Dear Monica Riva,

thank you very much for your suggestions for further improving our manuscript additionally to the very helpful reviewer comments. In the following you will find the marked-up manuscript with the additional discussion you proposed. To keep an overview I've separated these changes from the already proposed changes after the discussion phase which I additional enclosed in this document for reference.

Best regards Robert Reinecke.

Spatially distributed sensitivity of simulated global groundwater heads and flows to hydraulic conductivity, groundwater recharge and surface water body parameterization

Robert Reinecke¹, Laura Foglia³, Steffen Mehl⁵, Jonathan D. Herman⁴, Alexander Wachholz¹, Tim Trautmann¹, and Petra Döll^{1,2}

¹Institute of Physical Geography, Goethe University Frankfurt, Frankfurt am Main, Germany

²Senckenberg Leibniz Biodiversity and Climate Research Centre Frankfurt (SBiK-F), Frankfurt am Main, Germany

³Department of Land, Air and Water Resources, University of California, Davis, USA

⁴Department of Civil & Environmental Engineering, University of California, Davis, USA

⁵Department of Civil Engineering, California State University, Chico, USA

Correspondence: Robert Reinecke (reinecke@em.uni-frankfurt.de)

Abstract. In global hydrological models, groundwater storages and flows are generally simulated by linear reservoir models. Recently, the first global gradient-based groundwater models were developed in order to improve the repre-5 sentation of groundwater-surface water interactions, capil-

- lary rise, lateral flows and human water use impacts. However, the reliability of model outputs is limited by a lack of data and by uncertain model assumptions that are necessary due to the coarse spatial resolution. The impact of data qual-
- ¹⁰ ity is presented by showing the sensitivity of a groundwater model to changes in the only available global hydraulic conductivity data-set. To better understand the sensitivity of model output to uncertain spatially distributed parameters, we present the first application of a global sensitivity
- ¹⁵ method for a global-scale groundwater model using nearly 2000 steady-state model runs of the global gradient-based groundwater model G³M. By applying the Morris method in a novel domain decomposition approach that identifies global hydrological response units, spatially distributed pa-
- ²⁰ rameter sensitivities are determined for a computationally expensive model. Results indicate that globally simulated hydraulic heads are equally sensitive to hydraulic conductivity, groundwater recharge and surface water body elevation, though parameter sensitivities vary regionally. For large ar-
- ²⁵ eas of the globe, rivers are simulated to be either losing or gaining, depending on the parameter combination, indicating a high uncertainty of simulating the direction of flow between the two compartments. Mountainous and dry regions show a high variance in simulated head due to numerical instabilities

of the model, limiting the reliability of computed sensitivities ³⁰ in these regions. This is likely caused by the uncertainty in surface water body elevation. We conclude that maps of spatially distributed sensitivities can help to understand complex behaviour of models that incorporate data with varying spatial uncertainties. The findings support the selection of possible calibration parameters and help to anticipate challenges for a transient coupling of the model.

1 Introduction

Global groundwater dynamics have significantly changed due to human withdrawals, and are projected to continue 40 due to climate change (Taylor et al., 2013). Groundwater withdrawals have led to lowered water tables, decreased base flows, and groundwater depletion around the globe (Konikow, 2011; Scanlon et al., 2012; Wada et al., 2012; Döll et al., 2014; Wada, 2016). To represent groundwater-surface 45 water body interactions, lateral and vertical flows, and human water use impacts on head dynamics, it is necessary to simulate the depth and temporal variation of the groundwater table. Global-scale hydrological models have recently moved to include these processes by implementing a gradient-based 50 groundwater model approach (de Graaf et al., 2015; Reinecke et al., 2018)(de Graaf et al., 2015; Reinecke et al., 2019). This study is based on G³M (Reinecke et al., 2018) (Reinecke et al., 2019) one of the two global groundwater models capable of

calculating hydraulic head and surface water body interaction on a global scale. However, the lack of available input data and the necessary conceptual assumptions due to the coarse spatial resolution limit the reliability of model out-

⁵ put. These substantial uncertainties suggest an opportunity for diagnostic methods to prioritize efforts in data collection and parameter estimation.

Sensitivity analysis is a powerful tool to assess how uncertainty in model parameters affects model outcome, and can ¹⁰ provide insights about how the interactions between parameters influence the model results (Saltelli et al., 2008). Sensitivity methods can be separated into two classes: local and global methods. Local methods compute partial derivatives of the output with respect to an input factor at a fixed point

- ¹⁵ in the input space. By contrast, global methods explore the full input space, though at higher computational costs (Pianosi et al., 2016). The large number of model evaluations required can render global methods unfeasible for computationally demanding models, though increased computational
- ²⁰ resources have led to more widespread application e.g. (Herman et al., 2013b, a; Ghasemizade et al., 2017)(Herman et al., 2013a, b; Ghasemizade et al., 2017). For this reason, existing studies of global models either focus on exploring uncertainties by running their model with a limited set of different in-
- ²⁵ puts for a quasi local sensitivity analysis (Wada et al., 2014; Müller Schmied et al., 2014, 2016; Koirala et al., 2018) or applying computationally inexpensive methods based on a limited set of model evaluations (Schumacher et al., 2015). For example, de Graaf et al. (2015, 2017) determined the
- ³⁰ coefficient of variation for head results in a global groundwater model with 1000 model runs evaluating the impact of varying aquifer thickness, saturated conductivity and groundwater recharge. To the knowledge of the authors, the only other study that applied a global sensitivity analysis to a com-
- ³⁵ parably complex global model is Chaney et al. (2015). An overview of the application of different sensitivity analysis methods for hydrological models can be found in Song et al. (2015); Pianosi et al. (2016).

To address the issue of This study relies on the method of Morris (Morris, 1991) in the context of global sensitivity methods. Morris is a global sensitivity method as it provides an aggregated measure of local sensitivity coefficients for each parameter at multiple points across the input space and analyses the distribution properties (Razavi and Gupta,

- ⁴⁵ 2015). Compared to other global methods, like the more robust variance based methods e.g. Sobol (1993), Morris has drawbacks as it may provide false conclusions (Razavi and Gupta, 2015). The attribution of what is a direct effect (model response only due to one parametemplate and the set of interval in a factor of the set of th
- ter change) and what an effect of interaction (response to non-linear interaction of parameters on model output) is not trivial. Morris is prone to scale issues, that is that the step size of the analysis can have significant impact on the conclusions drawn especially for significantly non linear responses (Razavi and Gupta, 2015). In this study

we address this by limiting the parameter ranges of the multipliers where we suspect non-linearity in the model response. In general the choice of the chosen global sensitivity method may yield different results (Dell'Oca et al., 2017). On the other hand, Janetti et al. (2019) showed 60 for a regional scale groundwater study that different global methods showed similar results for hydraulic conductivity parameterization. Nevertheless, Morris is a well established and recognized method (Razavi and Gupta, 2015) that has the advantage of computational efficiency com- 65 pared to variance-based methods to screen the most sensitive parameters (Herman et al., 2013a). It requires significantly fewer model runs, compared to other global methods, to provide a meaningful ranking of sensitive parameters enabling the exploration of computationally demand-70 ing models (Herman et al., 2013a). The application of a global sensitivity method for a complex world-wide model of groundwater flows is unique, and Morris is currently the best available method to handle the computational constraints. 75

To reduce the number of necessary model runs when conducting global sensitivity analysis for computationally complex demanding models we introduce the concept of Global Hydrological Response Units (GHRUs) (Sect. 2.2.3) (similar to e.g. Hartmann et al. (2015)). Using the GHRUs ⁸⁰ we present an application of the well-established Morris method (Morris, 1991) to the Global Gradient-based Groundwater Model G³M (Reinecke et al., 2018). The Morris method has been successfully applied to a variety of models, ranging from hydrology (Zhan et al., 2013) to ecology models (Cariboni et al., 2007). It requires significantly fewer model runs, compared to other global methods, to provide a meaningful ranking of sensitive parameters (Herman et al., 2013a) enabling the exploration of computationally demanding models. (Reinecke et al., 2019).

G³M uses input from, and it is intended to be coupled and integrated into, the global hydrological model WaterGAP ⁹⁰ Global Hydrology Model (WGHM) (Döll et al., 2014). This study investigates the sensitivity of steady-state hydraulic heads and exchange flows between groundwater and surface water to variations in main model parameters (e.g. groundwater recharge and other model parameters like the riverbed ⁹⁵ conductance).

Sensitivities of the model are explored in three steps: (1) To understand the impact of improved input data, in particular hydraulic conductivity, we investigate the changes in simulated hydraulic head that result from changing the hydraulic conductivity data from the GLHYMPS 1.0 dataset (Gleeson et al., 2014) to 2.0 (Huscroft et al., 2018). (2) Based on prior experiments (de Graaf et al., 2015; Reinecke et al., 2018) (de Graaf et al., 2015; Reinecke et al., 2019) eight parameters are selected for a Monte Carlo experiment to investigate sensitivities of simulated hydraulic head and groundwatersurface water interactions. The parameters are sampled with a newly developed global region-based sampling strategy and build the framework for the (3) Morris analysis. Elementary Effects (EE), a metric of sensitivity, are calculated and 110 their means and variances ranked to determine global spatial distributions of parameter sensitivities and interactions. The derived global maps show, for the first time, the sensitivity and parameter interactions of simulated hydraulic head

- 5 and groundwater-surface water flows in the simulated steadystate global groundwater system to variations in uncertain parameters. Foremost, these maps help to guide future calibration efforts by identifying the most influential parameters and answer the question if the calibration should focus on differ-
- ¹⁰ ent parameters for different regions helping to understand regional deviations from observations. Additionally, they guide the further development of the model especially in respect to the coupling efforts highlighting which parameters will influence the coupled processes the most. Lastly, they show in
- ¹⁵ which regions global groundwater models might benefit the most from efforts in improving global datasets like global conductivity maps.

2 Methodology and Data

2.1 The model G^3M

- 20 G³M (Reinecke et al., 2018) (Reinecke et al., 2019) is a global groundwater model intended to be coupled with WaterGAP (Döll et al., 2003, 2012, 2014; Müller Schmied et al., 2014) and is based on the Open Source groundwater modelling framework G³M-f¹(Reinecke, 2018). It computes lateral and
- ²⁵ vertical groundwater flows as well as surface water exchanges for all land areas of the globe except Antarctica and Greenland on a resolution of 5' with two vertical layers with a thickness of each 100 m representing the aquifer. The groundwater flow between cells is computed as

$${}_{30} \frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right)$$
(1)

$$+\frac{Q}{\Delta x \Delta y \Delta z} = S_s \frac{\partial h}{\partial t} \tag{2}$$

where $K_{x,y,z}$ [LT⁻¹] is the hydraulic conductivity along the x,y, and z axis between the cells with size $\Delta x \Delta y \Delta z$, S_s [L⁻¹] the specific storage, h the hydraulic head [L], and Q ³⁵ [L³T⁻¹] the in- and outflows of the cells to or from external

sources e.g. groundwater recharge (R and surface water body flows (Q_{swb}) (see also Reinecke et al. (2019)[Eq.(1,2)]Reinecke et al. (2019)[Eq.(1,2)]). The evaluation presented in this study is based on a steady-state variant of the model representing a 40 quasi-natural equilibrium state, not taking into account human interference (a full description of the steady-state model and indented coupling can be found in Reinecke et al. (2018)Reinecke et al. (2019)). The stand-alone steady-state simulations were performed as initial step to identify the domi-45 nant parameters that are also likely important for controlmodel h_{swb} will be changed according to calculated river discharge calculated by WaterGAP (Fig. 1). Q_{swb} will be used to replace the current calculated flows in WaterGAP between groundwater and surface water bodies.

2.1.1 Groundwater recharge

Groundwater recharge (R) is based on mean annual R computed by WaterGAP 2.2c for the period 1901-2013. Human groundwater abstraction was not taken into account; not because it is not computed by WaterGAP but rather because there is no meaningful way to include it into a steady-state model which represents an equilibrium (abstractions do not equilibrize).

2.1.2 Hydraulic conductivity

Hydraulic conductivity (*K*) is derived from GLHYMPS 2.0 ⁶⁰ (Huscroft et al., 2018) (shown in Fig. 2 (a)). The original data was gridded to 5' by using an area-weighted average and used as *K* of the upper model layer. For the second layer, *K* of the first layer is reduced by an e-folding factor *f* used by Fan et al. (2013) (a calibrated parameter based on terrain slope) assuming that conductivity decreases exponentially with depth. Conductivity of the lower layer is calculated by multiplying the upper layer value by $exp(-50mf^{-1})^{-1}$ (Fan et al., 2013, Eq. 7).

Currently only two datasets, GLHMYPS 1.0 and 2.0 70 (Gleeson et al., 2014; Huscroft et al., 2018), are available and are used by a number of continental and global models (de Graaf et al., 2015; Maxwell et al., 2015; Keune et al., 2016; Reinecke et al., 2018)(de Graaf et al., 2015; Maxwell et al., 2015; Keune et al., 2016; Reinecke et al., 2019). GLHMYPS 1.0 75 (Gleeson et al., 2014) is compiled based on the global lithology map GLiM (Hartmann and Moosdorf, 2012) and data from 92 regional groundwater models and derives permeabilities (for the first 100 m vertically) based on Gleeson et al. (2011), differentiating the sediments into the categories fine-80 , coarse-grained, mixed, consolidated, and unconsolidated. Permafrost regions are assigned a K value of 10^{-13} ms⁻¹ based on Gruber (2012). Areas of deeply weathered laterite soil (mainly in tropical regions) are mapped as unconsolidated sediments as they dominate K (Gleeson et al., 2014). 85

The global permeability map was further improved with the development of GLHYMPS 2.0 by Huscroft et al. (2018). A two-layer set up was established in GLHYMPS 2.0 with the lower layer matching the original GLHYMPS 1.0. For the upper layer in GLHYMPS 2.0, a global database of unconsolidated sediments (Börker et al., 2018) was integrated into GLHYMPS 2.0 resulting in overall slightly increased *K* (Fig. 2 (a)). The thickness of the upper layer was deduced from the *depth-to-bedrock* information available from Soil-Grid (Hengl et al., 2017). No thickness was assigned to the power layer.

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ling transient groundwater flow. In the fully coupled transient

¹Available on globalgroundwatermodel.org



Figure 1. Parameterization and outputs of the G^3M model. Where Q_{swb} is the flow between the aquifer and surface water bodies, h is the simulated hydraulic head, K the hydraulic conductivity, E_{swb} the surface water body elevation, B_{swb} the bottom elevation of the surface water body, C_{swb} the conductance of the surface water bodies, and R the groundwater recharge. In the red the Outputs outputs and parameters that are foremost important for coupling.



Figure 2. Impact of hydraulic conductivity datasets GLHYMPS 1.0 and GLHYMPS 2.0. (a) GLHYMPS 2.0 $[ms^{-1}]$, (b) *K* differences, expressed as *K*(GLHYMPS 2.0)/*K*(GLHYMPS 1.0). Blue indicates higher values in GLHYMPS 2.0. (c) *h*(GLHYMPS 2.0) minus *h*(GLHYMPS 1.0) [m], (d) the sensitivity of *h* to change in the GLHYMPS dataset based on Eq. (7) (white indicates that no index could be calculated).

2.1.3 Surface water body conductance

The in- and outflows Q are described similar to MODFLOW as flows from the cell: a flow from the cell to a surface water body is negative and positive if the opposite is true. Thus 5 gains and losses from surface water bodies (lakes, wetlands and rivers) are described as

$$Q_{swb} = \begin{cases} C_{swb}(h_{swb} - h) & h > B_{swb} \\ C_{swb}(h_{swb} - B_{swb}) & h \le B_{swb} \end{cases}$$
(3)

where h is the simulated hydraulic head, h_{swb} is the head of the surface water body, and B_{swb} the bottom elevation. The conductance C_{swb} of the surface water body bed is calculated 10 as

$$C_{swb} = \frac{KLW}{h_{swb} - B_{swb}} \tag{4}$$

where K is the hydraulic conductivity, L the length and W the width of the surface water body. For lakes (including reservoirs) and wetlands, the conductances C_{lak} and C_{wet} ¹⁵ are estimated based on K of the aquifer and surface water

body area divided by a static thickness of 5 m ($h_{swb}-B_{swb}=5m$). For a steady-state simulation the surface water body data shows the maximum spatial extent of wetlands, an extent that is seldom reached in particular in case of wetlands in $_{5}$ dry areas. To account for that we assume for global wetlands

- $(C_{gl.wet})$ that only eighty percent of their maximum extent is reached in the steady-state. Global wetlands are defined as wetlands that are recharged by streamflow coming from an upstream 5' grid cell in WaterGAP (Reinecke et al., 2018) (Rei-
- ¹⁰ necke et al., 2019). For gaining rivers, the conductance is quantified individually for each grid cell following an approach proposed by Miguez-Macho et al. (2007). According to Miguez-Macho et al. (2007), the river conductance C_{riv} in a steady-state groundwater model needs to be set in a way
- ¹⁵ that the river is the sink for all the inflow to the grid cell (R and inflow from neighbouring cells) that is not transported laterally to neighbouring cells.

$$C_{riv} = \frac{R + Q_{eq_{lateral}}}{h_{eq} - h_{riv}} \quad h > h_{riv} \tag{5}$$

- where $Q_{eq_{lateral}}$ is the lateral flow based on the equilib-²⁰ rium head h_{eq} of Fan et al. (2013) and h_{riv} the head of the river ($E_{swb} = h_{swb,riv}$ in Table 1). These conductance equations are inherently empirical as they use a one-dimensional flow equation to represent the three-dimensional flow process that occurs between groundwater and surface water. Fu-
- ²⁵ ture efforts will investigate using approaches appropriate for large scale models, such as described by Morel-Seytoux et al. (2017). An extensive description on the chosen equations and implications can be found in Reinecke et al. (2018)Reinecke et al. (2019).

30 2.1.4 Surface water body elevation

The vertical location of surface water bodies has a great impact on model outcome (Reinecke et al., 2018)(Reinecke et al., 2019). Their vertical location h_{swb} is set to the 30th percentile of the 30" land surface elevation values of Fan et al.

- ³⁵ (2013) per 5' cell, e.g. the elevation that is exceeded by 70 % of the thousand hundred 30" elevation values within one 5' cell. B_{swb} is calculated based on that head elevation with different values for wetlands and lakes (Reinecke et al., 2018, Table 1)(Reinecke et al., 2019, Table 1). For rivers, B_{swb} is equal to $h_{riv} - 0.349 \times Q_{bankfull}^{0.341}$ (Allen et al., 1994), where
- $Q_{bankfull}$ is the bankfull river discharge in the 5' grid cell (Verzano et al., 2012).

2.1.5 Ocean boundary

The outer boundary condition in the model is described by 45 the ocean and uses an equation similar to MODFLOW's general head boundary condition as flow

$$Q_{ocean} = C_{oc}(h_{ocean} - h) \tag{6}$$

where h_{ocean} is the elevation of the ocean water table set 0 m worldwide and C_{oc} the conductance of the boundary con-

dition set to $10^{-6}m^2s^{-1}$ based on average K and aquifer 50 thickness.

2.2 Sensitivity Analysis

2.2.1 Sensitivity of simulated head to choice in hydraulic conductivity dataset

Parameterization of aquifer properties based on hydrogeological data is an important decision in groundwater modeling. We first investigate the effect of switching to a newly available global permeability dataset to explore the sensitivity of h to the variability in geologic data. The results are then compared to the effects of parameter variability, as quantified by the Monte Carlo experiments.

GLHYMPS 2.0 (Huscroft et al., 2018) provides an update of the only available global permeability map (Gleeson et al., 2014). To quantify how the new hydraulic conductivity estimates change the simulation outcome of the groundwater ⁶⁵ model we apply a basic sensitivity method.

$$S = \frac{\frac{h_2 - h_1}{h_1}}{\frac{K_2 - K_1}{K_1}}$$
(7)

where the sensitivity S of h to a change in K is calculated based on the change in h (h_1 is the hydraulic head calculated with GLHYMPS 1.0 and h_2 with GLHYMPS 2.0) ⁷⁰ and change in K_1 and K_2 the conductivity based on GL-HYMPS 1.0 and 2.0, respectively.

