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Understanding each other's models: a standard representation of global water models to support improvement, intercomparison, and communication

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Abstract. Global water models (GWMs) simulate the terrestrial water cycle, on the global scale, and are used to assess the impacts of climate change on freshwater systems. GWMs are developed within different modeling frameworks and consider different underlying hydrological processes, leading to varied model structures. Furthermore, the equations used to describe various processes take different forms and are generally accessible only from within the individual model codes. These factors

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have hindered a holistic and detailed understanding of how different models operate, yet such an understanding is crucial for explaining the results of model evaluation studies, understanding inter-model differences in their simulations, and identifying areas for future model development. This study provides a comprehensive overview of how state-of-the-art GWMs are designed. We analyze water storage compartments, water flows, and human water use sectors included in 16 GWMs that provide simulations for the Inter-Sectoral Impact Model Intercomparison Project phase 2b (ISIMIP2b). We develop a standard writing style for the model equations to further enhance model improvement, intercomparison, and communication. In this study, WaterGAP2 used the highest number of water storage compartments, 11, and CWatM used 10 compartments. Seven models used six compartments, while three models (JULES-W1, Mac-PDM.20, and VIC) used the lowest number, three compartments. WaterGAP2 simulates five human water use sectors, while four models (CLM4.5, CLM5.0, LPJmL, and MPI-HM) simulate only water used by humans for the irrigation sector. We conclude that even though hydrologic processes are often based on similar equations, in the end, these equations have been adjusted or have used different values for specific parameters or specific variables. Our results highlight that the predictive uncertainty of GWMs can be reduced through improvements of the existing hydrologic processes, implementation of new processes in the models, and high-quality input data.

1 Introduction

Many multi-model intercomparison projects (MIPs) have been designed to provide insights into various Earth system processes. Some MIPs examples include FireMIP for the fire regime and its drivers (Rabin et al., 2017); CMIP for past, present, and future climate changes and their drivers (Eyring et al., 2016; Kageyama et al., 2018); LakeMIP for physical and biogeochemical processes of lakes (Stepanenko et al., 2010; Thiery et al., 2014); AgMIP for crop growth (Rosenzweig et al., 2013), and WaterMIP or ISIMIP for the water cycle (Haddeland et al., 2011; Frieler et al., 2017). These MIPs provided many multi-model ensembles that consist of multiple models driven by the output of multiple other models. The multi-model ensembles offer the opportunity to inter-compare models for an increased understanding of process representation and inter-model differences as well as for model improvement. Hence, they have evaluated models' performance in the past and have focused on the models' agreement for the future. They also have encountered many challenges in how to inter-compare models and interpret various model results (Von Lampe et al., 2013), realize the standardization of data and scenarios, and integrate transdisciplinary knowledge in modeling (Rosenzweig et al., 2013), identify and reduce uncertainties (Sitch et al., 2008). In the end, many MIPs and their multi-model ensembles have been blocked in interpreting inter-model differences (Clark et al., 2011). They have underlined the need to go beyond good overall model performance and to improve process representation in the models (Guseva et al., 2020), integrate missing processes (Friend et al., 2013) and reduce uncertainties (Warszawski et al. 2013). Certainly, MIPs have also been affected by scientific complexity, input data quality, and technical infrastructure. Therefore, the modeling community is still testing and learning how to improve modeling and how to realize multi-model inter-comparison studies. For example, the Coupled Model Intercomparison Project (CMIP) adopted, after 20 years of existence, a new and more federated structure because of complex scientific questions, large amount of model outputs, challenges of technical infrastructure, and even cultural and organizational challenges (Eyring et al., 2016). CMIP also showed that robust similarities exist among models and, as a result, models are not strictly independent of each other given previous and legacy versions, and existing links among modeling communities who indirectly transfer some models' strengths and weaknesses by sharing their ideas and codes (Masson and Knutti, 2011; Knutti et al., 2013). Finally, few studies have

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undertaken model experiments on process representation and evaluated the models for specific events or characteristics specifically on the catchment scale (Boer-Euser et al., 2017; Duethmann et al., 2020). It has been concluded that there is no perfect model (Essery et al., 2013; Ullrich et al., 2017) and there is a need to understand better how models work.

Therefore, in this complex scientific context, the present study represents a step forward towards an increased understanding of process representation and inter-model differences. The three main goals are (i) to provide a better understanding of how state-of-the-art global water models are designed, (ii) to show similarities and differences among them, based on their equations, and (iii) to underline future research potential in global hydrological modeling.

