater flow increases with aridity or decreases
656 with frequency of perennial streams (Gleeson & Manning, 2008; Goderniaux et al., 2013; Schaller
657 and Fan, 2008); or
- 658 • human water use systematically redistributes water resources at the continental scale via non-
659 local atmospheric feedbacks (Al-Yaari et al., 2019; Keune et al., 2018).

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

672
673 Formal approaches are available to gather the opinions of experts and to integrate them into a joint
674 result, often called expert elicitation (Aspinall, 2010; Cooke, 1991; O'Hagan, 2019). Expert elicitation
675 strategies have been used widely to describe the expected behavior of environmental or man-made
676 systems for which we have insufficient data or knowledge to build models directly. Examples include
677 aspects of future sea-level rise (Bamber and Aspinall, 2013), tipping points in the Earth system (Lenton
678 et al., 2018), or the vulnerability of bridges to scour due to flooding (Lamb et al., 2017). In the
679 groundwater community, expert opinion is already widely used to develop system conceptualizations
680 and related model structures (Krueger et al., 2012; Rajabi et al., 2018; Refsgaard et al., 2006), or to
681 define parameter priors (Ross et al., 2009; Doherty and Christensen, 2011; Brunner et al., 2012;
682 Knowing and Werner, 2016; Rajabi and Ataie-Ashtiani, 2016). The term expert opinion may be
683 preferable to the term expert knowledge because it emphasizes a preliminary state of knowledge
684 (Krueger et al., 2012).

685
686 A critical benefit of expert elicitation is the opportunity to bring together researchers who have
687 experienced very different groundwater systems around the world. It is infeasible to expect that a single
688 person could have gained in-depth experience in modelling groundwater in semi-arid regions, in cold
689 regions, in tropical regions etc. Being able to bring together different experts who have studied one or a
690 few of these systems to form a group would certainly create a whole that is bigger than the sum of its



691 parts. If captured, it would be a tremendous source of knowledge for the evaluation of large-scale
692 groundwater models. A challenge though is to formalize this knowledge in such a way that it is still
693 usable by third parties that did not attend the expert workshop itself.

694
695 So, while expert opinion and judgment play a role in any scientific investigation (O'Hagan, 2019),
696 including that of groundwater systems, we rarely use formal strategies to elicit this opinion. It is also less
697 common to use expert opinion to develop hypotheses about the dynamic behavior of groundwater
698 systems, rather than just priors on its physical characteristics. Yet, it is intuitive that information about
699 system behavior can help in evaluating the plausibility of model outputs (and thus of the model itself).
700 This is what we call expert-based evaluation herein. Expert elicitation is typically done in workshops with
701 groups of a dozen or so experts (e.g. Lamb et al., 2018). Upscaling such expert elicitation in support of
702 global modeling would require some web-based strategy and a formalized protocol to engage a
703 sufficiently large number of people. Contributors could potentially be incentivized to contribute to the
704 web platform by publishing a data paper with all contributors as co-authors and a secondary analysis
705 paper with just the core team as coauthors. We recommend the community develop expert elicitation
706 strategies to identify effective hypotheses that directly link to the relevant large-scale hydrologic
707 processes of interest.

708 **4. TOWARDS A HOLISTIC EVALUATION OF GROUNDWATER REPRESENTATION IN LARGE-SCALE** 709 **MODELS**

710
711 Ideally, all three strategies (observation-based, model-based, expert-based) should be pursued
712 simultaneously because the strengths of one strategy might further improve others. For example,
713 expert- or model-based evaluation may highlight and motivate the need for new observations in certain
714 regions or at new resolutions. Or observation-based model evaluation could highlight and motivate
715 further model development or lead to refined or additional hypotheses. We thus recommend the
716 community significantly strengthens efforts to evaluate large-scale models using all three strategies.
717 Implementing these three model evaluation strategies may require a significant effort from the scientific
718 community, so we therefore conclude with two tangible community-level initiatives that would be
719 excellent first steps that can be pursued simultaneously with efforts by individual research groups or
720 collaborations of multiple research groups.

721
722 First, we need to develop a 'Groundwater Modeling Data Portal' that would both facilitate and
723 accelerate the evaluation of groundwater representation in continental to global scale models (Bierkens,
724 2015). Existing initiatives such as IGRAC's Global Groundwater Monitoring Network ([https://www-
725 igrac.org/special-project/ggm-global-groundwater-monitoring-network](https://www-igrac.org/special-project/ggm-global-groundwater-monitoring-network)) and HydroFrame
726 (www.hydroframe.org), are an important first step but were not designed to improve the evaluation of
727 large-scale models and the synthesized data remains very heterogeneous - unfortunately, even
728 groundwater level time series data often remains either hidden or inaccessible for various reasons. This
729 open and well documented data portal should include:

730 a) observations for evaluation (Table 1) as well as derived signatures (Section 3.1);



- 731 b) regional-scale models that meet the standards described above and could facilitate inter-scale
732 comparison (Section 3.2);
733 c) Schematizations, conceptual or perceptual models of large-scale models since these are the
734 basis of computational models; and
735 d) Hypothesis and other results derived from expert elicitation (Section 3.3).