2.2.2 Sensitivity of head and surface water body flow to choice in parameters

Along with K, additional parameters influence the model ⁷⁵ outcome. In this study we apply the method of Morris (Morris, 1991) as a screening method to identify which parameters are most important for the two main model outcomes, namely h and groundwater-surface water interactions (Q_{swb}). The Morris method provides a compromise between accuracy and computational cost in comparison to other Monte Carlo like methods (Campolongo et al., 2007). Each model execution represents an individually randomized One Factor At a Time (OAT) experiment, where one parameter is changed per simulation. Based on these model executions, the Morris method calculates an Elementary Effect (EE) d for every trajectory of a *i*-th parameter (in this study parameter multipliers).

$$d_i(\mathbf{X}) = \left(\frac{y(X_1, \dots, X_{i-1}, X_i + \Delta, X_{i+1}, \dots, X_k) - y(\mathbf{X})}{\Delta}\right)$$
(8)

where Δ is the trajectory step size for the parameter multiplier X_i , **X** is the vector of model parameters multipliers of ⁹⁰ size k and $y(\mathbf{X})$ the model output e.g. in the presented model h or Q_{swb} . The total effect of the *i*th parameter is computed as the absolute mean of the EEs for all trajectories and is denoted as μ * (Campolongo et al., 2007). The standard deviation of EEs (σ_i) is an aggregated measure of the intensity of the interactions of the *i*th parameter with the other parameters, representing the degree of non-linearity in model

- ⁵ response to changes in the *i*th parameter (Morris, 1991). The derived metrics μ * and σ_i both are measures of intensity (higher values are more sensitive/interactive) and do not represent absolute values of sensitivity. Both can only be interpreted meaningfully in comparison with values derived for ¹⁰ other parameters.
- To achieve that, $\mu *$ and σ_i are presented in this study in *ranks*. Thus, values for all parameters are ranked from highest to lowest, and the parameter with the highest value is selected as the most influential parameter. The parameter with 15 the second highest value (*rank* 2) is the second most influen-
- tial parameter and so on.

Previous experiments (de Graaf et al., 2015; Reinecke et al., 2018) (de Graaf et al., 2015; Reinecke et al., 2019) showed the importance of hydraulic conductivity, groundwater recharge, ²⁰ and surface water body elevation to the simulated hydraulic head. Together with the highly uncertain surface water body and ocean conductance we thus selected eight model parameters for the sensitivity analysis. The analysis was conducted my using randomly sampled multipliers in the ranges pre-²⁵ sented in Table 1.

Throughout the analysis the following parameters including the convergence criterion and spatial resolution stay fixed: global mean sea-level, bottom elevation of surface water bodies and their width, length. The baseline parame-

- ³⁰ ters are assumed equally to Reinecke et al. (2018)Reinecke et al. (2019). Hydraulic conductivity is based on a global data set (2.1.2), the conductance is calculated as previously shown (2.1.3), and the groundwater recharge baseline is equally to the mean annual values calculated by WaterGAP (2.1.1). Pa-
- ³⁵ rameter ranges were chosen to ensure that a high percentage of model realizations converge numerically. For example, the uncertainty of E_{swb} in the model is higher than the ranged used in this study, but the sampling range was restricted because the parameter is especially important for
- ⁴⁰ model convergence. Furthermore, the chosen river conductance approach uses *R* as parameter and includes a nonlinear threshold between losing and gaining surface water bodies, which strongly affects numeric stability. As in any global sensitivity analysis, the choice of parameter ranges involves ⁴⁵ some subjectivity that may influence the ranking of sensitive
- parameters in the results.

2.2.3 Global hydrological response units

Even though the number of model evaluations are comparably less for OAT-based experiments than for All-At-a-Time

⁵⁰ (Pianosi et al., 2016), varying every parameter independently in every spatial grid cell leads to an unfeasible amount of model runs. On the other hand, the use of global multipliers that vary a parameter uniformly for all computational cells



Figure 3. Map of k-means clustering categories each representing a GHRU (a). Each color identifies a region where the combination of all three parameters is similar.

may lead to inconclusive results, as the sensitivity for every cell to this change is spread to the whole computational domain. A possible solution would be to separate the globe into zones with similar geological characteristics based on the GLHYMPS dataset, but this may still result in an infeasible number of required simulations. Each simulation takes about 30 min to 1 h on a commodity computer (more if the parameters hinder a fast convergence).

To overcome these limitations, we introduce the use of a Global Hydrological Response Unit (GHRU). Every GHRU represents a region of similar characteristics regarding three characteristics: E_{swb} (Sect. 2.1.3,2.1.4), K (Sect. 2.1.2), and ⁶⁵ R (Sect. 2.1.1). This does not constitute a zoning approach often used for calibration in traditional regional groundwater modelling, only a separation into parameter multipliers. All multipliers for a given parameter for all regions are based on the same random distribution inside a given range of uncertainty for that parameter. Characteristics for each model cell are normalized to [0,1] and used to create a 3d point space (based on the three characteristics for each model cell). We apply a *k-means* (Lloyd, 1982) clustering algorithm to identify these regions.

K-means clustering partitions n points into k clusters where each point belongs to the cluster with a minimized pairwise squared distance to the mean in a cluster. Figure 3 (a) shows a map of k-means clustering (6 clusters) categories based on normalized three-dimensional space of E_{swb} , K, ⁸⁰ and R per grid cell.

The number of clusters was determined based on the feasible number of model evaluations. *k-means* constitutes an unsupervised machine learning approach that builds the required number of clusters automatically, thus it is necessary afterwards to examine what main characteristics these clusters represent (shown in Table 2). Characteristics are encoded as relative values (high (\uparrow), medium (\sim), low (\downarrow)) of the three parameter values based on their mean value per cluster. These characteristics are used to connect calculated parameter sensitivities to GHRUs when analyzing the results of the experiment.

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Parameter	P. Unit	Multiplier Range	Description
K	LT^{-1}	0.1 - 100	Saturated hydraulic conductivity
E_{swb} C_{lak}	$L^{2}T^{-1}$	0.5 - 2	Conductance of lakebed
C_{wet}	$L^2 T^{-1}$	0.5 - 2	Conductance of wetland bed
$C_{gl.wet}$	$L^2 T^{-1}$	0.5 - 2	Conductance of global wetland bed
C_{riv}	$L^2 T^{-1}$	0.5 - 2	Conductance of riverbed
R	LT^{-1}	0.5 - 2	Groundwater recharge
C_{oc}	$L^2 T^{-1}$	0.1 - 10	Conductance of the ocean boundary

Table 1. Range of parameter multipliers used in the Morris experiments. Each parameter multiplier is sampled in log space $(\log_{10}(Multiplier))$ with sampling based on Campolongo et al. (2007) and optimized with Ruano et al. (2012).

 C_{oc} is equal for all ocean cells

Table 2. Mean values of GHRU characteristics and their summarized description, where \uparrow is read as a relatively high value, \sim as medium, and \downarrow as low; e.g. $\uparrow\uparrow$ E indicates a cluster with very high and relatively high (\uparrow) average E_{swb} . Additionally, the last two columns show the percentage of cells per GHRU where $\mu *$ of h and Q_{swb} could be reliably determined (described in Sect. 3.2.6).

					% of reliable $\mu *$	
GHRU	$\mu(E_{swb})$ [m]	$\mu(K)[\mathrm{m~day^{-1}}]$	$\mu(R)$ [mm day ⁻¹]	GHRU description	h	Q_{swb}
1	454	10^{-4}	0.15	\sim E, \uparrow K, \sim R	9.54 %	6.58 %
2	286	10^{-6}	0.15	\downarrow E, ~ K, ~ R	12.07 %	14.41 %
3	4107	10^{-6}	0.13	$\uparrow\uparrow \mathrm{E},\sim\mathrm{K},\downarrow\mathrm{R}$	0.08~%	4.09 %
4	1355	10^{-6}	0.11	\uparrow E, \sim K, \downarrow R	3.17 %	17.19 %
5	303	10^{-6}	1.24	\downarrow E, \sim K, \uparrow R	31.62 %	26.37 %
6	194	10^{-4}	1.25	\downarrow E, \uparrow K, \uparrow R	29.00 %	14.36 %

2.2.4 Experiment Configuration

With seven parameters per GHRU plus the ocean boundary, 10 000 initial trajectories were sampled in total (Campolongo et al., 2007) and optimized using Ruano et al. (2012) result-5 ing in 1848 optimized trajectories for each parameter. Ran-

dom sampling might result in non-optimal coverage of the input space; thus a high number of trajectories is sampled first and only trajectories with a maximized spread are selected (Ruano et al., 2012). For 7 parameters (without ocean

¹⁰ boundary), *n* GHRUs (6 in this paper) we get a total number of parameters k = 42 + 1 where +1 stands for the ocean boundary, which is not varied by GHRU. We assume 42 for the number of optimized trajectories (Ruano et al., 2012) resulting in N = r(k+1) (Campolongo et al., 2007), where N ¹⁵ is the total number of simulation (1848).

The experiment resulted in 1848 simulations with an overall runtime of two months on a machine with 20 computational cores (enabled hyper-threading) and 188 GB RAM. Each simulation required about 8 GB of RAM and was as-²⁰ signed four computational threads while running the simulations in cohorts of 10 simulations at once. Each simulation was an OAT experiment (an extended explanation of OAT and other sensitivity experiment setups and methods

can be found in Pianosi et al. (2016)). Changes in parame-²⁵ ters were stacked over all experiments. Thus, an experiment may have changed R (also affecting C_{riv} for gaining conditions) while containing a C_{riv} multiplier from a previous experiment. Sampling and analysis was implemented with the Python library *SALib* (Herman and Usher, 2017). For each experiment, the model was run until it reached an equilibrium state (steady-state model). All other parameters and convergence criteria can be found in Reinecke et al. (2018) Reinecke et al. (2019). If a simulation failed (6 of 1848 did not converge) the missing results were substituted randomly from another simulation within the cohort to preserve the required ordering of parameter samples for the used Python implementation of Morris. This number is low enough that it does not bias the results in any significant way (Branger et al., 2015).

A converged simulation does not necessarily constitute a valid result for all computed cells. Numeric difficulties based ⁴⁰ on the model configuration (due to the selected parameter multipliers) may lead to cells with calculated h that are unreasonable. More specifically, a hydraulic head that is far above or below the land surface and/or leads to a large mass budget error. In the presented study these simulations are retained as a removal would require to either rerun simulations with a different convergence criterion (see Sect. 4) and include this in the analysis or modify the Morris method to allow removal of simulations.

Confidence intervals (95 %) are derived via bootstrapping using 1000 bootstrap resamples, following Archer et al. (1997).

3 Results

5 3.1 Sensitivity to updated GLHMYPS dataset

Global-scale hydrogeological data is limited. Figure 2 (b) shows the change in K between GLHYMPS 1.0 (Gleeson et al., 2014) and the upper layer of GLHYMPS 2.0 (Huscroft et al., 2018) where an overall increase can be observed due

- ¹⁰ to the change in unconsolidated sediments. Although unconsolidated sediments cover roughly 50 % of the world's terrestrial surface, their extent was underestimated in previous lithologic maps by half (Börker et al., 2018). The largest increase of K can be found between 50 and 70 °N because
- ¹⁵ of glacial sediments that were assigned high K values. Different lithologies, e.g. alluvial terrace sediments and glacial tills, have all been grouped into the hydrolithological category of sand. Areas of decreased conductivity are e.g. the Great Lakes, south of Hudson Bay, and parts of Somalia.
- ²⁰ The area around Hudson Bay was assumed to consist of unconsolidated sediments in GLHYMPS 1.0 (Gleeson et al., 2014) and was changed to consolidated. In Somalia, evaporites, which are known for low K, were incorporated from the Global Unconsolidated Sediments Map Database (GUM)

²⁵ (Börker et al., 2018). Furthermore, GUM provides a detailed mapping of loess and loess-like depositions, which were assigned lower K values. These regions can be observed to be the only regions with reduced K (Fig. 2 (b)). Overall, the increase in unconsolidated sediments is probably the main ³⁰ cause for the increased K.

Due to the change in K, the simulated h changes accordingly (Fig. 2(c)). In areas where the K decreased h increased e.g. eastern North America. Overall heads decreased, especially in central Russia by up to 10 to 100 m. A slight in-35 crease in head can be observed in areas with no change in

K. This can be either due to changes in groundwater flow patterns due to the overall increase in K or due to numerical noise.

Based on these results, a local sensitivity index was cal-⁴⁰ culated using Eq. (7), shown in Fig. 2 (d). White constitutes areas where either the relative change of K was zero or the head of the GLHYMPS 1.0 simulation was zero. Areas with a sensitivity index below (-)0.1 probably constitute variations that can be accounted to numerical differences in simulation

⁴⁵ outcome. Overall, h and K change in the opposite directions (positive values indicate a change into the same direction). An overall increase in K has led to a overall decrease in has the higher K values are able to transport more water for a given hydraulic gradient, especially along coastlines and

⁵⁰ mountainous areas. Increased sensitivity indexes can be observed at boundaries of areas of large spatial extent where the initial K was equal, whereas the h changes inside that area are relatively small (e.g. Arabian Peninsula). In regions where an increase in K leads to a decrease in head, an increase of h at the boundary to other hydrolithological structures can be observed. Areas with changing indexes next to each other, e.g. in the Sahara, possibly point to a numerically unstable model region with a general sensitivity to parameter changes. GLHYMPS 2.0 represents the best available global data for hydraulic conductivity, and the results of this initial experiment indicate a significant sensitivity to updating the model with this new dataset.

3.2 Monte Carlo experiments

To assess the variability of model outputs we used the Monte Carlo-like OAT experiments to analyze the outcomes of 1848 65 model realizations.

3.2.1 Variability of hydraulic head

The spatial distribution of variability in the main model output h provides insights into model stability and highlights regions which are most sensitive to parameter changes. Ob-70 servable differences between simulations can be caused by: (1) the parameter change of the OAT experiment, (2) the interactive effects due to combinations of parameter changes, (3) numerical noise (slight variations in outcome due to the nature of the numerical algorithm or floating point errors that 75 cannot be attributed to a specific parameter change), and (4) a non-optimal solution of the groundwater equation (Eq. (1)) even if the convergence criterion is met. The latter error (4) can be observed in regions of the model where a strong nonlinear relation may produce solutions that fit the convergence 80 criterion but should be considered non-valid, e.g., because of a mass-balance that is unacceptably inprecise.

Figure 4 shows the absolute coefficient of variation (ACV) of h per cell over all Monte Carlo experiments. The ACV is used to make a sound comparison of variance taking into ac-85 count the mean of the h value per cell (because the mean might be negative the absolute value is used). Yellow indicates that h changed little (mostly for regions with shallow groundwater), white to gray values indicate a growing difference in model results, and red values indicate a high variation 90 of h over all model realizations. The latter areas represent either very low R (Sahara, Australia, South Africa) or a high variance in elevations, e.g., Himalaya, Andes and the Rocky Mountains. These are expected to have a high sensitivity to parameter changes as the multiplier of E_{swb} produces the 95 highest shifts in regions with high elevation. Large changes in E_{swb} might cause a switch from gaining to losing conditions and vice versa (discussed in Sect. 3.2.2). Additionally, a change in R directly influences the conductance term C_{riv} that might also be changed by a multiplier. These combinations may yield conditions that are exceptionally challenging for the numerical solver. Switches between the two



Figure 4. Absolute coefficient of variation $(\sigma(h)\mu(|h|)^{-1})$ [%] of simulated *h* per cell over all Monte Carlo realizations. Yellow indicates that *h* results changed very little, white to gray values indicate a growing difference in model results, and red values indicate a very high variation of *h* over all model realizations.

conditions constitute a non-linearity in the equation which might require a smaller temporal step-size to be solved. In a nutshell, if an iteration leads to a gaining condition and the next to a losing condition, the switch renders the approxi-

⁵ mated heads of the preceding iterations invalid as the equation changed. In the worst case this can lead to an infinite switch between the two conditions without finding the correct solution.

Areas with a high variance in results will also produce ¹⁰ wide confidence intervals and are highlighted in Fig. A2.

Figure 5 relates the uncertainty in h, due to a change from GLHYMPS 1.0 to 2.0 to the interquartile range of h of all Monte Carlo realizations, thus uncertainty in h due to parameter variation. Parameter variation is the dominant cause for

- ¹⁵ h variability in mountainous regions, whereas the change in geologic data has a dominant impact in northern latitudes and the upper Amazon. In Australia, central Africa, and northern India the impact of increasing K is almost as high as the variability caused by the variation of parameters in the Monte
- $_{20}$ Carlo experiments. This suggests that a reduced uncertainty in K in these regions will improve the model results.

3.2.2 Variability of losing/gaining surface water bodies

Surface water bodies that provide focused, indirect groundwater recharge to the aquifer system are an impor-²⁵ tant recharge mechanism to support ecosystems alongside streams (Stonestrom, 2007). Especially in arid regions, they are important for agriculture and industrial development.

Losing or gaining surface water bodies are determined by h in relation to E_{swb} . When h drops below E_{swb} water is ³⁰ lost to the aquifer (Eq. (5)) Figure 6 shows for each grid cell the percentage of the model runs in which the surface water bodies in the cell lose water to the groundwater. Regions with a higher percentage are regions that are in losing conditions independently of the applied parameter changes.

 $_{\rm 35}$ Areas with the highest deviation in h (Fig. 4), thus the low-



Figure 5. Uncertainty in *h* caused by variability in geologic structure (dominant in blue to light blue) in relation to uncertainty in *h* caused by variability in parameters based on Monte Carlo simulations (dominant in brown to green) calculated as $\frac{|h1-h2|}{IQR(h_{mc})}$ where h1/2 is the simulated head based on GLHMYPS 1.0 and 2.0 and h_{mc} the simulated head of all Monte Carlo experiments.



Figure 6. Percentage of all Monte Carlo realizations that resulted in a losing surface water body in a specific cell.

est agreement over all model realizations, are similar to the regions where some parameter combinations lead to losing surface water bodies, while others lead to gaining surface water bodies (Fig. 6). Overall arid and mountainous regions show high percentages of Monte Carlo realizations with los- 40 ing conditions, with dominantly 20-50 % of the realizations resulting in losing surface water bodies. h in these regions falls below E_{swb} either due to low recharge or high gradients. Surface water-groundwater interaction in these regions should be more closely investigated to improve model performance. The Sahara region stands out with large areas that contain losing surface water bodies in almost all model realizations. Values close to 100 % are furthermore reached in the Great-Lakes, the Colorado Delta, the Andes, the Namib Desert, along the coast of Somalia, the Aral lake, lakes and 50 wetlands in northern Siberia, and partially in Australian wetlands. Wetlands in Australia and the Sahara are likely to be overestimated in size in the context of a steady-state model.

3.2.3 Parameter sensitivities as determined by the method of Morris

The global-scale sensitivity of h and Q_{swb} is summarized in Table 3 that lists the percentage fractions of all cells for 5 which a certain parameter has a certain rank regarding sensitivity and parameter interaction.

Overall, E_{swb} and R are the most important parameters for both model outputs over all ranks, followed by K. Q_{swb} is more sensitive to R than h, whereas h is more sensitive to E_{swb} . C_{riv} appears only dominant in the second and third rank for both model outputs. This means that for the majority of cells a change in E_{swb} and R, rather than C_{riv} dominates changes in Q_{swb} and h. K and R directly influence the cal-

culation of C_{riv} and thus show a higher sensitivity. The standard deviation of EEs (σ_i) is an aggregated measure of the intensity of the interactions of the *i*th parameter with the other parameters, representing the degree of nonlinearity in the model response to changes in the *i*th parameter Morris (1991). A high parameter interaction indicates

²⁰ that the total output variance rises due to the interaction of the parameter with other parameters.