This study supports intercomparison, improvement, and communication among models. It also provides the basis for 1. further water model (inter)comparison studies, including model outputs; 2. selecting the right model(s) for a given application; and 3. identifying data needs for a given analysis and application.

The target audience includes students, professors, the modeling community, the stakeholder community, and members of the general public interested in understanding large-scale models, and simulating climate change and its impacts.

Hence, we present the modeling approaches in simulating globally terrestrial water cycle in section 2. In section 3, we present key characteristics of the models included in the present study. In section 4, we review models and present their strengths and weaknesses. In section 5, we present similarities and differences among models. In section 6, we discuss challenges and future research potential in global hydrological modeling. In the end, we present our conclusions.

2. Modeling approaches in simulating terrestrial water cycle globally

The terrestrial water cycle is simulated globally by three different communities that have developed three types of models: (i) the climate community has developed land surface models (LSMs); (ii) the global hydrological community has developed global hydrological models (GHMs); (iii) the vegetation community has developed dynamic global vegetation models (DGVMs). These communities interact with each other, but generally focus on specific hydrological processes that are important for their research and are presented in the following subsections.

2.1 Differences in modeling approaches

The climate community is focused on climate simulations (long-term weather patterns in an area) and their changes over decades and centuries. LSMs simulate the water and energy exchanges between the land surface and the atmosphere, specifically focusing on vertical flow exchanges. Therefore, these models simulate the energy cycle, the water cycle, the carbon and nitrogen cycles, and vegetation and crop responses to temperature, precipitation, and CO_2 concentrations. Further, they represent the soil with a higher vertical resolution and represent evapotranspiration and snow dynamics in a more physical manner than the global hydrological models (GHMs; Döll et al., 2016; Pokhrel et al., 2016; Wada et al., 2017). Ultimately, they are fundamental components of global climate models (GCMs) and Earth system models (ESMs).

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The global hydrological community is focused on surface hydrologic processes, primarily river flow simulation and its daily to century-scale changes. GHMs simulate the water cycle with its water flows, water storage compartments, and human water use sectors. These models simulate water abstracted for the irrigation, domestic use, livestock, industry (manufacturing and electricity), and desalination sectors. One of their main foci is streamflow simulation and their ability to reproduce historical observations of this variable. They focus on lateral flows and only partly on vertical flows, comprehensively simulating the following surface water bodies: (i) lakes, (ii) wetlands, (iii) rivers.

The vegetation community is focused on vegetation distribution and growth in an area and over a time interval and is primarily interested in the global carbon cycle. DGVMs simulate shifting vegetation, driven by biogeochemistry, hydrology, and anthropogenic influences. These models simulate the vegetation composition and distribution as well as compartments and flows of carbon and water, for both natural and agricultural ecosystems. Specifically, they model the active response of vegetation to changes in air temperature, precipitation, and CO_2 concentrations.

The main driver that connects the processes simulated by these communities is solar energy, specifically, it links the water and energy budgets with vegetation processes. This can be exemplified by the latent heat flux of evaporation that describes the heat or the energy required to change the liquid water into water vapor. This heat or energy is locked in the humid air as water vapor, and is released when the humid air touches cold air and water vapor condensation starts. Therefore, continental evaporation is considered to be water loss by the global hydrological and vegetation modeling communities, but a water source (for cloud formation) by the climate community (those that simulate the atmosphere), with implications for agriculture and ecosystems (Abbott et al., 2019). Additionally, transpiration represents a water source for the vegetation community, necessary for photosynthesis and plant growth, and water loss for the global hydrological community.

Although these communities simulate the same hydrological processes, they use the same expressions or terminology with different, field-specific meanings. Some examples are presented in subsection 2.2.

In conclusion, all these models simulate the water cycle at the global scale despite fundamental differences in model structure, model parameterization, and output variables.

2.2 Ambiguity of terminologies used in hydrological modeling

This subsection highlights the same expressions used by the three communities, but with different meanings. For example, *climate forcings* (factors) are used by climate community to point out the natural and human-made factors that affect the Earth's climate. Natural factors include the Sun's energy, regular changes in the Earth's orbital cycle, and large volcanic eruptions, while human-made factors are greenhouse gas emissions and land use changes. The global hydrological community and vegetation community consider *climate forcings* as climate input data or climate variables for their models.