736 Meta-data documentation, data tagging, aggregation and services as well as consistent data structures
737 using well-known formats (netCDF, .csv, .txt) will be critical to developing a useful, dynamic and evolving
738 community resource. The data portal should be directly linked to harmonized input data such as forcings
739 (climate, land and water use etc.) and parameters (topography, subsurface parameters etc.), model
740 codes, and harmonized output data. Where possible, the portal should follow established protocols,
741 such as the Dublin Core Standards for metadata (<https://dublincore.org>) and ISIMIP protocols for
742 harmonizing data and modeling approach, and would ideally be linked to or contained within an existing
743 disciplinary repository such as HydroShare (<https://www.hydroshare.org/>) to facilitate discovery,
744 maintenance, and long-term support. Additionally, an emphasis on model objective, uncertainty and
745 regional differences as highlighted (Section 3) will be important in developing the data portal. Like
746 expert-elicitation, contribution to the data portal could be incentivized through co-authorship in data
747 papers and by providing digital object identifiers (DOIs) to submitted data and models so that they are
748 citable. By synthesizing and sharing groundwater observations, models, and hypotheses, this portal
749 would be broadly useful to the hydrogeological community beyond just improving global model
750 evaluation.

751
752 Second, we suggest ISIMIP, or a similar model intercomparison project, could be harnessed as a
753 platform to improve the evaluation of groundwater representation in continental to global scale models.
754 For example, in ISIMIP (Warszawski et al., 2014), modelling protocols have been developed with an
755 international network of climate-impact modellers across different sectors (e.g. water, agriculture,
756 energy, forestry, marine ecosystems) and spatial scales. Originally, ISIMIP started with multi-model
757 comparison (model-based model evaluation), with a focus on understanding how model projections
758 vary across different sectors and different climate change scenarios (ISIMIP Fast Track). However, more
759 rigorous model evaluation came to attention more recently with ISIMIP2a, and various observation data,
760 such as river discharge (Global Runoff Data Center), terrestrial water storage (GRACE), and water use
761 (national statistics), have been used to evaluate historical model simulation (observation-based model
762 evaluation). To better understand model differences and to quantify the associated uncertainty sources,
763 ISIMIP2b includes evaluating scenarios (land use, groundwater use, human impacts, etc) and key
764 assumptions (no explicit groundwater representation, groundwater availability for the future, water
765 allocation between surface water and groundwater), highlighting that different types of hypothesis
766 derived as part of the expert-based model evaluation could possibly be simulated as part of the ISIMIP
767 process in the future. While there has been a significant amount of research and publications on MIPs
768 including surface water availability, limited multi-model assessments for large-scale groundwater
769 studies exist. Important aspects of MIPs in general could facilitate all three model evaluation strategies:
770 community-building and cooperation with various scientific communities and research groups, and
771 making the model input and output publicly available in a standardized format.
772



773 Large-scale hydrologic and land surface models increasingly represent groundwater, which we envision
774 will lead to a better understanding of large-scale water systems and to more sustainable water resource
775 use. We call on various scientific communities to join us in this effort to improve the evaluation of
776 groundwater in continental to global models. As described by examples above, we have already started
777 this journey and we hope this will lead to better outcomes especially for the goals of including
778 groundwater in large-scale models that we started with above: improving our understanding of Earth
779 system processes; and informing water decisions and policy. Along with the community currently
780 directly involved in large-scale groundwater modeling, above we have made pointers to other
781 communities who we hope will engage to accelerate model evaluation: 1) regional hydrogeologists, who
782 would be useful especially in expert-based model evaluation (Section 3.3); 2) data scientists with
783 expertise in machine learning, artificial intelligence etc. whose methods could be useful especially for
784 observation- and model-based model evaluation (Sections 3.1 and 3.2); and 3) the multiple Earth
785 Science communities that are currently working towards integrating groundwater into a diverse range of
786 models so that improved evaluation approaches are built directly into model development. Together we
787 can better understand what has always been beneath our feet, but often forgotten or neglected.