 E_{swb} shows higher interactions for h than for Q_{swb} . C_{riv} shows a high interaction on the first rank even if it is not the dominant effect. This interaction is likely due to changes

- ²⁵ and K and R that directly influence the computation of C_{riv} . Both model outputs are sensitive to changes in R but show a relatively low degree of interaction for the first rank. A higher percentage of cells with an increased interaction of R is only visible in the second and third rank.
- ³⁰ Lakes and wetlands show low sensitivity and interaction in relation to total number of cells in Table 3 because they only exist in a certain percentage of cells. Table 4 shows the percentage fractions relative for cells with more than 25 % coverage of a lakes, global wetlands, and/or wetlands. The
- ³⁵ dominant parameter (by percentage) for all cells with respective surface water body is always E_{swb} for h (in 79.2 % of the lakes and in (79.9 %) 66.3 % of the (global)wetlands) and R (~54-77 % of all cells) for Q_{swb} . For the second rank the conductance of the surface water body $C_{lak,wet,gl.wet}$ dom-
- ⁴⁰ inated h, C_{riv} for Q_{swb} . Thus for lakes and wetlands E_{swb} and R are more relevant to h and Q_{swb} than the conductance of these surface water bodies.

3.2.4 Maps of global sensitivity

To show the spatial distribution of the parameters that affect ⁴⁵ h and Q_{swb} the most, ranked parameters were plotted for every cell in Fig. 7. The top of Fig. 7 represents the most sensitive parameters in terms of h (left) and Q_{swb} (right). Areas that should be judged with caution due to overlapping CIs are shown in Fig. A2.

⁵⁰ E_{swb} stands out for mountainous regions and regions with low recharge aligned with regions in Fig. 4 and Fig. A4 with spots of C_{riv} . E_{swb} is dominant for Q_{swb} e.g. Rocky Moun-

Table 3. Percentage fractions of simulated cells with parameter sensitivity $\mu *$ and parameter interaction σ per model output h and Q_{swb} , where the respective output is most sensitive to the listed parameter. For example h is the most sensitive to E_{swb} (Rank 1) in 57.2% of all grid cells, while K is the second most important parameter for h in 24.2% of those cells. Fractions are shown for the first three ranks.

		% of cells			D	.1. 2	
		Rar	ік І	Rar	1K Z	Rank 3	
Para.	Output	$\mu *$	σ	$\mu *$	σ	$\mu *$	σ
V	h	24.2	18.8	21.7	12.9	7.1	4.3
Λ	Q_{swb}	18.4	15.4	21.1	7.3	8.8	4.7
\mathbf{F}	h	57.2	46.3	14.8	19.9	13.4	18.9
E_{swb}	Q_{swb}	18.5	14.3	11.2	27.7	36.0	34.4
C	h	1.0	0.5	3.9	2.4	4.3	2.5
C_{lak}	Q_{swb}	0.5	0.6	2.2	0.9	2	0.9
C_{wet}	h	1.4	0.5	3.4	1.4	5.3	4.5
	Q_{swb}	0.5	0.8	3.6	2.1	4.2	2.8
C	h	0.9	0.9	1.8	10.2	8.4	8.1
$C_{gl.wet}$	Q_{swb}	0.4	0.8	2.3	15.2	9.4	7.8
C_{riv}	h	2.0	28.0	32.8	29.3	28.7	18.1
	Q_{swb}	1.4	62.6	47.8	16.2	28.8	10.0
R	h	13.4	4.1	22.7	23.6	33.8	43.2
	Q_{swb}	59.8	5.1	11.3	30.5	10.7	39.2
C_{oc}	h	1.3	1.0	0.3	0.2	0.5	0.4
	Q_{swb}	0.5	0.4	0.5	0.2	0.2	0.2

Percentage of cells with non-overlapping CIs (see App. 1 and Sect. 3.2.6) $\mu*:11.8~\%$ (h) and 13.3 % (Q_{swb}).

tains, Andes, Hijaz Mountains in Saudi Arabia and the Himalaya. R stands out in regions in the Tropical Convergence Zone with large R and in northern latitudes for Q_{swb} . K 55 seems to be equally spatially distributed for h as well as for Q_{swb} . It is most important for h in Australia, the northern Sahara, the Emirates, and across Europe. There seems to be no correlation between the initial K spatial distribution and a highly ranked K sensitivity. Areas with a dominant K are 60 possibly influenced by a high interaction with other model components (K shows a high interaction Table 3 that is also reflected spatially in Sect. 3.2.5). E_{swb} stands out in the Sahara where likely overestimated wetland extents (Reinecke et al., 2018) (Reinecke et al., 2019) have a high impact on h. Q_{swb} 65 seems to be more robust to show the effects in the highly variable regions and indicates the assumption that E_{swb} is also mainly responsible for the h variations observed in Sect. 3.2.1.

The second rank (second row in Fig. 7) shows values that ⁷⁰ are not as important as the top row but dominant over all other parameters. In the highly variable regions K and for parts of the Himalaya R are dominant in the second rank. The C_{wet} appears as dominant parameter in areas with large wetlands with a bigger impact on Q_{swb} results than on h. C_{lak} is clearly visible in parts of Nepal and along the Brahmaputra. In the Tropical Convergence Zone C_{riv} and K dominate for

		$\mu * (h)$	$\mu*($	(Q_{swb})
	% R. 1= E_{swb}	% R. 2= $C_{lak,wet,gl.wet}$	% R. 1= <i>R</i>	% R. 2=C _{riv}
Lakes	79.2	64.6	54.2	38.8
Wetlands	66.3	47.3	77.2	46.9
Gl. Wetlands	79.9	56.4	66.3	¹ 31.7

Table 4. Percentage fractions of the most frequent parameter for rank 1 and 2 of all cells with with more than 25 % coverage of a lakes, global wetland, or wetland.

 $^{1}C_{riv}$ =31.7 %, $C_{gl.wet}$ =40.6 %.

Percentage of second most frequent parameter not shown. Percentage in relation to cells with lakes, global wetland, or wetland > 25 %. Percentage-wise R. $1(\mu * (h))$ was always followed by R except for global wetlands were the second most frequent R. 1 was $C_{gl.wet}$. R. $1(\mu * (Q_{swb}))$ was followed percentage-wise by E_{swb} except for local wetlands with K, R. $2(\mu * (Q_{swb}))$ by $C_{lak,wet,gl.wet}$ except for global wetlands with C_{riv} .

 $Q_{swb},$ whereas results for h show a mix of $C_{gl.wet} \; C_{wet}$ and $C_{riv}.$

Zooming in on Europe (Fig. 8) for h, as an example, shows a similar trend to the global picture that R and K have the

- ⁵ highest impact on h along with E_{swb} . E_{swb} is dominant in mountainous regions like the Alps and the Apennines as well in regions with lots of surface water bodies e.g. southern part of Sweden in the area of lake Vättern and Vänern and in the Finnish Lakeland. R appears dominant in east Italy in the
- ¹⁰ lagoon of Venice and Marano, the Netherlands, and the wetlands in southwestern France. Almost invisible in the global picture is C_{oc} , a dominant parameter for most cells that have the ocean as boundary condition (only observable for *h*). Predominantly C_{riv} follows E_{swb} as second most important pa-¹⁵ rameter. Only visible in the second rank are the wetlands e.g. in west Scotland.

3.2.5 Maps of global parameter interaction

Similar to the spatial parameter sensitivities Fig. 9 shows the parameter interactions for h and Q_{swb} . Parallel to Fig. 7, the ²⁰ first row of Fig. 9 represents the most interactive parameters in terms of h change (left) and Q_{swb} (right). The highest interaction with other parameters can be observed for E_{swb} for regions with high h variability similar to Fig. 7. C_{riv} shows a high interaction in regions sensitive to R (compare Fig. 7) ²⁵ and is more visible for Q_{swb} .

K regions in the second rank are similar to where K already showed a high sensitivity for h (compare Fig. 7). In the Himalaya R and C_{riv} show a large spatial pattern. For Q_{swb} , $C_{gl.wet}$ is clearly visible where C_{riv} was most inter-³⁰ active before.

3.2.6 Sensitivity per GHRU

Average sensitivities and parameter interactions for each of the six GHRUs are shown in Fig. 10 (a). A dominant average per GHRU does not imply a rank 1 in each cell but rather ³⁵ provides an indication of its average importance per GHRU.

Each GHRU is described by the notation in Table 2. The shown average sensitivities and interactions are normalized

to [0,1] because the calculated $\mu *$ and σ present no absolute measure of sensitivity. Mean values of $\mu *$ and σ that are very close to zero are not shown in Fig. 10.

The values shown in Fig. 10 (a) should be judged with caution as they also include the regions Fig. A2 shown to be unreliable. Reliability means that due to overlapping CIs (any overlapping) the ranking of the parameters can't be clearly determined (compare Fig. A2 and additional explanation Fig. ⁴⁵ A1).

To judge the reliability of the outcomes per GHRU Table 2 shows the percentage of reliable results for h and Q_{swb} for each GHRU, where reliable results exclude over 80% of all sensitivity values.

Figure 10 (b) shows only cells with reliable results, based on their confidence intervals, resulting in 11.8 % of all grid cells for h and 13.3 % for Q_{swb} . GHRUs in high and very high elevations show low reliability concerning h results as expected (compare Fig. 4). Q_{swb} appears as more robust in 55 these regions.

Figure 10 (a) shows a similar picture to the two global maps (Fig. 7, 9). All GHRUs show a linear correlation of sensitivity and degree of interaction. The GHRU with average elevation, average recharge, and high K (GHRU 1) shows 60 higher average response in Q_{swb} than h. h is most sensitive to C_{riv} , and less sensitive to the other parameters. Q_{swb} is clearly most sensitive to K and $C_{gl.wet}$ and shows a high interaction in this GHRU. Lower-lying regions with average K and R (GHRU 2) show high sensitivity of h only to E_{swb} 65 with a high interaction while Q_{swb} is affected in decreasing order by $C_{gl.wet}$ and K. Results for h sensitivity in GHRU 3, with very high elevations, average K and low R, should be judged with caution because only a very low fraction is based on results with non-overlapping CIs (Table 2). Compared to 70 other GHRUs, 3 shows rather clustered sensitivities and parameter interactions. h is most sensitive to E_{swb} and R and Q_{swb} to C_{lak} , K, and C_{wet} . GHRU 4, which differs from GHRU 3 by its high but not very high land surface elevation, shows E_{swb} , K, and R as clearly most dominant and inter- 75 active parameter for Q_{swb} , followed by C_{wet} . Similar Q_{swb} is most sensitive to E_{swb} and K. In low-lying and rather flat

50

40



Figure 7. Ranking of parameter sensitivity of h (left) and Q_{swb} (right). The upper maps show the first rank, the middle the second, and the bottom the last rank by $\mu *$ values.



Figure 8. Zoom in of Europe of Fig. 7. Ranking of parameter sensitivity of h (left: rank 1, right: rank 2).

regions with high groundwater recharge (GHRU 5), sensitivities of h are close to zero except for K possibly because changes in h are to small in flat regions (compare Fig. 4) due to small h gradients. Q_{swb} is most sensitive to E_{swb} and

 $_{5} C_{gl.wet}$. GHRU 6 is relatively small and like GHRU 5 only occurs in the tropical zone (Fig. 3 (a)). In this GHRU, which differs from GHRU 5 only by K being high instead of average, the dominant parameters of Q_{swb} are similar to other GHRUs where E_{swb} is clearly the most dominant followed

¹⁰ by R and K. h shows a response to wetlands but again like in 5 a very low response to E_{swb} . Taking into account only the reliable regions changes the perception in Fig. 10 (b). GHRU 1 shows rather similar sensitivities and parameter interactions as compared to other GHRUs. *h* is most sensitive to E_{swb} , and only somewhat less sensitive to C_{riv} and C_{wet} . Q_{swb} is clearly most sensitive to C_{riv} and shows a high interaction in this GHRU. GHRU 2 shows high sensitivity of *h* only to E_{swb} with a high interaction while Q_{swb} is equally affected by *K*, E_{swb} and *R*. Results for *h* sensitivity in GHRU 3 are not very representative for the whole GHRU as only a very small fraction of cells shows reliable results (Table 2). Like in GHRU 2, Q_{swb}



Figure 9. Ranking of parameters interaction (σ of EE is an indicator for parameter interaction) based on h (left) and Q_{swb} (right). Parameters are ranked from top to bottom by Σ values.

is equally affected by by K, E_{swb} and R. GHRU 4 shows E_{swb} as clearly most dominant and interactive parameter for h, followed by K and C_{wet} . For GHRU 5, sensitivities of h could not be determined reliably possibly because changes $_{5}$ in h are to small in flat regions (compare Fig. 4) due to small h gradients. Q_{swb} is most sensitive to R (as rivers are gaining rivers that need to drain groundwater recharge) followed by K. In GHRU 6 the dominant parameters of Q_{swb} are the same as for GHRU 5 (except for E_{swb}) while h is most sen-

4 Discussion

This study presents a novel spatially distributed sensitivity analysis for a high-resolution global gradient-based groundwater model encompassing 4.3 million grid cells. While ¹⁵ these maps are challenging to interpret, they yield new ways of understanding model behaviour based on spatial differences and help to prepare calibration efforts by identifying parameters that are most influential in specific regions. Furthermore, they guide the future development of the model

²⁰ and the intended coupling efforts of the groundwater model to the hydrological model. Especially, the sensitivity of Q_{swb} and the importance of E_{swb} , which are the two major coupling components, are of interest.

However, the large number of grid cells with either statis-²⁵ tically zero sensitivity values (overlapping CI with zero) or unreliable results limit the relevance and applicability of the study results. The study suggests that the highly non-linear and conceptual approach to the surface water body conductance (in particular the sudden change of conductance between gaining and losing rivers) needs to be revised as it may affect the stability of transient model results. Additionally the results suggest that elevation of the water table of surface water bodies is a promising calibration parameter alongside with hydraulic conductivity.

The presented results need to be considered against the 35 backdrop of the high h variability of the Monte Carlo experiments (Sect. 3.2.1). Some of these simulations cannot be considered as a valid result for a h distribution. This is due to multiple model challenges: (1) the evaluated model approximates a differential equation and can show non-linear 40 behaviour for different parameterizations, (2) the equations used for rivers present a non-linear model component (switch between equations for gaining and losing conditions as well as relation to K and R), (3) the convergence criterion for the steady-state solution is solely based on a vector norm of 45 residuals (metric of changes of the solution inside the conjugate gradient approach) and maximum h change between iterations and do not contain an automated check for a reasonable mass balance. On the other hand, it is challenging to include a validation mechanism in the presented analysis 50 to alleviate these problems while maintaining a reasonable model runtime (as a stricter convergence criterion will most



Figure 10. Normalized average sensitivity and parameter interaction per GHRU for *h* and Q_{swb} (a). If a parameter is not present the mean sensitivity for that GHRU was close to zero (overlapping CI with zero). Does not include ocean parameter sensitivity. Mean characteristics, their symbols for each GHRU, and the reliability of the sensitivity measure (only μ * not σ) are shown in Table 2. (b) Only reliable results (after removing overlapping CI).

likely increase the number of necessary iterations) and/or number of necessary model runs. It is questionable whether results based on different convergence criteria can be compared. This would necessitate including the numeric stability 5 in the sensitivity analysis as well.

However, the results help to answer the research questions at hand. While overlapping CIs blur the ranking of the parameters in some regions, they still provide evidence on what parameters the calibration should focus and how the impor-

¹⁰ tance of parameters varies per region. The sensitivity of Q_{swb} to parameters, especially E_{swb} , will help to guide the future model development and coupling to the hydrological model. In general, the analysis helped to identify the elevation of surface water bodies as a focus for future research. Around 30 % of all μ * values had a confidence interval ¹⁵ that was larger than 10 % of the μ * value. This suggests that even more model runs are required and that large extents of the model experienced numerically unstable results as the spatial distribution of head variance and large confidence intervals overlap.

The selection of parameter ranges can influence the results of a sensitivity analysis significantly (Pianosi et al., 2016). Even parameters that are suspected of not being sensitive can show highly nonlinear behavior in certain parts of the parameter space that are only activated when one expands the ²⁵ ranges of the parameters. The presented ranges in this study do not explore the full assumed uncertainty range. Specifically, the small range of E_{swb} is likely influencing the out-

come of the parameter rankings. The range was chosen to allow a reasonable number of simulations to converge as the range of E_{swb} directly influences the numerical stability of the model. The presented results, however, do show that the

- ⁵ model output is highly sensitive to changes in E_{swb} in most areas of the globe. The response in mountainous regions can be attributed to applying E_{swb} as a multiplier, which has a higher impact in regions where the initial water body elevation is high. On the other hand, this is accounting for the fact
- ¹⁰ that the uncertainty of E_{swb} is largest in regions with highly variable topography per 5' grid cell.

The only previous sensitivity analysis of a global gradientbased groundwater model to out knowledge was done by de Graaf et al. (2015). Based on varying K, aquifer thick-¹⁵ ness, and R, the coefficient of variation of the steady-state hydraulic head was computed (de Graaf et al., 2015, Fig. 5).

- From that analysis it was determined that K has the highest impact and aquifer thickness the lowest. It is not clear how the coefficient of variation determined these outcomes. The ²⁰ relatively low impact of aquifer thickness was observed also
- by Reinecke et al. (2018) Reinecke et al. (2019). Therefore, this parameter was not included in this study. Both de Graaf et al. (2015) and this study show a high h variance in parts of Australia and the Sahara (de Graaf et al., 2015, Fig. 5) possibly
- ²⁵ due to the low initial R. Variations in the mountainous regions, on the other hand, are not reflected in de Graaf et al. (2015) as their analysis did not vary E_{swb} .

Besides the large h variance, which is likely the main cause for the low percentage of reliable cells, the confidence

- ³⁰ intervals of the sensitivity indices in this experiment suggest that additional simulations are necessary to determine more reliable results. Additionally, the small parameter ranges, required for stable model runs, influenced the overall outcome and might be a reason for cells with inconclusive results.
- For cells with lakes and wetlands, E_{swb} dominates over the variations in conductance for h (Table 4), confirming the importance in determining the surface water body elevation. For Q_{swb} , on the other hand, R is most influential in these cells even though it does not affect the conductance equation
- ⁴⁰ for these surface water bodies. Apparently, available recharge is driving the interaction more than it influences changes in head. In regions with high recharge (GHRU 5) Q_{swb} was more robust to parameter changes than *h*. This is possibly due to the generally lower response in Q_{swb} to changes in
- ⁴⁵ E_{swb} , which can be explained by the constant flow for losing surface water bodies (incl. rivers) as soon as h drops below E_{swb} . Thus changes is E_{swb} do not affect Q_{swb} afterwards (as long as the surface water body remains in losing conditions). Both model outcomes show a high sensitivity to R⁵⁰ while the interaction of R is only visible at the 3rd rank sug-
- gesting that if R changes other parameter changes do not influence the model response further.

Separating the complex global domain into a selected number of GHRUs enables a sensitivity analysis in accor-⁵⁵ dance with computational constraints (e.g. maximum number of core hours). It alleviates the drawbacks of global-scale multipliers while keeping a reasonable number of total simulations. The presented decomposition based on three parameters E_{swb} , K, and R was guided by the high sensitivity of model output to these parameters. Other factors like lithology and surface water body characteristics should be investigated as additional characteristics for GHRUs.

5 Conclusions

For the first time, spatially distributed sensitivities of the global steady-state distribution of hydraulic head and flows 65 between the groundwater and the surface water bodies were calculated and presented. We found the Morris sensitivity analysis method can yield insights for computationally challenging (concerning computation time and numerical difficulties) models with reasonable computational demand. This 70 study applied a novel approach for domain decomposition into GHRUs. Applying parameter multipliers simultaneously to all grid cells within each of the six GHRUs allowed a more meaningful sensitivity calculation, than it would be possible if the parameters would have varied simultaneously in all 75 grid cells, while maintaining a feasible the number of simulations.

Based on only a small fraction of grid cells for which parameters could be ranked reliably according to their importance for simulated model output, steady-state hydraulic 80 heads (h) were found to be comparably affected by hydraulic conductivity (K), groundwater recharge (R) and the elevation of the water table of surface water bodies (E_{swb}) . Rankings for individual grid cells varies, but globally none of the three dominates with respect to h. The simulated flows 85 between groundwater and surface water bodies (Q_{swb}) are clearly most sensitive to R. This is due to the model parameterization of river conductance that is computed as a function of R, assuming under steady-state conditions, groundwater discharge to rivers should tend to increase with in-90 creasing R (Eq. (5)). The results indicate that changes in R between timesteps for a fully coupled transient model could pose a challenge to the model convergence and that the equations might need to be reconsidered for a fully coupled model. In general the uncertainty due to the parameteriza- 95 tion of groundwater-surface water exchange flows (E_{swb} and $C_{riv.al.wet.wet.lak}$) needs to be further investigated as they have a high impact on h distribution and Q_{swb} .