Another example is *dynamic vegetation*, which has two meanings among these communities: 1. *active vegetation* defines vegetation that actively changes in an area because of changes in the CO_2 concentration, that is CO_2 assimilation through plant stomata in the photosynthesis process and because of changes in air temperature and precipitation; 2. *dynamic vegetation*, also called *vegetation competition*, defines vegetation that changes its geographical distribution from one geographical area to

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another because of competitive and biogeographical processes determined by climate change (geographical distribution of plants) or human activities. In the present study, we use *active vegetation* to highlight if models include the photosynthesis scheme in their structure. Generally, it is recommended to include this process in models because elevated CO_2 concentrations cause physiological and structural effects on plants and indirectly influence runoff and evapotranspiration over a geographical area. The physiological effect reduces the opening of leaf stomata because less water is needed to assimilate carbon, leading to decreased transpiration and, indirectly, increased runoff. The structural effect or fertilization effect causes an increase in plant growth and leads to increased transpiration per unit area and, indirectly, a decreased runoff (Gerten et al., 2014). However, Singh et al. (2020) demonstrated that increased leaf area under elevated CO_2 concentrations (structural effect) might counterbalance the increased water use efficiency (physiological effect).

In the end, because of differing and complementary perceptions and details of their models, it is important that these communities interact, identify their similarities and differences, share experiences, learn from different experiments, undertake joint experiments, present and discuss their results, and discuss how they influence and depend on each other and how hydrological modeling can be improved. Therefore, collaboration among these communities will result in new multi-model intercomparison projects and multi-model ensembles that will facilitate new analyses, comparisons, understandings, and improvements.

3 Global water models included in the study

3.1 Description of the modeling experiment

The GWMs analyzed in this study contribute with simulations to the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP). This project was initiated by the Potsdam Institute for Climate Impact Research (PIK) and the International Institute for Applied Systems Analysis (IIASA) in 2012. It includes a strategy and a framework to create, compare, and explain climate-impact projections in various sectors and at varying scales (Warszawski et al., 2014). ISIMIP has gone through various simulation phases (Fast Track, 2a/2b, currently 3a/3b), each designed with a specific focus topic that has dictated the protocol framework, including specific simulation scenarios and common input datasets. All models participating in ISIMIP have to comply with its simulation protocol (Frieler et al., 2017). The ISIMIP project has been offering a forum where scientists from, currently, 13 sectors, including the global water sector, bring their expertise, experience, and knowledge together to extend the frontier of research on climate change and its cross-sectoral impact assessments. In its second phase (ISIMIP 2b), most models are run with a daily temporal resolution and with a spatial resolution of 0.5° × 0.5° (~55 km × 55 km at the Equator). The models of the global water sector contribute to an experiment setup designed to assess the impact of historical and future warming under the Paris Agreement. These models are driven by the same climate input datasets under representative concentration pathways (RCPs) and socioeconomic scenarios (SSPs). The time span of the simulations is divided into pre-industrial (1661–1860), historical (1861–2005) and future (RCP2.6, RCP6.0, and RCP8.5). The requested output datasets provide quantitative information to identify the major drivers of historical impacts, to examine the impacts of additional

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warming, and to assess the impacts from different future socioeconomic development scenarios. More details regarding the ISIMIP framework can be found on the ISIMIP webpage (https://www.isimip.org/) and in Frieler et al., 2017. However, one recommendation for the ISIMIP community will be to increase the number of regional studies and pilot studies that could validate global studies, which could be another effective way of studying climate change.

3.2 Steps taken to realize the standard writing style of model equations

All models that provide simulations for the global water sector in ISIMIP2b are included in this paper, although some of them have not yet finished their simulations for this phase. The rationale of describing models is based on how models simulate the water cycle. Therefore, in this study, a global water model describes the dynamic behavior of a hydrological system that includes input variables, state variables, parameters, constants, and output variables (Bierkens and van Geer, 2007). State variables define the state of the water in a compartment or storage at the beginning of the simulation, and can change in space and time, for example, with canopy water storage. Their variation is caused by a variation of the input variables, for example, precipitation. State variables are related to the input variables and output variables through parameters. Parameters may change in space, but do not change in time. Parameters and coefficients represent numbers that describe a particular characteristic of reality, of the model, of the catchment area or flow domain such as runoff coefficient, soil porosity, hydraulic conductivity of different soil horizons, maximum soil water storage, maximum canopy water storage, and mean residence time in the saturated zone (Beven, 2012). Some processes are parameterized, meaning that their values are precisely marked in the computer code and are not calculated by the model itself. Originally, to parameterize by itself means to describe a process or a phenomenon by the use of parameters. Therefore, in hydrological modeling many parameterization methods or techniques (equations running in some algorithms) have been implemented to simulate hydrological processes. Ultimately, a model also uses constants, properties of the model that do not change in space and time, and "output variables," which vary in space and time. Hence, we describe GWMs based on the equations implemented for eight water storage compartments, five human water use sectors, and desalination. The analyzed water storage compartments are (1) canopy, (2) snow, (3) soil, (4) groundwater, (5) lake, (6) wetland, (7) reservoir, and (8) river. The human water use sectors are (1) irrigation, (2) domestic (households), (3) livestock, (4) manufacturing, (5) electricity.