788

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795

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800

801 **Code/Data availability:**

802 No code or data were used in the writing of this manuscript

803

804 **Competing interests:**

805 The authors declare no competing interests.

806

807

808



809 **Table 1. Available observations for evaluating the groundwater component of large-scale models**

810

Data type	Strengths	Limitations	Data availability and spatial resolution
Available observations already used to evaluate large-scale models			
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	IGRAC Global Groundwater Monitoring Network ; Fan et al., 2013; USGS 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 European Groundwater Drought Initiative 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 $\approx 100,000 \text{ km}^2$ (Scanlon et al. 2016) which are then processed as groundwater storage change
Storage change (regional aquifers)	Regionally integrated response of aquifer	Bias towards North America and Europe	Konikow 2011 Döll et al., 2014a Regional aquifers (10,000s to 100,000s km^2)
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 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. 2014 National-scale data down-scaled to grid
Streamflow	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 data sources ; large to small basin.
Evapotranspiration	Widely available; related to groundwater recharge	Not a direct groundwater observations	Various datasets (Miralles et al., 2016); gridded

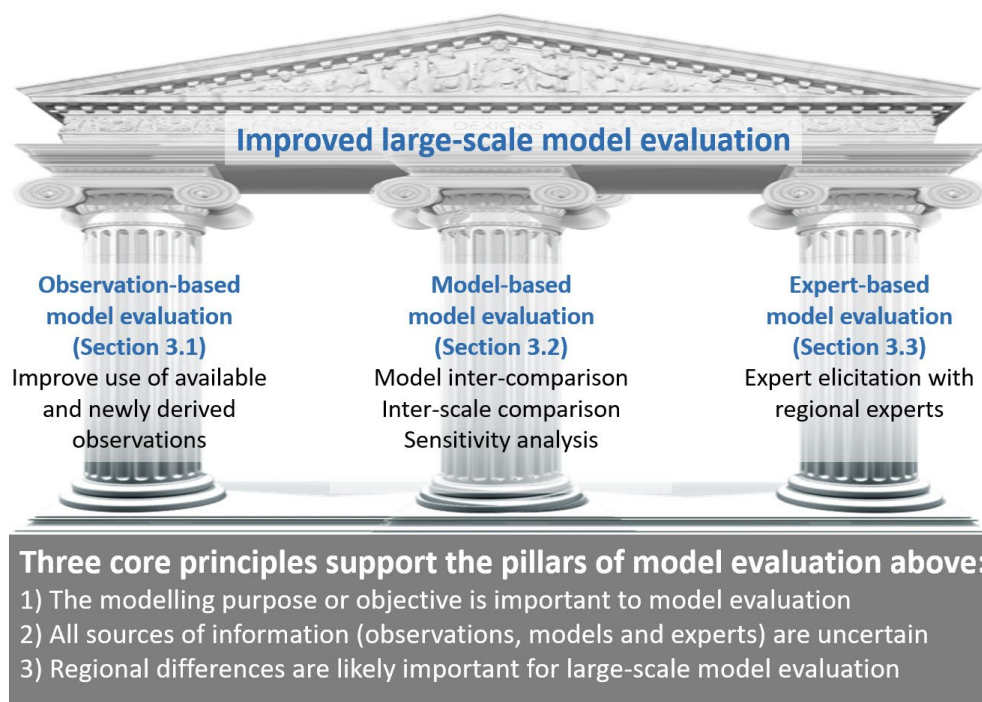


	or discharge (for shallow water tables)		
Available observations not being used to evaluate large-scale models			
Baseflow index (BFI) or baseflow recession (k)	Possible integrator of groundwater contribution to streamflow over a basin	BFI and k values vary with method; baseflow may be dominated by upstream 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 streams 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 (e.g. Springer, & Stevens, 2009) but not globally; 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 (Gleeson et al., 2016; Jasechko et al., 2017) but no global data for heat or other chemistry; Point measurements at existing wells or surface water features
Surface elevation data (leveling, GPS,	Provides information about changes in surface	Provides indirect information and needs a geomechanical	Leveling data, GPS data and lidar observations mostly limited to



radar/lidar) an in particular land subsidence observations	elevation that are related to groundwater head variations or groundwater head decline	model to translate to head. Introduces additional uncertainty of geomechanical properties.	areas of active subsidence (e.g. Minderhoud et al., 2019,2020) and not always open. Global data on elevation change are available from the Sentinel 1 mission.
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 816 **Figure 1: Improved large-scale model evaluation rests on three pillars: observation-, model-, and**
 817 **expert-based model evaluation. We argue that each pillar is an essential strategy so that all three**
 818 **should be simultaneously pursued by the scientific community. The three pillars of model evaluation**
 819 **all rest on three core principles related to 1) model objectives, 2) uncertainty and 3) regional**
 820 **differences.**



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