In high mountainous regions (Rocky Mountains, Andes, Ethiopian Highlands, Arabian Peninsula, Himalaya) and regions with low recharge (Sahara, southern Africa) the computed h showed an unreasonably high variance due to the numeric instability of the simulations in these areas. In case of high elevations and thus large variations in E_{swb} or in case of low groundwater recharge, it is not possible to solve steady-state groundwater flow equations with arbitrary parameter combinations and a constant convergence parameter. Q_{swb} was found to somewhat be more robust than h in these regions. These results suggest that the parameterization of E_{swb} needs to be reconsidered and is a likely parameter for future calibration.

- ⁵ The lack of reliable data at the global scale, in particular hydraulic conductivity data with high horizontal and vertical resolution, hinders the development of global groundwater models. A simple sensitivity analysis on the impact of small changes to an existing global hydraulic conductivity dataset
- ¹⁰ (GLHYMPS 1.0 (Gleeson et al., 2014) to 2.0 (Huscroft et al., 2018)) showed that knowledge about the distribution of K is pivotal for the simulation of h as even slight changes in K may change model results by up to 100 m.

The presented study results refer to the uncoupled steady-¹⁵ state groundwater model G³M. As G³M is currently being integrated into the global hydrological model WaterGAP, future work will extend this sensitivity analysis to fully coupled transient simulations.

1 Appendix

- ²⁰ Results of the method of Morris need to be contemplated in a ranking based scheme that relies on metrics that summarize the calculated EEs. Figure A1 shows the conceptual issues that are entailed with this ranking approach. The absolute mean (μ *) of all EEs of parameter 1 (P1) might be bigger
- ²⁵ than μ * of P2 but as their CIs are overlapping a clear ranking is not possible. On the other hand it is evident that P1 and P2 are clearly more sensitive than P3. An overlapping suggests that even if the mu* values are different a ranking should be considered with care as the two parameters could
- ³⁰ be equally important or in some regions inside one GRHU their importance could be the other way around. But even if they overlap, the mu* provides a valuable measure of the overall importance of the parameters also in comparison with much less important parameters.
- Additionally, not only the overlapping should be considered but also the size of the CI in comparison to the mu*. It is a useful indicator on whether the sampling of the parameter space was to small and more simulations are required to gain a clearer picture. 15% is an arbitrary value that we

⁴⁰ considered an appropriate boundary. Other studies used 10% (Herman et al., 2013a) or 3.5% (Vanrolleghem et al., 2015). Figure A2 shows regions where the applied sampling was sufficient (CIs where smaller than 15% of the calculated μ * of the first rank) and regions where more simulations, or a

⁴⁵ more sophisticated approach to ensure numerical stability, is required.

Author contributions. RR led conceptualization, formal analysis, methodology, software, visualization, and writing of the original draft. JH, LF, SM, TT supported review and editing as well as the ⁵⁰ development of the methodology. AW supported visualization and writing of original draft of section 3.1. PD supervised the work of



Figure A1. Illustration of derivation of presented metrics. Blue circles show the two criteria used to judge the quality of the results.

RR and made suggestions regarding analysis, structure, and wording of the text and design of tables and figures.

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Figure A2. Confidence interval (95) in relation to the μ * for rank 1 of *h* and Q_{swb} . Yellow regions indicate a sufficient sampling size.

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Author Response

We thank both reviewers for their thoughtful comments and questions. They helped us in particular to improve the consistency of the manuscript, frame the scientific advances this study provides and clarify the approach.

Our answers to referees' comments are written in italics.

Response Referee #1

1.1

The working principles of the global groundwater model G3M should be explained in more details, otherwise I find it very difficult to fully understand the SA set-up and results. For example, on P. 2 L. 32, it would be good to expand a bit on the connection betweenG3M and WaterGAP (which variables are exchanged from one model to the other and why this is important to improve WaterGAP predictions). In Section 2.1 I would insert a schematic figure of the links between the key variables of the G3M model (h, Qsub, Bswb, etc.) - it would makes it easier to follow Eq. (1), (2), etc. and understand the role of the input data and parameters subject to the sensitivity analysis. Also, the mathematical descriptions in Sec. 2.1.3 to 2.1.5 is a bit messy and possibly incomplete. Variable h in Eq. (1) is undefined and there is no further equation or description of how it is calculated. Variable Q on L. 17 does not appear in Eq. (1) (unless by Q the authors actually mean Qswb). Many sentences in Sec. 2.1.3 are rather unclear - see more specific comments in the last section of my review.

The model G³M and the governing equations are described in Reinecke (2018) in full detail. Because the presented study was not intended as a model description paper we choose to keep the description as light as possible. On the other hand, we agree with Ref.1 that in order to understand the results of the SA a more thorough description is necessary. We thank the Ref. for pointing out unclear sentences in such a detailed manner (see 1.12 for corrections).

A description of variable h (hydraulic head) has been added to former Eq. (1). The full groundwater equation can be found in Reinecke (2018) Eq. (1). The equation has been added as new Eq. (1) for sake of completeness.

An additional Figure 1 has been added and the description now reads (P. 4):

$$\frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right)$$
(1)
+
$$\frac{Q}{\Delta x \Delta y \Delta z} = S_s \frac{\partial h}{\partial t}$$
(2)

Where K_{x,y,z} [LT^-1] is the hydraulic conductivity along the x,y, and z axis between the cells, S_s [L^-1] the specific storage, h the hydraulic head [L], and Q [L^3T^-1] the in- and outflows of the cells to or from external sources e.g. groundwater recharge (R and surface water body flows (Q_swb) (see also Reinecke et al. (2018) [Eq.(1,2)]).

The evaluation presented in this study is based on a steady-state variant of the model representing a quasi-natural equilibrium state, not taking into account human interference (a full description of the steady-state model and indented coupling can be found in Reinecke et al. (2018)).

The stand-alone steady-state simulations were performed as initial step to identify the dominant parameters that are also likely important for controlling transient groundwater flow.

In the fully coupled transient model h_{swb} will be changed according to calculated river discharge calculated by WaterGAP (Fig. 1).

Q_swb will be used to replace the current calculated flows in WaterGAP between groundwater and surface water bodies.



Figure 1. Parameterization and outputs of the G³M model. Where Q_swb is the flow between the aquifer and surface water bodies, h is the simulated hydraulic head, K the hydraulic conductivity, E_swb the surface water body elevation, B_swb the bottom elevation of the surface water body, C_swb the conductance of the surface water bodies, and R the groundwater recharge. In red the outputs and parameters that are foremost important for coupling.

1.2

The ultimate goal of the SA should be more clearly stated. The Introduction ends with the statement (P. 3 L. 10): "The derived global maps show ,for the first time, the sensitivity and parameter interactions of simulated hydraulic head and groundwater-surface water flows in the simulated steady-state global groundwater system to variations in these uncertain inputs." Still, this does not clarify what are these maps useful for. Will they serve to set priorities for improvement of "input data"? Or to decide which parameters should be calibrated and which can be set to default values? Or maybe as a "sanity check" test, i.e. to prove that the dominant parameters are as expected for each particular output in each particular region? This needs to be clarified. At present, the manuscript Introduction only states which "sensitivities of the model are explored" (P. 3 L. 3) but it does not say what research questions this exploration is meant to answer.

We agree with the assessment that the ultimate goal of the SA needs to be stated more clearly. The introduction has been aligned to address that.

Now reads (P. 2 L. 78-88):

Foremost, these maps help to guide future calibration efforts by identifying the most influential parameters and answer the question if the calibration should focus on different parameters for different regions helping to understand regional deviations from observations.

Additionally, they guide the further development of the model especially in respect to the coupling efforts highlighting which parameters will influence the coupled processes the most.

Lastly, they show in which regions global groundwater models might benefit the most from efforts in improving global datasets like global conductivity maps.

1.3

One of the key ideas that make SA applicable to such a spatially complex model, is the use of Global Hydrological Response Units (i.e. groups of hydrologically similar cells to which the same parameter perturbations can be applied) as described in Sec. 2.2.3. This is a simple but effective approach that could be of interest to a wide audience of modellers who deals with large-scale models and may confront similar problems when applying MC simulations or SA. Hence it should be mentioned in the Introduction or it may go unnoticed by interested readers. Also, it would probably be good to recognise that similar approaches have been used before, for example (if I get this right) by Hartman et al. 2015 (A large-scale simulation model to assess karstic groundwater recharge over Europe and the Mediterranean, GMD).

We thank the Ref. for pointing out the importance of the concept and that similar approaches have been used before.

The introduction now reads (P.2 L. 37 ff):

To address the issue of conducting global sensitivity analysis for computationally complex models we introduce the concept of Global Hydrological Response Units (GHRUs) (Sect. 2.2.3) (similar to e.g. Hartmann et al. (2015)).

Using the GHRUs we present an application of the well-established Morris method (Morris, 1991) with the Global Gradient-based Groundwater Model G³M (Reinecke et al., 2018).

1.4

Reliability and meaningfulness of the SA results. The authors say that many model runs needed to be discarded from the SA because the simulation outputs were unreasonable, and that the sensitivity indices for many cells were not reliable because estimation errors were too large. I think these two issues are very important as they may undermine the usefulness of the entire analysis. As such, they need to be explained and discussed more clearly. Specifically: P. 9 L. 4: "A converged simulation does not necessarily constitute a valid result for all computed cells. Numeric difficulties based on the model configuration (due to the selected parameter multipliers) may lead to cells with calculated h that are unreasonable." This needs further clarification. First, how is an unreasonable value of h defined? Second, what do you do with simulation runs that provide unreasonable h values? Do you retain them in the SA? If so, sensitivity estimates may be affected by simulation results that you consider unreasonable. Is this acceptable? Table 2 (last column) and Table 3 (footnote): majority of the cells do not provide "reliable" sensitivity estimates (i.e. Cls of sensitivity estimates are overlapping). Again, the criterion by which CIs are deemed overlapping and hence sensitivity estimates are considered unreliable needs to be explained more clearly. Appendix 1 covers the topic but is very concise and not very clear. The sentence on P. 22 L. 1 seems to suggest that the 'reliability criterion' is based on the fact that the CI be smaller than 15% of the calculated $\mu *$ of the first rank - if so, where is the 15% threshold coming from? And is this criterion really related with the fact that CIs overlap? I suppose one could have CIs of P2 and P3 that overlap even if each of them is smaller than 15% of P1. Figure A1 does not help clarifying the matter. The 15% threshold does not appear in there, and many other things are confusing. For example, in P2 why the text "CI

95%" only refers to half of the CI (instead of all the CI)? In P3, why σ ' comes out' of an arrow starting from the CI of μ *? Please clarify

No model runs where discarded due to unreasonable model outputs. This would be challenging in two aspects: (1) it requires a metric of what is unreasonable e.g. min, max head values and/or water budget error and rerun the simulations with e.g. a stricter convergence criterion (see discussion) and (2) an approach on how to either change the Morris method to incorporate non-valid simulations or a simulations method for the discarded simulations. Both are challenging and should be approached in future research.

This issue is now highlighted more clearly in section 2.2.4 (P. 6 L. 88 – P. 7 L. 7):

"Numeric difficulties based on the model configuration (due to the selected parameter multipliers) may lead to cells with calculated h that are unreasonable.

More specifically, a hydraulic head that is far above or below the land surface and/or leads to a large mass budget error.

In the presented study these simulations are retained as a removal would require to either rerun simulations with a different convergence criterion (see Sect. 4) and include this in the analysis or modify the Morris method to allow removal of simulations."

The overlapping CIs and the 15% criterion are two different metrics to judge the quality of the SA results. The overlapping is a binary property (any or none) and the 15% is a relation of the μ * to the CI. An overlapping suggests that even if the μ * values are different a ranking should be considered with care as the two parameters could be equally important or in some regions inside one GRHU their importance could be the other way around. But even if they overlap the μ * provides a valuable measure of the overall importance of the parameters also in comparison with much less important parameters (if the two most important overlap in CI it might be still evident that they are much more important than other parameters). The 15% is an arbitrary value that the authors considered to be a useful indicator whether the sampling of the parameter space was too small and more simulations are required to gain a clearer picture. Other publications used 10% (Herman et al., 2013) or 3.5% (Vanrolleghem et al., 2015).

The appendix was revised (incl. Figure A1) and now reads:



New Fig. A1

"An overlapping suggests that even if the mu^{*} values are different a ranking should be considered with care as the two parameters could be equally important or in some regions inside one GRHU their importance could be the other way around.

But even if they overlap, the mu^{*} provides a valuable measure of the overall importance of the parameters also in comparison with much less important parameters.

Additionally, not only the overlapping should be considered but also the size of the CI in comparison to the mu*.

It is a useful indicator on whether the sampling of the parameter space was too small and more simulations are required to gain a clearer picture.

15% is an arbitrary value that we considered an appropriate boundary. Other studies used 10% (Herman et al., 2013) or 3.5% (Vanrolleghem et al., 2015)."

The implications of "unreliable" results are now more clearly highlighted in section 3 (P. 11, L. 3):

"Reliability means that due to overlapping CIs (any overlapping) the ranking of the parameters can't be clearly determined (compare Fig. A2 and additional explanation Fig. A1)."

1.5

Last, are the SA results really useful if so many cells provide unreliable results? This is difficult for me to say given that, as pointed out in [2] above, the ultimate goal of the analysis is not totally clear. For example, if the ultimate goal was to identify the 2-3 key controls of the model behaviour in each different region, then an overlap between the Cls of the first and second ranked parameters would not be too much of the problem: the key message of which are the 2 most important parameters would still emerge clearly from the SA. So I am not suggesting that the SA results presented here are not useful - I just think the manuscript should clarify better what can and what cannot be inferred from such results, and what the implications are for the future improvement or use of the model. At present, it sounds a bit like the authors produced SA maps and draw some conclusions, then checked the Cls and realised most of the regions in those maps are actually unreliable. This is unconvincing. I would approach the issue from another angle: given the questions you wanted to answer, is still possible to answer them despite the overlapping Cls?

See 1.2 and 1.4. Furthermore, the discussion has been extended by (P. 13 L. 28 ff):

"While these maps are challenging to interpret, they yield new ways of understanding model behaviour based on spatial differences and help to prepare calibration efforts by identifying parameters that are most influential in specific regions.

Furthermore, they guide the future development of the model and the intended coupling efforts of the groundwater model to the hydrological model.

Especially, the sensitivity of Q_swb and the importance of E_swb, which are the two major coupling components, are of interest."

And P.13 L. 70 ff:

"However, the results help to answer the research questions at hand.

While overlapping CIs blur the ranking of the parameters in some regions, they still provide evidence on what parameters the calibration should focus and how the importance of parameters varies per region.

The sensitivity of Q_swb to parameters, especially E_swb, will help to guide the future model development and coupling to the hydrological model.

In general, the analysis helped to identify the elevation of surface water bodies as a focus for future research."

1.6

Global-scale hydrological models have recently moved to include these processes by implementing a gradient-based groundwater model approach (de Graaf et al., 2015; Reinecke et al., 2018)." It would be good to be a bit more specific here. How many gradient-based groundwater models are currently available at the global scale? One (to which both cited papers contributed) or two (one developed by de Graff et al 2015 and a different one by Reinecke et al 2018)? And if the Reinecke model cited here is (as I guess) the G3Mmodel that is then analysed in this paper (as introduced on L. 26), then it would be good to clarify the point. If G3M is the only (or one of the two) global model currently able to simulate global groundwater heads and flows, then the relevance of this manuscript is higher than the manuscript currently communicates.

 $G^{3}M$ is currently one of two models (the other being developed by de Graaf et al. for the global hydrological model PCRGLOBWB) that are capable to calculate gradient-based hydraulic heads and interactions to surface water bodies.

To clarify we added the following sentence (P. 1 L. 52):

This study is based on $G^{3}M$ (Reinecke 2018) one of the two global groundwater models capable of calculating hydraulic head and surface water body interaction on a global scale.

1.7

Throughout the manuscript there is some confusion around the difference between "input data" and "parameters". I understand that "input data" essentially refer to theGLHYMPS dataset, of which two versions (1.0 and 2.0) are tested and compared(point (1) on P. 3 L.3). However, such input data are used to estimate the hydraulic conductivity K, which is also one of the parameters that are later made randomly vary in the Monte Carlo experiments. Therefore there is some overlap between the two concepts (input data = parameter in the case of K, if I get this right?). This is difficult to grasp if the authors do not clarify the point. Again, having a schematic of the key relationships between variables would probably help here.

This is correct there is some overlapping and the current use of the keywords is confusing. We are thankful for the suggestion of the schematic figure to clarify the input parameters (see 1.1 new Figure 1).

Additionally, multiple uses of "input" have been replaced by "parameter" (see mark-up document).

1.8

"Based on previous experiments..." I think it would be good to add some more information about the selection of the 8 parameters to be subject to SA. Mentioning "previous experiments" is too vague. How many other parameters are there in the model that are held fixed? What did these previous experiments show that made you choose those 8 in particular? Also, if the SA is conducted by varying the parameter multipliers, then the choice of the baseline parameter values that are perturbed by the multipliers may be critical. How were this baseline values estimated?

The section was extended with the following to answer these questions (P. 5 L. 70 ff):

"Previous experiments (de Graaf et al., 2015; Reinecke et al., 2018) showed the importance of hydraulic conductivity, groundwater recharge, and surface water body elevation to the simulated hydraulic head.

Together with the highly uncertain surface water body and ocean conductance we thus selected eight model parameters presented as multipliers inTable 1.

Throughout the analysis the following parameters including the convergence criterion and spatial resolution stay fixed: global mean sea-level, bottom elevation of surface water bodies and their width, length.

The baseline parameters are assumed equally to Reinecke et al. (2018).

Hydraulic conductivity is based on a global data set (2.1.2), the conductance is calculated as previously shown (2.1.3), and the groundwater recharge baseline is equally to the mean annual values calculated by WaterGAP (2.1.1)."

1.9

P. 2 L. 30: "the Morris method does not provide the variance decomposition "The sentence suggests that not providing the variance decomposition is a problem perse, but I do not understand why that should be the case. Many global SA methods (e.g. regional SA, density-based methods, etc.) do not provide variance decomposition as they define output sensitivity based on other principles than " contribution to outputvariance" - yet they can perfectly fit their purpose. So I think this sentence is misleadingand should be revised or removed.

Was removed.

1.10

P. 6 L. 10-15: I suppose you must have used the (most common and most sensible) implementation of the Morris method where sensitivity* is given by the mean absolute value of the Elementary Effects. Still neither Eq. (6) or the text mention using absolute values. Please clarify.

*Yes, this is described in Line 15 ff. directly below equation (6): "*The total effect of the ith parameter is computed as the absolute mean of the EEs and is denoted as mu* (Campolongo et al. 2007.)"

We corrected the missing "absolute mean".

1.11

P. 15: "The number of clusters was determined based on the feasible number of model evaluations"

P. 8 L. 2: "With seven parameters per GHRU plus the ocean boundary, 10,000 basepoints were sampled in total (Campolongo et al., 2007) and optimized using Ruano etal. (2012). The experiment resulted in 1848 simulations"

This is very confusing. How is the number of clusters (n) related to the total number of model evaluations (N)? I would think: $N = r \times (n \times 8 + 1)$, where 8 is the number of parameters in Table 1 (hence $n \times 6$ gives the total number of multipliers to be sampled in the application of the Morris method) and r is the number of Elementary Effects for the Morris method. However, as the authors use n = 6 clusters and N = 1848 model evaluations, I cannot figure out a feasible value for r! This needs to be explained more clearly. Also, I do not understand what the term "base points" refer to? It clearly cannot be the number of points from with OAT perturbations are applied, so what is it?

We agree that the number of simulations need a more extensive explanation. The number of basepoints refers to the number of initial trajectories that are randomly sampled to select an optimized number of trajectories from as suggested by Campolongo et al. 2007 and Ruano et al 2012.