It was extremely challenging to label processes as being similar or different among the 16 models because a unique equation can be implemented in various ways (e.g., discrete vs. analytical form, focusing on flows or water storage compartments) or parameterized differently. Therefore, we created a standard writing style for GWMs equations and used the same symbols to write those equations, thereby highlighting their similarities and differences in a consistent way. In the end, the standard writing style facilitated comparison among models, but it has also raised many challenges, mainly because we decided to write self-explanatory equations that could be understandable by readers with or without knowledge in hydrology.

In the supplement, we report tables containing various equations for each water storage compartment, human water use sector, and their related water flows (tables and figures in the supplementary information are denoted by an "S" in their numbering). All variables have been harmonized and their units have been standardized (Tables S1–S83).

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We made the standard writing style of the model equations following some steps. Firstly, we analyzed the nomenclature of each model with the purpose of identifying the best practices. Secondly, we assembled a list with water storage compartments, flows, and human water use sectors included in the models. Thirdly, we established clear definitions for all variables that have been collected inside a glossary of terms. Finally, we collated all model equations of each inflow and outflow for each water storage compartment and human water use sector.

Multiple subscripts or superscripts are required to properly identify water storage compartments, flows, and human water use sectors because of the large number of compartments that are included in the model structures. Thus, we selected "S" to describe water storage, "P" to describe everything connected to precipitation, "E" everything related to evaporation, "R" everything related to runoff, "Q" everything related to streamflow and outflow, and "A" for water abstractions. We used two letters for subscripts and superscripts, ideally, the first two letters of the word, for example, "ca" for canopy; "sn" for snow; "so" for soil, and so on (see list of symbols and glossary in the Supplement), while we used the first letter of each word in case of compounds words such as groundwater ("gw") or surface water ("sw"). We separated subscripts and superscripts from one another using comma. Some of these decisions correspond with some habits that exist in the hydrological community (e.g., *gw* and *sw*) and we decided to keep them to make a comfortable and easy workflow for modelers and readers. We did not write full words for subscripts and superscripts, because equations became too long and difficult to read and understand.

In the end, the standard writing style of the equations is useful and necessary for finding similarities and differences among models for each water storage, human water use sector, and water flow. In addition, it can be leveraged for explaining the different model outputs, for classification of the models based on cluster analysis, and for selecting the right model for the right application. It can also be used for drawing a standard schematic visualization of the water cycle, for describing models on ISIMIP and ISIpedia platforms (the open climate-impacts encyclopedia, a part of the ISIMIP, https://www.isipedia.org/), and for understanding how models work. It should be noted that these equations are available only for model versions used for ISIMIP2b.

3.3 Key characteristics of the global water models

The present model intercomparison study is based on the lists presented in Tables 1 to 5 that show water storage compartments, flows, and use sectors included in the GWMs. Generally, the model description is separated into two parts: the hydrological part and human water use part. The hydrological part includes the water cycle processes described as water storage compartments and flows, with flow presented as inflow and outflow of each water storage, while the water use part includes human water use, specifically water abstracted from the groundwater or surface waters. In the supplement, we provide tables that present an overview of the GWMs, helping readers to understand similarities and differences among models, identify included water storage and flows, and get an overview of hydrological knowledge complexity behind models (Tables S1–S103).

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In this study, six models are LSMs: CLM4.5, CLM5.0, DBH, JULES-W1, MATSIRO, and ORCHIDEE. Nine models are GHMs: CWatM, H08, Mac-PD20, mHM, MPI-HM, PCR-GLOBWB, VIC, WaterGAP2, and WAYS. One model is a DGVM (LPJmL, Tables 6 and 12).