The paragraph reads now (P. 6 L. 50 ff):

"With seven parameters per GHRU plus the ocean boundary, 10 000 initial trajectories were sampled in total (Campolongo et al., 2007) and optimized using Ruano et al. (2012) resulting in 1848 optimized trajectories for each parameter.

Random sampling might result in non-optimal coverage of the input space; thus a high number of trajectories is sampled first and only trajectories with a maximized spread are selected (Ruano et al., 2012).

For 7 parameters (without ocean boundary), n GHRUs (6 in this paper) we get a total number of parameters k=42+1 where +1 stands for the ocean boundary, which is not varied by GHRU.

We assume 42 for the number of optimized trajectories (Ruano et al., 2012) resulting in N = r(k+1) (Campolongo et al., 2007), where N is the total number of simulation (1848)."

1.12 Typos and grammar

1.12.1

P. 1 L. 4: "the reliability of model outputs is limited by a lack of data as well as model assumptions required due to the necessarily coarse spatial resolution." Something not right with this sentence, maybe better: "the reliability of model outputs is limited by lack of data and by uncertain model assumptions that are necessary due to the coarse spatial resolution."

Now reads (P. 1 L. 6):

"However, the reliability of model outputs is limited by a lack of data and by uncertain model assumptions that are necessary due to the coarse spatial resolution."

1.12.2

P. 1 L. 14: "numerical difficulties". Unclear. Is it a problem of numerical instability? Or what else? "difficulties" is not a technical term.

Now reads "instability" (P. 1 L. 28).

1.12.3

P. 2 L. 26: "an application of with the Global ..." should be "an application of ... to the Global ..."

Corrected.

1.12.4

P. 2 L. 29: "sensitivity parameters" should be "sensitive parameters"

Corrected.

1.12.5

P. 3 L. 15 and L. 23: "to be coupled with WGHM".... "computed by WaterGAP 2.2c". I suppose WGHM and WaterGAP 2.2c are the same model, if so please use one name, otherwise explain the difference.

For clarification only WaterGAP is used now.

1.12.6

P. 3 L. 25: "to include it into a stead-state model represents a natural equilibrium "Something missing/wrong in this sentence, please revise.

Now reads (P. 3 L. 22):

"Human groundwater abstraction was not taken into account; not because it is not computed by WaterGAP but rather because there is no meaningful way to include it into a steady-state model which represents an equilibrium (abstractions do not equilibrize)."

1.12.7

P. 3 L. 26: "shown in Fig. 2(a)". Figure 2 is cited before Figure 1, which is odd. Maybe change the Figure order?

Has been moved and is now new Fig.2 (because auf new additional Fig. 1).

1.12.8

P. 4 L. 16-17: "The in- and outflows are described similar to MODFLOW as flows from the cell Q, thus losing and gaining surface water bodies (lakes, wetlands and rivers)are described as" Very unclear. "from the cell Q" seems to suggest that "Q" is the index of the cell, which from the subsequent equation clearly is not. Also, it is unclear here if the spatial unit of interest is a grid cell (as in the text) or a surface water body (as in the equation) - if there is a difference between the two? Last, the subject of the sentence changes from "flows" to "surface water bodies" but the subsequent equation defines (again) flows (Qswb) not water bodies. So maybe rephrase as "gains and losses from surface water bodies (lakes, wetlands and rivers) are described as" (?)

Q is not the index but rather the symbol for the multiple flows a cell can contain (e.g. Q_wetland, Q_river etc.).

Now reads (P. 3 L. 65ff):

"The in- and outflows Q are described similar to MODFLOW as flows from the cell: a flow from the cell to a surface water body is negative and positive if the opposite is true.

Thus gains and losses from surface water bodies (lakes, wetlands and rivers) are described as"

1.12.9

P. 4 L. 21: "For lakes (including reservoirs) Clak and wetlands Cwet, Cswb is estimated...". Unclear what is the difference between one variable and another. Maybe the authors mean: " For lakes (including reservoirs) and wetlands, the conductances Clak and Cwet are estimated ..."

Now reads (P. 3 L. 77 ff):

"For lakes (including reservoirs) and wetlands, the conductances C_lak and C_wet are estimated based on K of the aquifer and surface water body area divided by a static thickness of 5 m."

1.12.10

P. 4 L. 15-30: "To account for that we assume ... the river is the sink for all the inflow to the grid cell ... that is not transported ...". Very long, convoluted sentences that can be hardly followed - please revised.

Now reads (P. 3 L. 84-96):

"To account for that we assume for global wetlands (C_gl.wet) that only eighty percent of their maximum extent is reached in the steady-state.

Global wetlands are defined as wetlands that are recharged by streamflow coming from an upstream 5' grid cell in WaterGAP (Reinecke et al., 2018).

For gaining rivers, the conductance is quantified individually for each grid cell following an approach proposed by Miguez-Macho et al. (2007).

According to Miguez-Macho et al. (2007), the river conductance C_riv in a steady-state groundwater model needs to be set in a way that the river is the sink for all the inflow to the grid cell (R and inflow from neighbouring cells) that is not transported laterally to neighbouring cells."

1.12.11

P. 5 L. 22: "the sensitivity of caused by variability" should be: "the sensitivity of ... to the variability"

Corrected.

1.12.12

P. 5 L. 23: "The results are then compared to the variability in parameters of the MonteCarlo experiments." Unclear. I suppose what can be compared is the variations of outputs, not the variability of inputs. Hence the sentence should sound something like: "The results are then compared to the effects of parameter variability, as quantified by the Monte Carlo experiments."

Now reads (P. 5 L. 19):

"The results are then compared to the effects of parameter variability, as quantified by the Monte Carlo experiments."

1.12.13

P. 6 L. 5: "(Sect. 2)". Circular reference: this is actually Section 2!

Removed.

1.12.14

P. 6 L. 10: "model evaluation responses". Unnecessarily confusing. I would just say: "model executions".

Corrected.

1.12.15

P. 6 L. 19: "To achieve that, μ * and σ i are presented as ranked parameters". This is not understandable. What do the authors mean by "ranked parameters"? Please clarify.

Now reads (P. 5 64 ff):

"To achieve that, mu* and sigma_i are presented in this study in ranks.

Thus, values for all parameters are ranked from highest to lowest, and the parameter with the highest value is selected as the most influential parameter.

The parameter with the second highest value (rank 2) is the second most influential parameter and so on."

1.12.16

P. 6 L. 22: "we identified eight uncertain model parameters presented as multipliers in Table 1". Again, unclear. I guess this means that eight uncertain parameters were selected for the SA, and the analysis was performed by multiplying each parameter by a random multiplier (sampled from ranges specified in Table 1). If so, please clarify.

Now reads (P. 5 L. 76):

"The analysis was conducted my using randomly sampled multipliers in the ranges presented in Table 1."

1.12.17

P. 7 L. 6: "(Sect. 2.1.4)" Possibly wrong reference? E is defined in Sec. 2.1.3.

h_swb is defined in 2.1.3 but more closely discussed in 2.1.4.

We added 1.3 as reference as well.

1.12.18

P. 10 L. 3: "3.2 Monte Carlo experiments". I find it a bit confusing that the results re-ported here are sometimes referred to as "Monte Carlo experiments", some other times as "Morris method". I would choose one term (possibly the latter, as it is more precise) and stick to it.

We decided to refer to the setup as Monte Carlo experiments because the analysis also contains results that are only connected to the Morris method through its random nature e.g. the percentage of gaining and losing rivers. We wanted to emphasise that through the sensitivity analysis additional large amounts of data are created that can be analysed in the context of a classical Monte Carlo setup.

1.12.19

P. 10 L. 11: "the groundwater equation": which equation? please clarify.

Now refers to new Eq 1.

1.12.20

P. 11 L. 20:"... are determined by h in relation to Eswb." Vague. Explain what the relationship is.

Added additional sentence (P. 9 L. 4):

"When h drops below E_swb water is lost to the aquifer (Eq. (5))"

1.12.21

P. 11 L. 21: "the the surface": remove one "the"

Removed.

1.12.22

P. 11 L. 22: "independent of": should be "independently of"

Corrected.

1.12.23

P. 17 L. 3: "as most sensitive" should be "is most sensitive"

Corrected.

1.12.24

P. 18 L. 15: "grid cells with either zero sensitivity value" This is strange. If the sensitivity estimate is exactly zero, that should suggest there must be some calculation error.

Thank you for that important note. We intended to say statistically zero i.e. and overlap of the CI with zero.

The sentence has been changed and now reads (P. 13 L. 37 ff):

"However, the large number of grid cells with either statistically zero sensitivity values (overlapping CI with zero) or unreliable results limit the relevance and applicability of the study results."

1.12.25

P. 18 L. 22: "the evaluated model is a numerical model and thus behaves differently for different parameterizations" This sentence does not mean much. Every model subject to SA is a numerical model and all models behave differently if one changes the parameter values. Please clarify what you mean to say here.

Every model subjected to SA is a mathematical model. In our view a numerical model is a model that uses some sort of numerical time-stepping. We understand that the current phrasing might be misleading.

Now reads (P. 13 L. 52):

"(1) the evaluated model approximates a differential equation and can show non-linear behaviour for different parameterizations,"

Response Referee #2

2.1

Page 2 Line 22 "To the knowledge of the authors": What about Widen-Nilsson et al.(2007)?

The paper of Wilden-Nilsson et al. (2007) presents a global runoff model with different parameter sets and use the model realisations in a quasi-calibration approach. The sensitivity analysis was not carried out by applying a global sensitivity method and the paper does not show any sensitivities values.

On the other hand, we agree that the current sentence might be misleading in what we want to convey.

The manuscript has been changed and now reads (P. 2 L. 31):

"To the knowledge of the authors, the only other study that applied a global sensitivity analysis to a comparably complex global model is Chaney et al. (2015). "

2.2

Page 3 Line 8 "Elementary Effects (EE)": To improve readability, this term needs a briefexplanation.

Now reads (P. 2 L. 71):

"Elementary Effects (EE), a metric of sensitivity, are calculated and their means and variances ranked to determine global spatial distributions of parameter sensitivities and interactions."

2.3

Page 3 Line 18 "two vertical layers with a thickness of 100m": Do you mean totally 200m? What does each layer represent?

Yes in total the two layers are 200 m in thickness. Each layer represents the first 100 and 200 m of the aquifer.

Now reads (P. 2 L. 95):

"It computes lateral and vertical groundwater flows as well as surface water exchanges for all land areas of the globe except Antarctica on a resolution of 5' with two vertical layers with a thickness of each 100 m representing the aquifer."

2.4

Page 4 Line 2 "exp(-50mf-1)-1": What is m?

The SI unit meter.

2.5

Page 4 Line 16 "G3M is a conceptual model with one river in every 5' grid cell": What is a "river" in a groundwater model? Perhaps this sentence would be better read 'The interaction of groundwater and surface water bodies (lakes, wetlands, and rivers) is conceptualized in G3M as follows.

Has been removed for clarity.

2.6

Page 4 Equation 1: h must be defined. A simple schematic diagram is needed to explain h, Bswb, hswb, L, and W. Actually I still cannot clearly figure out the relationship of these terms.

See 1.1.

2.7

Page 4 Line 24 "a static thickness of 5m": Do you mean the difference between hswb and Bswb in Equation 1 is always 5m?

Yes (for lakes and wetlands).

Now reads (P. 3 L. 77):

"For lakes (including reservoirs) and wetlands, the conductances C_lak and C_wet are estimated based on K of the aquifer and surface water body area divided by a static thickness of 5 m (h_swb - B_swb = 5 m)."

2.8

Page 5 Line 1 "Eswb and hswb,riv": Define these terms.

(Lines numbers refer to initial document)

E_swb is defined in Line 1 and 2: "..(E_swb = h_swb,riv .."

h_riv is defined in Line 1 "... and h_riv the head of the river..".

h_swb is defined on page 4 line 19: "where h_swb is the head of the surface water body.

2.9

Page 5 Line 2 "These conductance equations are inherently empirical": Unclear. Equations 1-3 show physical relationships (although quite simplified). What are the "empirical" aspects?

The empirical aspects are that the connection between a groundwater and surface water is a threedimensional flow process which is being simplified to a one-dimensional flow linked through a single conductance parameter.

Now reads (P. 4 L. 3):

"These conductance equations are inherently empirical as they use a one-dimensional flow equation to represent the three-dimensional flow process that occurs between groundwater and surface water."

2.10

Page 5 Equation 4 "haq": Define this term.

Now reads h.

2.11

Page 6 Line 10 "Elementary Effect (EE) for a given value of X for the ith model input": What are the value and the input? Because this is a parameter sensitivity test, I thought X was parameter, but it didn't work. Anyway, the terms 'value' and 'input' are highly confusing to me.

Now reads (P. 5 L. 45):

"Based on these model executions, the Morris method calculates an Elementary Effect (EE) d for every trajectory of a i-th parameter (in this study parameter multipliers).

2.12

Page 6 Line 14 "y(X) the model output.": What are outputs? For example, the ground-water level (h) is an output?

Now reads (P. 5 L. 51):

"..y(X) the model output e.g. in the presented model h or Q_swb."

2.13

Page 6 Line 14 "The total effect of ith parameters": What does "total" mean here? Here the term "parameters" appears in addition to "values" and "inputs".

See 2.11 and now reads (P. 5 L. 52): "The total effect of the ith parameter is computed as the absolute mean of the EEs for all trajectories and is denoted as mu* (Campolongo et al., 2007)."

2.14

Page 6 Line 24 "Eswb in the model is higher than the range used in this study": Indeed it looks extremely small in Table 1.

Yes this is why the rest of the sentence states: "…, but the sampling range was restricted because the parameter is especially important for model convergence."

2.15

Page 8 Line 3 "optimized using Ruano et al. (2012)": Optimized to what? What was the objective function?

The objective function is the maximized spread of trajectories. See 1.11.

Added text (P. 6 L. 54 ff): "Random sampling might result in non-optimal coverage of the input space; thus a high number of trajectories is sampled first and only trajectories with a maximized spread are selected (Ruano et al., 2012)."

2.16

Page 9 Line 30 "at boundaries of large areas where K changed": What are "large areas"? Are there any "small areas"?

Now reads (P. 8 L. 9):

"Increased sensitivity indexes can be observed at boundaries of areas of large spatial extent where the initial K was equal, whereas the h changes inside that area are relatively small (e.g. Arabian Peninsula)."

2.17

Page 10 Line 12 "latter error": Do you mean the last error (4) or the latter two errors (3-4)?

Mainly 4. This has been clarified and now reads (P. 8 L. 37):

"The latter error (4) can be observed in regions of the model where a strong non-linear relation may produce solutions that fit the convergence criterion but should be considered non-valid, e.g., because of a mass-balance that is unacceptably inprecise.

2.18

Page 11 Line 4"the multiplier of Eswb produces the highest shifts in regions with high elevation that might cause a switch from gaining to losing conditions and vice versa": Hard to read

Now reads (P. 8 53 ff):

"These are expected to have a high sensitivity to parameter changes as the multiplier of E_swb produces the highest shifts in regions with high elevation.

Large changes in E_swb might cause a switch from gaining to losing conditions and vice versa (discussed in Sect.3.2.2)."

2.19

Page 11 Line 7 "these combinations may yield conditions that are exceptionally challenging for the numerical solver.": Hard to understand what the authors meant here. Clarify the logic.

Now reads (P. 8 L. 59):

"These combinations may yield conditions that are exceptionally challenging for the numerical solver.

Switches between the two conditions constitute a non-linearity in the equation which might require a smaller temporal step-size to be solved.

In a nutshell, if an iteration leads to a gaining condition and the next to a losing condition, the switch renders the approximated heads of the preceding iterations invalid as the equation changed.

In the worst case this can lead to an infinite switch between the two conditions without finding the correct solution."

2.20

Page 11Line 22 "independent of the applied parameter changes": Why is this independent? I am confused because the change in parameters should be the only source of difference in sensitivity simulations.

Regions with a higher percentage of simulations that show losing conditions can be considered to be not influenced by the applied parameter changes. Only a few of the parameter changes caused them not to be in a losing condition.

2.21

Page 12 Line 1 "lowest agreement": Do you mean the lowest percentage (0-1%) or the lowest agreement (50%)?

The sentence refers to Fig 3. Which shows an absolute coefficient of variation which is 0-4.5 %. Thus the lowest agreement of model realizations and the highest deviation in h refer to the highest percentage in this figure.

2.22

Page 15 Figure 6 "Parameters are ranked from top to bottom": Only three panels for eight parameters. What does "bottom" mean? The third or the eighth?

The maps show all 8 parameters for the first 3 ranks. To clarify figure now reads:

"The upper maps show the first rank, the middle the second, and the bottom the last rank by mu* values."

2.23

Page 18 Line 24 "a vector norm of residuals": Explain what it means.

Now reads (P. 13 L. 58):

".. based on a vector norm of residuals (metric of changes of the solution inside the conjugate gradient approach) and maximum h change between iterations and do not contain an automated check for a reasonable mass balance."

2.24

Page 19 Figure 9 "If a parameter is not present the mean sensitivity for that GHRU was close to zero": Because the axes are logarithmic, "close to zero" sounds a bit odd. Consider rephrasing the overall caption because this figure is particularly hard to understand.

See also 1.12.24

Sentence in caption now reads:

"If a parameter is not present the mean sensitivity for that GHRU was close to zero (overlapping CI with zero)."

References

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Spatially distributed sensitivity of simulated global groundwater heads and flows to hydraulic conductivity, groundwater recharge and surface water body parameterization

Robert Reinecke¹, Laura Foglia³, Steffen Mehl⁵, Jonathan D. Herman⁴, Alexander Wachholz¹, Tim Trautmann¹, and Petra Döll^{1,2}

¹Institute of Physical Geography, Goethe University Frankfurt, Frankfurt am Main, Germany

²Senckenberg Leibniz Biodiversity and Climate Research Centre Frankfurt (SBiK-F), Frankfurt am Main, Germany

³Department of Land, Air and Water Resources, University of California, Davis, USA

⁴Department of Civil & Environmental Engineering, University of California, Davis, USA

⁵Department of Civil Engineering, California State University, Chico, USA

Correspondence: Robert Reinecke (reinecke@em.uni-frankfurt.de)

Abstract. In global hydrological models, groundwater storages and flows are generally simulated by linear reservoir models. Recently, the first global gradient-based groundwater models were developed in order to improve the represen-

- 5 tation of groundwater-surface water interactions, capillary rise, lateral flows and human water use impacts. However, the reliability of model outputs is limited by a lack of data as well as model assumptions required and by uncertain model assumptions that are necessary due to the necessarily coarse
- ¹⁰ spatial resolution. The impact of data quality is presented by showing the sensitivity of a groundwater model to changes in the only available global hydraulic conductivity data-set. To better understand the sensitivity of model output to uncertain spatially distributed parameter inputsparameters, we
- ¹⁵ present the first application of a global sensitivity method for a global-scale groundwater model using nearly 2000 steadystate model runs of the global gradient-based groundwater model G³M. By applying the Morris method in a novel domain decomposition approach that identifies global hydro-
- ²⁰ logical response units, spatially distributed parameter sensitivities are determined for a computationally expensive model. Results indicate that globally simulated hydraulic heads are equally sensitive to hydraulic conductivity, groundwater recharge and surface water body elevation, though pa-
- ²⁵ rameter sensitivities vary regionally. For large areas of the globe, rivers are simulated to be either losing or gaining, depending on the parameter combination, indicating a high uncertainty of simulating the direction of flow between the two compartments. Mountainous and dry regions show a

high variance in simulated head due to numerical difficulties instabilities of the model, limiting the reliability of computed sensitivities in these regions. This instability is likely caused by the uncertainty in surface water body elevation. We conclude that maps of spatially distributed sensitivities can help to understand complex behaviour of models that incorporate data with varying spatial uncertainties. The findings support the selection of possible calibration parameters and help to anticipate challenges for a transient coupling of the model.

1 Introduction

Global groundwater dynamics have significantly changed ⁴⁰ due to human withdrawals, and are projected to continue due to climate change (Taylor et al., 2013). Groundwater withdrawals have led to lowered water tables, decreased base flows, and groundwater depletion around the globe (Konikow, 2011; Scanlon et al., 2012; Wada et al., 2012; ⁴⁵ Döll et al., 2014; Wada, 2016). To represent groundwatersurface water body interactions, lateral and vertical flows, and human water use impacts on head dynamics, it is necessary to simulate the depth and temporal variation of the groundwater table. Global-scale hydrological models have ⁵⁰ recently moved to include these processes by implementing a gradient-based groundwater model approach (de Graaf et al., 2015; Reinecke et al., 2018). This study is based on G³M (Reinecke et al., 2018) one of the two global groundwater models capable of calculating hydraulic head and surface water body interaction on a global scale. However, the lack of available input parameter data and the necessary conceptual assumptions due to the coarse spatial resolution limit the s reliability of model output. These substantial uncertainties

suggest an opportunity for diagnostic methods to prioritize efforts in data collection and parameter estimation.

Sensitivity analysis is a powerful tool to assess how uncertainty in model inputs parameters affects model outcome, 10 and can provide insights about how the interactions between

- parameters influence the model results (Saltelli et al., 2008). Sensitivity methods can be separated into two classes: local and global methods. Local methods compute partial derivatives of the output with respect to an input factor at a fixed
- ¹⁵ point in the input space. By contrast, global methods explore the full input space, though at higher computational costs (Pianosi et al., 2016). The large number of model evaluations required can render global methods unfeasible for computationally demanding models, though increased computational
 ²⁰ resources have led to more widespread application e.g.
- (Herman et al., 2013b, a; Ghasemizade et al., 2017)(Herman et al.groundwate Gharfareizwater interactions. The parameters are For this reason, existing studies of global models either focus on exploring uncertainties by running their model with a limited set of different inputs for a quasi local sensitivity
- ²⁵ analysis (Wada et al., 2014; Müller Schmied et al., 2014, 2016; Koirala et al., 2018) or applying computationally inexpensive methods based on a limited set of model evaluations (Schumacher et al., 2015). For example, de Graaf et al. (2015, 2017) determined the coefficient of variation for head
- ³⁰ results in a global groundwater model with 1000 model runs evaluating the impact of varying aquifer thickness, saturated conductivity and groundwater recharge. To the knowledge of the authors, Chaney et al. (2015) is the only study of a global (land surface) model which carried out an extensive
- ³⁵ global the only other study that applied a global sensitivity analysis to assess how model parameter uncertainty affects prediction of hydrologic extremesa comparably complex global model is Chaney et al. (2015). An overview of the application of different sensitivity sensitivity analysis methods ⁴⁰ for hydrological models can be found in Song et al. (2015);
- Pianosi et al. (2016).

We To address the issue of conducting global sensitivity analysis for computationally complex models we introduce the concept of Global Hydrological

- ⁴⁵ Response Units (GHRUs) (Sect. 2.2.3) (similar to e.g. Hartmann et al. (2015)). Using the GHRUs we present an application of the well-established Morris method (Morris, 1991) with to the Global Gradient-based Groundwater Model G³M (Reinecke et al., 2018). The Morris method has
- ⁵⁰ been successfully applied to a variety of models, ranging from hydrology (Zhan et al., 2013) to ecology models (Cariboni et al., 2007). It requires significantly fewer model runs, compared to other global methods, to provide a meaningful ranking of sensitivity sensitive parameters (Herman

55 et al., 2013a) enabling the exploration of computationally

demanding models. One drawback is that the Morris method does not provide the variance decomposition obtained with variance-based measures like Sobol (1993).

G³M uses input from, and it is intended to be coupled and integrated into, the global hydrological model WaterGAP ⁶⁰ Global Hydrology Model (WGHM) (Döll et al., 2014). This study investigates the sensitivity of steady-state hydraulic heads and exchange flows between groundwater and surface water to variations in main model <u>inputs parameters</u> (e.g. groundwater recharge and other model parameters like the ⁶⁵ riverbed conductance).

Sensitivities of the model are explored in three steps: (1) To understand the impact of improved input data, in particular hydraulic conductivity, we investigate the changes in simulated hydraulic head that result from changing the hydraulic conductivity data from the GLHYMPS 1.0 dataset (Gleeson et al., 2014) to 2.0 (Huscroft et al., 2018). (2) Based on prior experiments (de Graaf et al., 2015; Reinecke et al., 2018) eight parameters are selected for a Monte Carlo experiment to investigate sensitivities of simulated hydraulic head and 75

sampled with a newly developed global region-based sampling strategy and build the framework for the (3) Morris analysis. Elementary Effects (EE), a metric of sensitivity, are calculated and their means and variances ranked to determine 80 global spatial distributions of parameter sensitivities and interactions. The derived global maps show, for the first time, the sensitivity and parameter interactions of simulated hydraulic head and groundwater-surface water flows in the simulated steady-state global groundwater system to variations 85 in these uncertain inputsuncertain parameters. Foremost, these maps help future calibration efforts by identifying the most influential parameters and answer the question if the calibration should focus on different parameters for different regions helping to understand regional deviations 90 from observations. Additionally, they guide the further development of the model especially in respect to the coupling efforts highlighting which parameters will influence the coupled processes the most. Lastly, they show in which regions global groundwater models might benefit the 95 most from efforts in improving global datasets like global conductivity maps.

2 Methodology and Data

2.1 The model G³M

 $G^{3}M$ (Reinecke et al., 2018) is a global groundwater model ¹⁰⁰ intended to be coupled with WGHM-WaterGAP (Döll et al., 2003, 2012, 2014; Müller Schmied et al., 2014) and is based on the Open Source groundwater modelling framework $G^{3}M$ -f¹(Reinecke, 2018). It computes lateral and vertical groundwater flows as well as surface water exchanges for ¹⁰⁵

¹Available on globalgroundwatermodel.org

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all land areas of the globe except Antarctica and Greenland on a resolution of 5' with two vertical layers with a thickness of each 100 m representing the aquifer. The groundwater flow between cells is computed as

$$= \frac{\partial}{\partial x} \left(K_x \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial h}{\partial z} \right)$$
(1)

$$+\frac{Q}{\Delta x \Delta y \Delta z} = S_s \frac{\partial h}{\partial t}$$
(2)

where $K_{x,y,z}$ [LT⁻¹] is the hydraulic conductivity along the x,y, and z axis between the cells with size $\Delta x \Delta y \Delta z$, S_s [L⁻¹] the specific storage, h the hydraulic head [L], and Q to [L³T⁻¹] the in- and outflows of the cells to or from external

- sources e.g. groundwater recharge (R and surface water body flows (Q_{swb}) (see also Reinecke et al. (2018)[Eq.(1,2)]). The evaluation presented in this study is based on a steady-state variant of the model representing a quasi-natural equilib-
- ¹⁵ rium state, not taking into account human interference (a full description of the steady-state model and indented coupling can be found in Reinecke et al. (2018)). The stand-alone steady-state simulations were performed as initial step to identify the dominant parameters that are also likely important for a standard state of the standard state.
- ²⁰ tant for controlling transient groundwater flow. In the fully coupled transient model h_{swb} will be changed according to calculated river discharge calculated by WaterGAP (Fig. 1). Q_{swb} will be used to replace the current calculated flows in WaterGAP between groundwater and surface water bodies.

25 2.1.1 Groundwater recharge

Groundwater recharge (R) is based on mean annual R computed by WaterGAP 2.2c for the period 1901-2013. Human groundwater abstraction was not taken into account; not because it is not computed by WaterGAP but rather because ³⁰ there is no meaningful way to include it into a steady-state model represents a natural equilibrium-which represents an

equilibrium (abstractions do not equilibrize).

2.1.2 Hydraulic conductivity

- Hydraulic conductivity (K) is derived from GLHYMPS 2.0 ³⁵ (Huscroft et al., 2018) (shown in Fig. 2 (a)). The original data was gridded to 5' by using an area-weighted average and used as K of the upper model layer. For the second layer, K of the first layer is reduced by an e-folding factor f used by Fan et al. (2013) (a calibrated parameter based on terrain ⁴⁰ slope) assuming that conductivity decreases exponentially
- with depth. Conductivity of the lower layer is calculated by multiplying the upper layer value by $exp(-50mf^{-1})^{-1}$ (Fan et al., 2013, Eq. 7).
- Currently only two datasets, GLHMYPS 1.0 and 2.0 ⁴⁵ (Gleeson et al., 2014; Huscroft et al., 2018), are available and are used by a number of continental and global models (de Graaf et al., 2015; Maxwell et al., 2015; Keune et al.,

2016; Reinecke et al., 2018). GLHMYPS 1.0 (Gleeson et al., 2014) is compiled based on the global lithology map GLiM (Hartmann and Moosdorf, 2012) and data from 92 regional groundwater models and derives permeabilities (for the first 100 m vertically) based on Gleeson et al. (2011), differentiating the sediments into the categories fine-, coarse-grained, mixed, consolidated, and unconsolidated. Permafrost regions are assigned a K value of 10^{-13} ms⁻¹ based on Gruber (2012). Areas of deeply weathered laterite soil (mainly in tropical regions) are mapped as unconsolidated sediments as they dominate K (Gleeson et al., 2014).

The global permeability map was further improved with the development of GLHYMPS 2.0 by Huscroft et al. (2018). ⁶⁰ A two-layer set up was established in GLHYMPS 2.0 with the lower layer matching the original GLHYMPS 1.0. For the upper layer in GLHYMPS 2.0, a global database of unconsolidated sediments (Börker et al., 2018) was integrated into GLHYMPS 2.0 resulting in overall slightly increased K(Fig. 2 (a)). The thickness of the upper layer was deduced from the *depth-to-bedrock* information available from Soil-Grid (Hengl et al., 2017). No thickness was assigned to the lower layer.

2.1.3 Surface water body conductance

 $G^{3}M$ is a conceptual model with one river in every 5' grid eell. The in- and outflows Q are described similar to MOD-FLOW as flows from the cellQ, thus losing and gaining : a flow from the cell to a surface water body is negative and positive if the opposite is true. Thus gains and losses from surface water bodies (lakes, wetlands and rivers) are described as

$$Q_{swb} = \begin{cases} C_{swb}(h_{swb} - h) & h > B_{swb} \\ C_{swb}(h_{swb} - B_{swb}) & h \le B_{swb} \end{cases}$$
(3)

where <u>h</u> is the simulated hydraulic head, h_{swb} is the head of the surface water body, and B_{swb} the bottom elevation. The conductance C_{swb} of the surface water body bed is calculated as

$$C_{swb} = \frac{KLW}{h_{swb} - B_{swb}} \tag{4}$$

where K is the hydraulic conductivity, L the length and W the width of the surface water body. For lakes (including ⁸⁵ reservoirs) C_{lak} and wetlands C_{wet} , C_{swb} is and wetlands, the conductances C_{lak} and C_{wet} are estimated based on K of the aquifer and surface water body area divided by a static thickness of 5 m ($h_{swb} - B_{swb} = 5m$). For a steady-state simulation the surface water body data shows the maximum spatial extent of wetlands, an extent that is seldom reached in particular in case of wetlands in dry areas. To account for that we assume for global (surface water bodies recharged by streamflow coming from an upstream 5' grid cell) wetlands ($C_{ql.wet}$) that only eighty percent of their maximum extent ⁹⁵

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Figure 1. Parameterization and outputs of the G^3M model. Where Q_{swb} is the flow between the aquifer and surface water bodies, *h* is the simulated hydraulic head, *K* the hydraulic conductivity, E_{swb} the surface water body elevation, B_{swb} the bottom elevation of the surface water body. C_{swb} the conductance of the surface water bodies, and *R* the groundwater recharge. In red the outputs and parameters that are foremost important for coupling.



Figure 2. Impact of hydraulic conductivity datasets GLHYMPS 1.0 and GLHYMPS 2.0. (a) GLHYMPS 2.0 $[ms^{-1}]$, (b) *K* differences, expressed as *K*(GLHYMPS 2.0)/*K*(GLHYMPS 1.0). Blue indicates higher values in GLHYMPS 2.0. (c) *h*(GLHYMPS 2.0) minus *h*(GLHYMPS 1.0) [m], (d) the sensitivity of *h* to change in the GLHYMPS dataset based on Eq. (7) (white indicates that no index could be calculated).

is reached in the steady-state. Global wetlands are defined as wetlands that are recharged by streamflow coming from an upstream 5' grid cell in WaterGAP (Reinecke et al., 2018). For gaining rivers, the conductance is quantified individu-

⁵ ally for each grid cell following an approach proposed by Miguez-Macho et al. (2007). The value of river conductance C_{riv} , according According to Miguez-Macho et al. (2007), in a groundwater flow the river conductance C_{riv} in a steady-state groundwater model needs to be set to such a values that, for steady-state conditions, in a way that the river is the sink for all the inflow to the grid cell (R and inflow from neighbouring cells) that is not transported laterally to neighbouring cellssuch that.

$$C_{riv} = \frac{R + Q_{eq_{lateral}}}{h_{eq} - h_{riv}} \quad h > h_{riv} \tag{5}$$

where $Q_{eq_{lateral}}$ is the lateral flow based on the equilibrium ¹⁵ head h_{eq} of Fan et al. (2013) and h_{riv} the head of the river $(E_{swb} = h_{swb,riv}$ in Table 1). These conductance equations are inherently empirical as they use a one-dimensional flow equation to represent the three-dimensional flow process that occurs between groundwater and surface water. Future efforts will investigate using approaches appropriate for large scale models, such as described by Morel-Seytoux et al. 5 (2017). An extensive description on the chosen equations and

implications can be found in Reinecke et al. (2018).

2.1.4 Surface water body elevation

The vertical location of surface water bodies has a great impact on model outcome (Reinecke et al., 2018). Their vertical location h_{swb} is set to the 30th percentile of the 30" land surface elevation values of Fan et al. (2013) per 5' cell, e.g. the elevation that is exceeded by 70 % of the thousand hundred 30" elevation values within one 5' cell. B_{swb} is calculated based on that head elevation with different values for wetlands and lakes (Reinecke et al., 2018, Table 1). For rivers, B_{swb} is equal to $h_{riv} - 0.349 \times Q_{bankfull}^{0.341}$ (Allen et al., 1994), where $Q_{bankfull}$ is the bankfull river discharge in the 5' grid cell (Verzano et al., 2012).

2.1.5 Ocean boundary

20 The outer boundary condition in the model is described by the ocean and uses an equation similar to MODFLOW's general head boundary condition as flow

$$Q_{ocean} = C_{oc}(h_{ocean} - h_{aq}) \tag{6}$$

where h_{ocean} is the elevation of the ocean water table set 0 ²⁵ m worldwide and C_{oc} the conductance of the boundary condition set to $10^{-6}m^2s^{-1}$ based on average K and aquifer thickness.

2.2 Sensitivity Analysis

2.2.1 Sensitivity of simulated head to choice in hydraulic conductivity dataset

Parameterization of aquifer properties based on hydrogeological data is an important decision in groundwater modeling. We first investigate the effect of switching to a newly available global permeability dataset to explore the sensitivity of simulated budgenlin head (h) coursed by to the unri-

 $_{35}$ ity of simulated hydraulic head (h) caused by to the variability in geologic data. The results are then compared to the variability in parameters of effects of parameter variability, as quantified by the Monte Carlo experiments.

GLHYMPS 2.0 (Huscroft et al., 2018) provides an update 40 of the only available global permeability map (Gleeson et al., 2014). To quantify how the new hydraulic conductivity estimates change the simulation outcome of the groundwater model we apply a basic sensitivity method.

$$S = \frac{\frac{h_2 - h_1}{h_1}}{\frac{K_2 - K_1}{K_1}} \tag{7}$$

where the sensitivity S of h to a change in K is calculated ⁴⁵ based on the change in h (h_1 is the hydraulic head calculated with GLHYMPS 1.0 and h_2 with GLHYMPS 2.0) and change in K_1 and K_2 the conductivity based on GL-HYMPS 1.0 and 2.0, respectively.

2.2.2 Sensitivity of head and surface water body flow to 50 choice in parameters

Along with K, additional parameters influence the model outcome(Sect. 2). In this study we apply the method of Morris (Morris, 1991) as a screening method to identify which parameters are most important for the two main model out-55 comes, namely h and groundwater-surface water interactions (Q_{swb}) . The Morris method provides a compromise between accuracy and computational cost in comparison to other Monte Carlo like methods (Campolongo et al., 2007). Each model execution represents an individually randomized One 60 Factor At a Time (OAT) experiment, where one parameter is changed per simulation. Based on these model evaluation responses executions, the Morris method calculates an Elementary Effect (EE) d for a given value of X for the every trajectory of a *i*th model input-th parameter (in this study 65 parameter multipliers).

$$d_i(\mathbf{X}) = \left(\frac{y(X_1, \dots, X_{i-1}, X_i + \Delta, X_{i+1}, \dots, X_k) - y(\mathbf{X})}{\Delta}\right)$$
(8)

where Δ is the trajectory step size for the parameter multiplier X_i , X is the vector of model parameters multipliers of size k and $y(\mathbf{X})$ the model output e.g. in the presented model 70 h or Q_{sub} . The total effect of the *i*th parameter is computed as the absolute mean of the EEs for all trajectories and is denoted as μ * (Campolongo et al., 2007). The standard deviation of EEs (σ_i) is an aggregated measure of the intensity of the interactions of the *i*th parameter with the other pa-75 rameters, representing the degree of non-linearity in model response to changes in the *i*th parameter (Morris, 1991). The derived metrics $\mu *$ and σ_i both are measures of intensity (higher values are more sensitive/interactive) and do not represent absolute values of sensitivity. Both can only be inter- 80 preted meaningfully in comparison with values derived for other parameters.

To achieve that, $\mu *$ and σ_i are presented as in this study in *rankedparameters*. $\mu *$ *ranks*. Thus, values for all parameters are ranked from highest to lowest, and the parameter with the highest value is selected as the most influential parameter. The parameter with the second highest value (*rank* 2) is the second most influential parameter and so on.

Based —	on		ous	-experiments	
(de Graaf et	al., 2015;	Reinecke et a	al., 2018) w	e	90
identified	-eight	uncertain	model		
presented	as mult	ipliers in	-Previous	experiments	
(de Graaf et	al., 2015;	Reinecke et a	al., 2018) sh	lowed the	

importance of hydraulic conductivity, groundwater recharge, and surface water body elevation to the simulated hydraulic head. Together with the highly uncertain surface water body and ocean conductance we thus selected eight model

5 parameters for the sensitivity analysis. The analysis was conducted my using randomly sampled multipliers in the ranges presented in Table 1.

Throughout the analysis the following parameters including the convergence criterion and spatial resolution

- 10 stay fixed: global mean sea-level, bottom elevation of surface water bodies and their width, length. The baseline parameters are assumed equally to Reinecke et al. (2018). Hydraulic conductivity is based on a global data set (2.1.2), the conductance is calculated as previously shown (2.1.3),
- 15 and the groundwater recharge baseline is equally to the mean annual values calculated by WaterGAP (2.1.1). Parameter ranges were chosen to ensure that a high percentage of model realizations converge numerically. For example, the uncertainty of E_{swb} in the model is higher than the ranged
- 20 used in this study, but the sampling range was restricted because the parameter is especially important for model convergence. Furthermore, the chosen river conductance approach uses R as input parameter and includes a nonlinear threshold between losing and gaining surface water bodies,
- 25 which strongly affects numeric stability. As in any global sensitivity analysis, the choice of parameter ranges involves some subjectivity that may influence the ranking of sensitive parameters in the results.

Global hydrological response units 2.2.3

- 30 Even though the number of model evaluations are comparably less for OAT-based experiments than for All-At-a-Time (Pianosi et al., 2016), varying every parameter independently in every spatial grid cell leads to an unfeasible amount of model runs. On the other hand, the use of global multipliers
- 35 that vary a parameter uniformly for all computational cells may lead to inconclusive results, as the sensitivity for every cell to this change is spread to the whole computational domain. A possible solution would be to separate the globe into zones with similar geological characteristics based on
- 40 the GLHYMPS dataset, but this may still result in an infeasible number of required simulations. Each simulation takes about 30 min to 1 h on a commodity computer (more if the parameters hinder a fast convergence).

To overcome these limitations, we introduce the use of a 45 Global Hydrological Response Unit (GHRU). Every GHRU represents a region of similar characteristics regarding three characteristics: E_{swb} (Sect. 2.1.3, 2.1.4), K (Sect. 2.1.2), and R (Sect. 2.1.1). This does not constitute a zoning approach often used for calibration in traditional regional groundwater

50 modelling, only a separation into parameter multipliers. All multipliers for a given parameter for all regions are based on the same random distribution inside a given range of uncertainty for that parameter. Characteristics for each model cell



Figure 3. Map of k-means clustering categories each representing a GHRU (a). Each color identifies a region where the combination of all three parameters is similar.

are normalized to [0,1] and used to create a 3d point space (based on the three characteristics for each model cell). We 55 apply a k-means (Lloyd, 1982) clustering algorithm to identify these regions.

K-means clustering partitions n points into k clusters where each point belongs to the cluster with a minimized pairwise squared distance to the mean in a cluster. Figure 3 (a) shows a map of k-means clustering (6 clusters) categories based on normalized three-dimensional space of E_{swb} , K, and R per grid cell.

The number of clusters was determined based on the feasible number of model evaluations. k-means constitutes an 65 unsupervised machine learning approach that builds the required number of clusters automatically, thus it is necessary afterwards to examine what main characteristics these clusters represent (shown in Table 2). Characteristics are encoded as relative values (high (\uparrow), medium (\sim), low (\downarrow)) of the three 70 input parameter values based on their mean value per cluster. These characteristics are used to connect calculated parameter sensitivities to GHRUs when analyzing the results of the experiment.

2.2.4 Experiment Configuration

With seven parameters per GHRU plus the ocean boundary, 10 000 base points initial trajectories were sampled in total (Campolongo et al., 2007) and optimized using Ruano et al. (2012) - resulting in 1848 optimized trajectories for each parameter. Random sampling might result in 80 non-optimal coverage of the input space; thus a high number of trajectories is sampled first and only trajectories with a maximized spread are selected (Ruano et al., 2012). For 7 parameters (without ocean boundary), n GHRUs (6 in this paper) we get a total number of parameters k = 42 + 185 where +1 stands for the ocean boundary, which is not varied by GHRU. We assume 42 for the number of optimized trajectories (Ruano et al., 2012) resulting in N = r(k+1)(Campolongo et al., 2007), where N is the total number of simulation (1848).

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Parameter	P. Unit	Multiplier Range	Description
K	$LT^{-1}LT^{-1}$	0.1 - 100	Saturated hydraulic conductivity
E_{swb}	⊬ L	$10^{-0.001}$ - $10^{0.001}$	SWB elevation
C_{lak}	$L^2 T^{-1} L^2 T^{-1}$	0.5 - 2	Conductance of lakebed
C_{wet}	$\frac{L^2 T^{-1}}{L^2 T^{-1}} L^2 T^{-1}$	0.5 - 2	Conductance of wetland bed
$C_{gl.wet}$	$L^2 T^{-1} L^2 T^{-1}$	0.5 - 2	Conductance of global wetland bed
C_{riv}	$L^2 T^{-1} L^2 T^{-1}$	0.5 - 2	Conductance of riverbed
R	$LT^{-1}LT^{-1}$	0.5 - 2	Groundwater recharge
C_{oc}	$\frac{L^2 T^{-1}}{L^2 T^{-1}}$	0.1 - 10	Conductance of the ocean boundary

Table 1. Range of parameter multipliers used in the Morris experiments. Each parameter multiplier is sampled in log space $(\log_{10}(Multiplier))$ with sampling based on Campolongo et al. (2007) and optimized with Ruano et al. (2012).

 C_{oc} is equal for all ocean cells

Table 2. Mean values of GHRU characteristics and their summarized description, where \uparrow is read as a relatively high value, \sim as medium, and \downarrow as low; e.g. $\uparrow\uparrow$ E indicates a cluster with very high and relatively high (\uparrow) average E_{swb} . Additionally, the last two columns show the percentage of cells per GHRU where μ * of h and Q_{swb} could be reliably determined (described in SeeSect. 3.2.6).

					% of rel	iable $\mu *$
GHRU	$\mu(E_{swb})$ [mm]	$\mu(K)[$ m/day $m day^{-1}]$	$\mu(R)[$ mm/day $mm day^{-1}]$	GHRU description	h	Q_{swb}
1	454	10^{-4}	0.15	\sim E, \uparrow K, \sim R	9.54 %	6.58 %
2	286	10^{-6}	0.15	\downarrow E, ~ K, ~ R	12.07 %	14.41 %
3	4107	10^{-6}	0.13	$\uparrow\uparrow$ E, \sim K, \downarrow R	0.08~%	4.09 %
4	1355	10^{-6}	0.11	\uparrow E, \sim K, \downarrow R	3.17 %	17.19 %
5	303	10^{-6}	1.24	\downarrow E, ~ K, \uparrow R	31.62 %	26.37 %
6	194	10^{-4}	1.25	\downarrow E, \uparrow K, \uparrow R	29.00 %	14.36 %

The experiment resulted in 1848 simulations with an overall runtime of two months on a machine with 20 computational cores (enabled hyper-threading) and 188 GB RAM. Each simulation required about 8 GB of RAM and was assigned four computational threads while running the simulations in cohorts of 10 simulations at once. Each simulation was an OAT experiment (an extended explanation of OAT and other sensitivity experiment setups and methods can be found in Pianosi et al. (2016)). Changes in parameto ters were stacked over all experiments. Thus, an experiment

- may have changed R (also affecting C_{riv} for gaining conditions) while containing a C_{riv} multiplier from a previous experiment. Sampling and analysis was implemented with the Python library *SALib* (Herman and Usher, 2017). For each
- ¹⁵ experiment, the model was run until it reached an equilibrium state (steady-state model). All other parameters and convergence criteria can be found in Reinecke et al. (2018). If a simulation failed (6 of 1848 did not converge) the missing results were substituted randomly from another simulation
- ²⁰ within the cohort to preserve the required ordering of parameter samples for the used Python implementation of Morris. This number is low enough that it does not bias the results in any significant way (Branger et al., 2015).

A converged simulation does not necessarily constitute ²⁵ a valid result for all computed cells. Numeric difficulties based on the model configuration (due to the selected parameter multipliers) may lead to cells with calculated h that are unreasonable. More specifically, a hydraulic head that is far above or below the land surface and/or leads to a large mass budget error. In the presented study these simulations are retained as a removal would require to either rerun simulations with a different convergence criterion (see Sect. 4) and include this in the analysis or modify the Morris method to allow removal of simulations.

Confidence intervals (95 %) are derived via bootstrapping using 1000 bootstrap resamples, following Archer et al. (1997).

3 Results

3.1 Sensitivity to updated GLHMYPS dataset

Global-scale hydrogeological data is limited. Figure 2 (b) ⁴⁰ shows the change in *K* between GLHYMPS 1.0 (Gleeson et al., 2014) and the upper layer of GLHYMPS 2.0 (Huscroft et al., 2018) where an overall increase can be observed due to the change in unconsolidated sediments. Although unconsolidated sediments cover roughly 50 % of the world's terrestrial surface, their extent was underestimated in previous lithologic maps by half (Börker et al., 2018). The largest increase of *K* can be found between 50 and 70 °N because

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of glacial sediments that were assigned high K values. Different lithologies, e.g. alluvial terrace sediments and glacial tills, have all been grouped into the hydrolithological category of sand. Areas of decreased conductivity are e.g. the

- 5 Great Lakes, south of Hudson Bay, and parts of Somalia. The area around Hudson Bay was assumed to consist of unconsolidated sediments in GLHYMPS 1.0 (Gleeson et al., 2014) and was changed to consolidated. In Somalia, evaporites, which are known for low K, were incorporated from
- 10 the Global Unconsolidated Sediments Map Database (GUM) (Börker et al., 2018). Furthermore, GUM provides a detailed mapping of loess and loess-like depositions, which were assigned lower K values. These regions can be observed to be the only regions with reduced K (Fig. 2 (b)). Overall, the
- 15 increase in unconsolidated sediments is probably the main cause for the increased K.

Due to the change in K, the simulated h changes accordingly (Fig. 2(c)). In areas where the K decreased h increased e.g. eastern North America. Overall heads decreased, espe-

- 20 cially in central Russia by up to 10 to 100 m. A slight increase in head can be observed in areas with no change in K. This can be either due to changes in groundwater flow patterns due to the overall increase in K or due to numerical noise.
- Based on these results, a local sensitivity index was cal-25 culated using Eq. (7), shown in Fig. 2 (d). White constitutes areas where either the relative change of K was zero or the head of the GLHYMPS 1.0 simulation was zero. Areas with a sensitivity index below (-)0.1 probably consti-
- 30 tute variations that can be accounted to numerical differences in simulation outcome. Overall, h and K change in the opposite directions (positive values indicate a change into the same direction). An overall increase in K has led to a overall decrease in h as the higher K values are able
- 35 to transport more water for a given hydraulic gradient, especially along coastlines and mountainous areas. Increased sensitivity indexes can be observed at boundaries of large areas where areas of large spatial extent where the initial K changed was equal, whereas the h changes inside that
- 40 area are relatively small (e.g. Arabian Peninsula). In regions where an increase in K leads to a decrease in head, an increase of h at the boundary to other hydrolithological structures can be observed. Areas with changing indexes next to each other, e.g. in the Sahara, possibly point to a numeri-
- 45 cally unstable model region with a general sensitivity to parameter changes. GLHYMPS 2.0 represents the best available global data for hydraulic conductivity, and the results of this initial experiment indicate a significant sensitivity to updating the model with this new dataset. Impact of hydraulic 50 conductivity datasets GLHYMPS 1.0 and GLHYMPS 2.0.
- (a) GLHYMPS 2.0 ms⁻¹, (b) K differences, expressed as K(GLHYMPS 2.0)/K(GLHYMPS 1.0). Blue indicates higher values in GLHYMPS 2.0. (c) h(GLHYMPS 2.0) minus h(GLHYMPS 1.0) m, (d) the sensitivity of h to

change in the GLHYMPS dataset based on Eq. (7) (white 55 indicates that no index could be calculated).

3.2 Monte Carlo experiments

To assess the variability of model outputs we used the Monte Carlo-like OAT experiments to analyze the outcomes of 1848 model realizations.

Variability of hydraulic head 3.2.1

The spatial distribution of variability in the main model output h provides insights into model stability and highlights regions which are most sensitive to parameter changes. Observable differences between simulations can be caused by: 65 (1) the parameter change of the OAT experiment, (2) the interactive effects due to combinations of parameter changes, (3) numerical noise (slight variations in outcome due to the nature of the numerical algorithm or floating point errors that cannot be attributed to a specific parameter change), 70 and (4) a non-optimal solution of the groundwater equation (Eq. (1)) even if the convergence criterion is met. The latter error (4) can be observed in regions of the model where a strong non-linear relation may produce solutions that fit the convergence criterion but should be considered non-valid, 75 e.g., because of a mass-balance that is not in an acceptably preciseunacceptably inprecise.

Figure 4 shows the absolute coefficient of variation (ACV) of h per cell over all Monte Carlo experiments. The ACV is used to make a sound comparison of variance taking into ac-80 count the mean of the h value per cell (because the mean might be negative the absolute value is used). Yellow indicates that h changed little (mostly for regions with shallow groundwater), white to gray values indicate a growing difference in model results, and red values indicate a high varia- 85 tion of h over all model realizations. The latter areas represent either very low R (Sahara, Australia, South Africa) or a high variance in elevations, e.g., Himalaya, Andes and the Rocky Mountains. These are expected to have a high sensitivity to parameter changes as the multiplier of E_{swb} pro- $_{90}$ duces the highest shifts in regions with high elevationthat . Large changes in E_{swb} might cause a switch from gaining to losing conditions and vice versa (discussed in Sect. 3.2.2). Additionally, a change in R directly influences the conductance term C_{riv} that might also be changed by a multiplier. These combinations may yield conditions that are exceptionally challenging for the numerical solver. Switches between the two conditions constitute a non-linearity in the equation which might require a smaller temporal step-size to be solved. In a nutshell, if an iteration leads to a gaining 100 condition and the next to a losing condition, the switch renders the approximated heads of the preceding iterations invalid as the equation changed. In the worst case this can lead to an infinite switch between the two conditions without finding the correct solution. 105

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Figure 4. Absolute coefficient of variation $(\sigma(h)\mu(|h|)^{-1})$ [%] of simulated *h* per cell over all Monte Carlo realizations. Yellow indicates that *h* results changed very little, white to gray values indicate a growing difference in model results, and red values indicate a very high variation of *h* over all model realizations.



Figure 5. Uncertainty in *h* caused by variability in geologic structure (dominant in blue to light blue) in relation to uncertainty in *h* caused by variability in parameters based on Monte Carlo simulations (dominant in brown to green) calculated as $\frac{|h1-h2|}{IQR(h_{mc})}$ where h1/2 is the simulated head based on GLHMYPS 1.0 and 2.0 and h_{mc} the simulated head of all Monte Carlo experiments.

Areas with a high variance in results will also produce wide confidence intervals and are highlighted in Fig. A2.

Figure 5 relates the uncertainty in h, due to a change from GLHYMPS 1.0 to 2.0 to the interquartile range of h of all ⁵ Monte Carlo realizations, thus uncertainty in h due to parameter variation. Parameter variation is the dominant cause for h variability in mountainous regions, whereas the change in geologic data has a dominant impact in northern latitudes and the upper Amazon. In Australia, central Africa, and northern ¹⁰ India the impact of increasing K is almost as high as the vari-

ability caused by the variation of parameters in the Monte Carlo experiments. This suggests that a reduced uncertainty in K in these regions will improve the model results.

3.2.2 Variability of losing/gaining surface water bodies

¹⁵ Surface water bodies that provide focused, indirect groundwater recharge to the aquifer system are an important recharge mechanism to support ecosystems alongside



Figure 6. Percentage of all Monte Carlo realizations that resulted in a losing surface water body in a specific cell.

streams (Stonestrom, 2007). Especially in arid regions, they are important for agriculture and industrial development.

Losing or gaining surface water bodies are determined by 20 h in relation to E_{swb} . When h drops below E_{swb} water is lost to the aquifer (Eq. (5)) Figure 6 shows for each grid cell the percentage of the model runs in which the the surface water bodies in the cell lose water to the groundwater. Regions with a higher percentage are regions that are in losing conditions 25 independent independently of the applied parameter changes. Areas with the highest deviation in h (Fig. 4), thus the lowest agreement over all model realizations, are similar to the regions where some parameter combinations lead to losing surface water bodies, while others lead to gaining surface 30 water bodies (Fig. 6). Overall arid and mountainous regions show high percentages of Monte Carlo realizations with losing conditions, with dominantly 20-50 % of the realizations resulting in losing surface water bodies. h in these regions falls below E_{swb} either due to low recharge or high gradients. Surface water-groundwater interaction in these regions should be more closely investigated to improve model performance. The Sahara region stands out with large areas that contain losing surface water bodies in almost all model realizations. Values close to 100 % are furthermore reached in 40 the Great-Lakes, the Colorado Delta, the Andes, the Namib Desert, along the coast of Somalia, the Aral lake, lakes and wetlands in northern Siberia, and partially in Australian wetlands. Wetlands in Australia and the Sahara are likely to be overestimated in size in the context of a steady-state model. 45

3.2.3 Parameter sensitivities as determined by the method of Morris

The global-scale sensitivity of h and Q_{swb} is summarized in Table 3 that lists the percentage fractions of all cells for which a certain parameter has a certain rank regarding sensitivity and parameter interaction.

Overall, E_{swb} and R are the most important parameters for both model outputs over all ranks, followed by K. Q_{swb} is more sensitive to R than h, whereas h is more sensitive

Table 3. Percentage fractions of simulated cells with parameter sensitivity μ^* and parameter interaction σ per model output h and Q_{swb} , where the respective output is most sensitive to the listed parameter. For example h is the most sensitive to E_{swb} (Rank 1) in 57.2% of all grid cells, while K is the second most important parameter for h in 24.2% of those cells. Fractions are shown for the first three ranks.

		Rar	1 nk	% of cells Rank 2		Rank 3	
Para.	Output	μ*	σ	$\mu *$	σ	$\mu *$	σ
T.7	h	24.2	18.8	21.7	12.9	7.1	4.3
K	Q_{swb}	18.4	15.4	21.1	7.3	8.8	4.7
F	h	57.2	46.3	14.8	19.9	13.4	18.9
E_{swb}	Q_{swb}	18.5	14.3	11.2	27.7	36.0	34.4
C	h	1.0	0.5	3.9	2.4	4.3	2.5
O_{lak}	Q_{swb}	0.5	0.6	2.2	0.9	2	0.9
a	h	1.4	0.5	3.4	1.4	5.3	4.5
C_{wet}	Q_{swb}	0.5	0.8	3.6	2.1	4.2	2.8
C	h	0.9	0.9	1.8	10.2	8.4	8.1
$C_{gl.wet}$	Q_{swb}	0.4	0.8	2.3	15.2	9.4	7.8
C	h	2.0	28.0	32.8	29.3	28.7	18.1
C_{riv}	Q_{swb}	1.4	62.6	47.8	16.2	28.8	10.0
R	h	13.4	4.1	22.7	23.6	33.8	43.2
	Q_{swb}	59.8	5.1	11.3	30.5	10.7	39.2
C	h	1.3	1.0	0.3	0.2	0.5	0.4
U_{oc}	Q_{swb}	0.5	0.4	0.5	0.2	0.2	0.2

Percentage of cells with non-overlapping CIs (see App. 1 and Sect. 3.2.6) μ *: 11.8 % (*h*) and 13.3 % (*Q*_{*swb*}).

to E_{swb} . C_{riv} appears only dominant in the second and third rank for both model outputs. This means that for the majority of cells a change in E_{swb} and R, rather than C_{riv} dominates changes in Q_{swb} and h. K and R directly influence the cal-5 culation of C_{riv} and thus show a higher sensitivity.

The standard deviation of EEs (σ_i) is an aggregated measure of the intensity of the interactions of the *i*th parameter with the other parameters, representing the degree of nonlinearity in the model response to changes in the *i*th param-¹⁰ eter Morris (1991). A high parameter interaction indicates that the total output variance rises due to the interaction of the parameter with other parameters.

 E_{swb} shows higher interactions for h than for Q_{swb} . C_{riv} shows a high interaction on the first rank even if it is not 15 the dominant effect. This interaction is likely due to changes and K and R that directly influence the computation of C_{riv} . Both model outputs are sensitive to changes in R but show a relatively low degree of interaction for the first rank. A higher percentage of cells with an increased interaction of R is only 20 visible in the second and third rank.

Lakes and wetlands show low sensitivity and interaction in relation to total number of cells in Table 3 because they only exist in a certain percentage of cells. Table 4 shows the percentage fractions relative for cells with more than 25 % ²⁵ coverage of a lakes, global wetlands, and/or wetlands. The dominant parameter (by percentage) for all cells with respective surface water body is always E_{swb} for h (in 79.2 % of the lakes and in (79.9 %) 66.3 % of the (global)wetlands) and R (~54-77 % of all cells) for Q_{swb} . For the second rank the conductance of the surface water body $C_{lak,wet,gl.wet}$ dominated h, C_{riv} for Q_{swb} . Thus for lakes and wetlands E_{swb} and R are more relevant to h and Q_{swb} than the conductance of these surface water bodies.

3.2.4 Maps of global sensitivity

To show the spatial distribution of the parameters that affect ³⁵ h and Q_{swb} the most, ranked parameters were plotted for every cell in Fig. 7. The top of Fig. 7 represents the most sensitive parameters in terms of h (left) and Q_{swb} (right). Areas that should be judged with caution due to overlapping CIs are shown in Fig. A2. ⁴⁰

 E_{swb} stands out for mountainous regions and regions with low recharge aligned with regions in Fig. 4 and Fig. A4 with spots of C_{riv} . E_{swb} is dominant for Q_{swb} e.g. Rocky Mountains, Andes, Hijaz Mountains in Saudi Arabia and the Himalaya. R stands out in regions in the Tropical Convergence 45 Zone with large R and in northern latitudes for Q_{swb} . Kseems to be equally spatially distributed for h as well as for Q_{swb} . It is most important for h in Australia, the northern Sahara, the Emirates, and across Europe. There seems to be no correlation between the initial K spatial distribution and 50 a highly ranked K sensitivity. Areas with a dominant K are possibly influenced by a high interaction with other model components (K shows a high interaction Table 3 that is also reflected spatially in Sect. 3.2.5). E_{swb} stands out in the Sahara where likely overestimated wetland extents (Reinecke 55 et al., 2018) have a high impact on h. Q_{swb} seems to be more robust to show the effects in the highly variable regions and indicates the assumption that E_{swb} is also mainly responsible for the h variations observed in Sect. 3.2.1.

The second rank (second row in Fig. 7) shows values that the are not as important as the top row but dominant over all other parameters. In the highly variable regions K and for parts of the Himalaya R are dominant in the second rank. The C_{wet} appears as dominant parameter in areas with large wetlands with a bigger impact on Q_{swb} results than on h. C_{lak} is the clearly visible in parts of Nepal and along the Brahmaputra. In the Tropical Convergence Zone C_{riv} and K dominate for Q_{swb} , whereas results for h show a mix of $C_{gl.wet}$ C_{wet} and C_{riv} .

Zooming in on Europe (Fig. 8) for h, as an example, shows ⁷⁰ a similar trend to the global picture that R and K have the highest impact on h along with E_{swb} . E_{swb} is dominant in mountainous regions like the Alps and the Apennines as well in regions with lots of surface water bodies e.g. southern part of Sweden in the area of lake Vättern and Vänern and in the Finnish Lakeland. R appears dominant in east Italy in the lagoon of Venice and Marano, the Netherlands, and the wetlands in southwestern France. Almost invisible in the global

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Table 4. Percentage fractions of the most frequent parameter for rank 1 and 2 of all cells with with more than 25 % coverage of a lakes, global wetland, or wetland.

		$\mu * (h)$	μst ((Q_{swb})
	% R. 1= <i>E</i> _{swb}	% R. 2= $C_{lak,wet,gl.wet}$	% R. 1= <i>R</i>	% R. 2=C _{riv}
Lakes	79.2	64.6	54.2	38.8
Wetlands	66.3	47.3	77.2	46.9
Gl. Wetlands	79.9	56.4	66.3	¹ 31.7

 $^{1}C_{riv}$ =31.7 %, $C_{gl.wet}$ =40.6 %.

Percentage of second most frequent parameter not shown. Percentage in relation to cells with lakes, global wetland, or wetland > 25 %. Percentage-wise R. $1(\mu * (h))$ was always followed by R except for global wetlands were the second most frequent R. 1 was $C_{gl.wet}$. R. $1(\mu * (Q_{swb}))$ was followed percentage-wise by E_{swb} except for local wetlands with K, R. $2(\mu * (Q_{swb}))$ by $C_{lak,wet,gl.wet}$ except for global wetlands with C_{riv} .



Figure 7. Ranking of parameter sensitivity of h (left) and Q_{swb} (right). Parameters are ranked from top to The upper maps show the first rank the middle the second, and the bottom the last rank by μ * values.

picture is C_{oc} , a dominant parameter for most cells that have the ocean as boundary condition (only observable for h). Predominantly C_{riv} follows E_{swb} as second most important parameter. Only visible in the second rank are the wetlands e.g. 5 in west Scotland.

3.2.5 Maps of global parameter interaction

Similar to the spatial parameter sensitivities Fig. 9 shows the parameter interactions for h and Q_{swb} . Parallel to Fig. 7, the first row of Fig. 9 represents the most interactive parameters in terms of h shapes (left) and Q_{swb} .

¹⁰ in terms of h change (left) and Q_{swb} (right). The highest interaction with other parameters can be observed for E_{swb} for regions with high h variability similar to Fig. 7. C_{riv} shows

a high interaction in regions sensitive to R (compare Fig. 7) and is more visible for Q_{swb} .

K regions in the second rank are similar to where K already showed a high sensitivity for h (compare Fig. 7). In the Himalaya R and C_{riv} show a large spatial pattern. For Q_{swb} , $C_{gl.wet}$ is clearly visible where C_{riv} was most interactive before.

20

3.2.6 Sensitivity per GHRU

Average sensitivities and parameter interactions for each of the six GHRUs are shown in Fig. 10 (a). A dominant average per GHRU does not imply a rank 1 in each cell but rather provides an indication of its average importance per GHRU.



Figure 8. Zoom in of Europe of Fig. 7. Ranking of parameter sensitivity of h (left: rank 1, right: rank 2).



Figure 9. Ranking of parameters interaction (σ of EE is an indicator for parameter interaction) based on h (left) and Q_{swb} (right). Parameters are ranked from top to bottom by Σ values.

Each GHRU is described by the notation in Table 2. The shown average sensitivities and interactions are normalized to [0,1] because the calculated μ * and σ present no absolute measure of sensitivity. Mean values of μ * and σ that are very 5 close to zero are not shown in Fig. 10.

The values shown in Fig. 10 (a) should be judged with caution as they also include the regions Fig. A2 shown to be unreliable. Reliability means that due to overlapping CIs (any overlapping) the ranking of the parameters can't be clearly

determined (compare Fig. A2 and additional explanation Fig. 10 A1).

To judge the reliability of the outcomes per GHRU Table 2 shows the percentage of reliable results for h and Q_{swb} for each GHRU, where reliable results exclude over 80% of all sensitivity valuesbecause their CI overlapped (compare Fig. 15 A2 and explanation Fig. A1).

Figure 10 (b) shows only cells with reliable results, based on their confidence intervals, resulting in 11.8 % of all grid cells for h and 13.3 % for Q_{swb} . GHRUs in high and very

high elevations show low reliability concerning h results as expected (compare Fig. 4). Q_{swb} appears as more robust in these regions.

Figure 10 (a) shows a similar picture to the two global

- ⁵ maps (Fig. 7, 9). All GHRUs show a linear correlation of sensitivity and degree of interaction. The GHRU with average elevation, average recharge, and high K (GHRU 1) shows higher average response in Q_{swb} than h. h as is most sensitive to C_{riv} , and less sensitive to the other parameters. Q_{swb}
- ¹⁰ is clearly most sensitive to K and $C_{gl.wet}$ and shows a high interaction in this GHRU. Lower-lying regions with average K and R (GHRU 2) show high sensitivity of h only to E_{swb} with a high interaction while Q_{swb} is affected in decreasing order by $C_{gl.wet}$ and K. Results for h sensitivity in GHRU 3,
- ¹⁵ with very high elevations, average K and low R, should be judged with caution because only a very low fraction is based on results with non-overlapping CIs (Table 2). Compared to other GHRUs, 3 shows rather clustered sensitivities and parameter interactions. h is most sensitive to E_{swb} and R and
- ²⁰ Q_{swb} to C_{lak} , K, and C_{wet} . GHRU 4, which differs from GHRU 3 by its high but not very high land surface elevation, shows E_{swb} , K, and R as clearly most dominant and interactive parameter for Q_{swb} , followed by C_{wet} . Similar Q_{swb} is most sensitive to E_{swb} and K. In low-lying and rather flat
- ²⁵ regions with high groundwater recharge (GHRU 5), sensitivities of h are close to zero except for K possibly because changes in h are to small in flat regions (compare Fig. 4) due to small h gradients. Q_{swb} is most sensitive to E_{swb} and $C_{gl.wet}$. GHRU 6 is relatively small and like GHRU 5 only

³⁰ occurs in the tropical zone (Fig. 3 (a)). In this GHRU, which differs from GHRU 5 only by K being high instead of average, the dominant parameters of Q_{swb} are similar to other GHRUs where E_{swb} is clearly the most dominant followed by R and K. h shows a response to wetlands but again like ³⁵ in 5 a very low response to E_{swb} .

Taking into account only the reliable regions changes the perception in Fig. 10 (b). GHRU 1 shows rather similar sensitivities and parameter interactions as compared to other GHRUs. h is most sensitive to E_{swb} , and only somewhat less 40 sensitive to C_{riv} and C_{wet} . Q_{swb} is clearly most sensitive to C_{riv} and shows a high interaction in this GHRU. GHRU 2 shows high sensitivity of h only to E_{swb} with a high interaction while Q_{swb} is equally affected by K, E_{swb} and R. Results for h sensitivity in GHRU 3 are not very represen-45 tative for the whole GHRU as only a very small fraction of cells shows reliable results (Table 2). Like in GHRU 2, Q_{swb} is equally affected by by K, E_{swb} and R. GHRU 4 shows E_{swb} as clearly most dominant and interactive parameter for h, followed by K and C_{wet} . For GHRU 5, sensitivities of h 50 could not be determined reliably possibly because changes in h are to small in flat regions (compare Fig. 4) due to small

h gradients. Q_{swb} is most sensitive to *R* (as rivers are gaining rivers that need to drain groundwater recharge) followed by *K*. In GHRU 6 the dominant parameters of Q_{swb} are the

same as for GHRU 5 (except for E_{swb}) while h is most sensitive to C_{lak} .

4 Discussion

This study presents a novel spatially distributed sensitivity analysis for a high-resolution global gradient-based groundwater model encompassing 4.3 million grid cells. While 60 these maps are challenging to interpret, they yield new ways of understanding model behavior and can help to focus efforts in collecting observation data for specific regionsfor future calibration. behaviour based on spatial differences and help to prepare calibration efforts by identifying parameters 65 that are most influential in specific regions. Furthermore, they guide the future development of the model and the intended coupling efforts of the groundwater model to the hydrological model. Especially, the sensitivity of Q_{swb} and the importance of E_{sub} , which are the two major coupling 70 components, are of interest.

However, the large number of grid cells with either statistically zero sensitivity values (overlapping CI with zero) or unreliable results limit the relevance and applicability of the study results. The study suggests that the highly nonlinear and conceptual approach to the surface water body conductance (in particular the sudden change of conductance between gaining and losing rivers) needs to be revised as it may affect the stability of transient model results. Additionally the results suggest that elevation of the water table of surface water bodies is a promising calibration parameter alongside with hydraulic conductivity.

The presented results need to be considered against the backdrop of the high h variability of the Monte Carlo experiments (Sect. 3.2.1). Some of these simulations cannot be 85 considered as a valid result for a h distribution. This is due to multiple model challenges: (1) the evaluated model is a numerical model and thus behaves differently approximates a differential equation and can show non-linear behaviour for different parameterizations, (2) the equations used for 90 rivers present a non-linear model component (switch between equations for gaining and losing conditions as well as relation to K and R), (3) the convergence criterion for the steady-state solution is solely based on a vector norm of residuals (metric of changes of the solution inside the 95 conjugate gradient approach) and maximum h change between iterations and do not contain an automated check for a reasonable mass balance. On the other hand, it is challenging to include a validation mechanism in the presented analysis to alleviate these problems while maintaining a rea- 100 sonable model runtime (as a stricter convergence criterion will most likely increase the number of necessary iterations) and/or number of necessary model runs. It is questionable whether results based on different convergence criteria can be compared. This would necessitate including the numeric 105 stability in the sensitivity analysis as well.



Figure 10. Normalized average sensitivity and parameter interaction per GHRU for *h* and Q_{swb} (a). If a parameter is not present the mean sensitivity for that GHRU was close to zero (overlapping CI with zero). Does not include ocean parameter sensitivity. Mean characteristics, their symbols for each GHRU, and the reliability of the sensitivity measure (only μ * not σ) are shown in Table 2. (b) Only reliable results (after removing overlapping CI).

However, the results help to answer the research questions at hand. While overlapping CIs blur the ranking of the parameters in some regions, they still provide evidence on what parameters the calibration should focus and how the

⁵ importance of parameters varies per region. The sensitivity of Q_{swb} to parameters, especially E_{swb} , will help to guide the future model development and coupling to the hydrological model. In general, the analysis helped to identify the elevation of surface water bodies as a focus for future ¹⁰ research.

Around 30 % of all μ * values had a confidence interval that was larger than 10 % of the μ * value. This suggests that even more model runs are required and that large extents of the model experienced numerically unstable results as the spatial distribution of head variance and large confito dence intervals overlap.

The selection of parameter ranges can influence the results of a sensitivity analysis significantly (Pianosi et al., 2016). Even parameters that are suspected of not being sensitive can show highly nonlinear behavior in certain parts of the parameter space that are only activated when one expands the ranges of the parameters. The presented ranges in this study do not explore the full assumed uncertainty range. Specifically, the small range of E_{swb} is likely influencing the outcome of the parameter rankings. The range was chosen to allow a reasonable number of simulations to converge as the range of E_{swb} directly influences the numerical stability of the model. The presented results, however, do show that the model output is highly sensitive to changes in E_{swb} in most areas of the globe. The response in mountainous regions can be attributed to applying E_{swb} as a multiplier, which has a higher impact in regions where the initial water body eleva-

 $_{5}$ tion is high. On the other hand, this is accounting for the fact that the uncertainty of E_{swb} is largest in regions with highly variable topography per 5' grid cell.

The only previous sensitivity analysis of a global gradientbased groundwater model to out knowledge was done by

- ¹⁰ de Graaf et al. (2015). Based on varying K, aquifer thickness, and R, the coefficient of variation of the steady-state hydraulic head was computed (de Graaf et al., 2015, Fig. 5). From that analysis it was determined that K has the highest impact and aquifer thickness the lowest. It is not clear how
- ¹⁵ the coefficient of variation determined these outcomes. The relatively low impact of aquifer thickness was observed also by Reinecke et al. (2018). Therefore, this parameter was not included in this study. Both de Graaf et al. (2015) and this study show a high h variance in parts of Australia and the
- ²⁰ Sahara (de Graaf et al., 2015, Fig. 5) possibly due to the low initial R. Variations in the mountainous regions, on the other hand, are not reflected in de Graaf et al. (2015) as their analysis did not vary E_{swb} .

Besides the large h variance, which is likely the main ²⁵ cause for the low percentage of reliable cells, the confidence intervals of the sensitivity indices in this experiment suggest that additional simulations are necessary to determine more reliable results. Additionally, the small parameter ranges, required for stable model runs, influenced the overall outcome ³⁰ and might be a reason for cells with inconclusive results.

For cells with lakes and wetlands, E_{swb} dominates over the variations in conductance for h (Table 4), confirming the importance in determining the surface water body elevation. For Q_{swb} , on the other hand, R is most influential in these ³⁵ cells even though it does not affect the conductance equation for these surface water bodies. Apparently, available recharge is driving the interaction more than it influences changes in

head. In regions with high recharge (GHRU 5) Q_{swb} was more robust to parameter changes than h. This is possibly ⁴⁰ due to the generally lower response in Q_{swb} to changes in E_{swb} , which can be explained by the constant flow for losing

surface water bodies (incl. rivers) as soon as h drops below E_{swb} . Thus changes is E_{swb} do not affect Q_{swb} afterwards (as long as the surface water body remains in losing condi-45 tions). Both model outcomes show a high sensitivity to R

while the interaction of R is only visible at the 3rd rank suggesting that if R changes other parameter changes do not influence the model response further.

Separating the complex global domain into a selected ⁵⁰ number of GHRUs enables a sensitivity analysis in accordance with computational constraints (e.g. maximum number of core hours). It alleviates the drawbacks of global-scale multipliers while keeping a reasonable number of total simulations. The presented decomposition based on three param-⁵⁵ eters E_{swb} , K, and R was guided by the high sensitivity of model output to these parameters. Other factors like lithology and surface water body characteristics should be investigated as additional characteristics for GHRUs.

5 Conclusions

For the first time, spatially distributed sensitivities of the 60 global steady-state distribution of hydraulic head and flows between the groundwater and the surface water bodies were calculated and presented. We found the Morris sensitivity analysis method can yield insights for computationally challenging (concerning computation time and numerical diffi-65 culties) models with reasonable computational demand. This study applied a novel approach for domain decomposition into GHRUs. Applying parameter multipliers simultaneously to all grid cells within each of the six GHRUs allowed a more meaningful sensitivity calculation, than it would be possible 70 if the parameters would have varied simultaneously in all grid cells, while maintaining a feasible the number of simulations.

Based on only a small fraction of grid cells for which parameters could be ranked reliably according to their im-75 portance for simulated model output, steady-state hydraulic heads (h) were found to be comparably affected by hydraulic conductivity (K), groundwater recharge (R) and the elevation of the water table of surface water bodies (E_{swb}) . Rankings for individual grid cells varies, but globally none of 80 the three dominates with respect to h. The simulated flows between groundwater and surface water bodies (Q_{swb}) are clearly most sensitive to R. This is due to the model parameterization of river conductance that is computed as a function of R, assuming under steady-state conditions, ground-85 water discharge to rivers should tend to increase with increasing R (Eq. (5)). The results indicate that changes in R between timesteps for a fully coupled transient model could pose a challenge to the model convergence and that the equations might need to be reconsidered for a fully coupled 90 model. In general the uncertainty due to the parameterization of groundwater-surface water exchange flows (E_{swb} and $C_{riv,gl.wet,wet,lak}$) needs to be further investigated as they have a high impact on h distribution and Q_{swb} .

In high mountainous regions (Rocky Mountains, Andes, ⁹⁵ Ethiopian Highlands, Arabian Peninsula, Himalaya) and regions with low recharge (Sahara, southern Africa) the computed h showed an unreasonably high variance due to the numeric instability of the simulations in these areas. In case of high elevations and thus large variations in E_{swb} or in ¹⁰⁰ case of low groundwater recharge, it is not possible to solve steady-state groundwater flow equations with arbitrary parameter combinations and a constant convergence parameter. Q_{swb} was found to somewhat be more robust than h in these regions. These results suggest that the parameterization of ¹⁰⁵ E_{swb} needs to be reconsidered and is a likely parameter for future calibration. The lack of reliable data at the global scale, in particular hydraulic conductivity data with high horizontal and vertical resolution, hinders the development of global groundwater models. A simple sensitivity analysis on the impact of small

- ⁵ changes to an existing global hydraulic conductivity dataset (GLHYMPS 1.0 (Gleeson et al., 2014) to 2.0 (Huscroft et al., 2018)) showed that knowledge about the distribution of K is pivotal for the simulation of h as even slight changes in K may change model results by up to 100 m.
- ¹⁰ The presented study results refer to the uncoupled steadystate groundwater model G³M. As G³M is currently being integrated into the global hydrological model WaterGAP, future work will extend this sensitivity analysis to fully coupled transient simulations.

15 1 Appendix

Results of the method of Morris need to be contemplated in a ranking based scheme that relies on metrics that summarize the calculated EEs. Figure A1 shows the conceptual issues that are entailed with this ranking approach. The absolute ²⁰ mean (μ *) of all EEs of parameter 1 (P1) might be bigger than μ * of P2 but as their CIs are overlapping a clear ranking

is not possible. On the other hand it is evident that P1 and P2 are clearly more sensitive than P3. Illustration of derivation of presented metrics. An overlapping suggests that even if $_{25}$ the mu* values are different a ranking should be considered

- with care as the two parameters could be equally important or in some regions inside one GRHU their importance could be the other way around. But even if they overlap, the *mu** provides a valuable measure of the overall importance of
- ³⁰ the parameters also in comparison with much less important parameters.

Additionally, not only the overlapping should be considered but also the size of the CI in comparison to the mu_* . It is a useful indicator on whether the

- ³⁵ sampling of the parameter space was to small and more simulations are required to gain a clearer picture. 15% is an arbitrary value that we considered an appropriate boundary. Other studies used 10% (Herman et al., 2013a) or 3.5% (Vanrolleghem et al., 2015).
- ⁴⁰ Figure A2 shows regions where the applied sampling was sufficient (CIs where smaller than 15% of the calculated μ * of the first rank) and regions where more simulations, or a more sophisticated approach to ensure numerical stability, is required.
- ⁴⁵ Author contributions. RR led conceptualization, formal analysis, methodology, software, visualization, and writing of the original draft. JH, LF, SM, TT supported review and editing as well as the development of the methodology. AW supported visualization and writing of original draft of section 3.1. PD supervised the work of ⁵⁰ RR and made suggestions regarding analysis, structure, and word-

ing of the text and design of tables and figures.



Figure A1. Illustration of derivation of presented metrics. Blue circles show the two criteria used to judge the quality of the results.

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Figure A2. Confidence interval (95) in relation to the μ * for rank 1 of *h* and Q_{swb} . Yellow regions indicate a sufficient sampling size.

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