Twelve models have a daily temporal resolution (Table 6), while MATSIRO has an hourly temporal resolution. Four models (CLM4.5, CLM5.0, MATSIRO, and ORCHIDEE) have 30-min temporal resolution, downscaling their daily forcing to a 30-min time step to solve the energy budget. JULES-W1 has a higher temporal resolution (1-hour) to solve the energy budget. Fifteen models run with a spatial resolution of 0.5°. ORCHIDEE runs with a spatial resolution of 1.0° and has its outputs converted to 0.5° spatial resolution. All models divide the land into grids of discrete "cells" (excluding Greenland and Antarctica) and, in addition, some models include subgrids for some components: CLM4.5 and CLM5.0 for vegetation, surface runoff and evapotranspiration; H08 for land cover (via 19 crop types); CWatM for land cover (6 land cover types) and snow (10 elevation zones); MPI-HM for surface runoff and evapotranspiration; PCR-GLOBWB for vegetation and land cover; WaterGAP2 and MATSIRO for snow; VIC for vegetation and elevation. Further, MATSIRO divides a subgrid cell in snow-covered and snow-free portions with flows and storages resolved separately for these portions, both for land and canopy surfaces.

Nine models (CLM4.5, CLM5.0, CWatM, H08, LPJmL, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2) use the 30-min global drainage direction map DDM30 (Döll and Lehner, 2002), a raster map with a spatial resolution of 0.5° × 0.5° (~ 50 km × 50 km), to outline the drainage directions of surface water collected by creeks, rivulets, and rivers. In this map, 66,896 discrete grid cells are connected to each other by their specific drainage direction and are organized into drainage basins that drain from the Earth's land surface (excluding Antarctica) into the ocean or into an inland sink. The mHM uses a river network (0.5° × 0.5°) upscaled from HydroSHEDS (Lehner et al., 2006). ORCHIDEE uses the river network from the Simulated Topological Networks (STN-30p: Vörösmarty et al., 2000). Five models (DBH, JULES-W1, Mac-PDM.20, VIC, and WAYS) do not use any river routing scheme for the ISIMIP2b; therefore, they do not compute streamflow.

MATSIRO and LPJmL use prescribed data for the domestic (household) and industry sectors; therefore, they do not consider the two-way interaction between water system and humans. In hydrological modeling and in the ISIMIP2b, the word "prescribed" has two meanings: (i) data which are simulated by other models and provided by the ISIMIP2b framework as input (https://www.isimip.org/gettingstarted/details/38/); (ii) data obtained from satellite observations, other datasets, or maps. Prescribed data highlight some limitations of the models or underline the lack of some processes that were intentionally or non-intentional removed from the model structure, according to the purpose of the model development or other priorities such as time.

Six GHMs perform calibration of their hydrological components, using different approaches (Table 6). CWatM calibrates monthly or daily streamflow for 12 catchments using the Distributed Evolutionary Algorithms in Python (DEAP) approach (Burek et al., 2020), while WaterGAP2 uses a beta function for the calibration of 1,319 gauged hydrological stations considering runoff as a nonlinear function of soil moisture. WaterGAP2 uses a runoff coefficient and two correction factors to calibrate the simulated and observed streamflow (Müller Schmied et al., 2014). Mac-PDM.20 is calibrated using the

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generalized likelihood uncertainty estimation (GLUE) approach, comprising a 100,000-member ensemble based on different model parameterizations run with Watch Forcing Data and evaluated against Global Runoff Data Centre (GRDC) streamflow data (Smith, 2016). In mHM, calibration of global model parameters is performed against the daily observed streamflow of GRDC stations, along with gridded global fields of FLUXNET evaporation (Jung et al., 2011) and a GRACE terrestrial water storage anomaly, using the ERA5 climate forcing (Landerer and Swenson, 2012). VIC uses the source datasets and parameter sets from Nijssen et al. (2001), namely the AVHRR-derived landcover dataset (Hansen et al., 2000) and the FAO soil textures (FAO, 1995), and is sub-sampled to 0.5° × 0.5° via a nearest-neighbor approach. WAYS is calibrated against data from the International Satellite Land Surface Climatology Project (ISLSCP) Initiative II of the University of New Hampshire or GRDC composite monthly runoff data (Fekete et al., 2011), from 1986 to 1995 at a 0.5° spatial resolution. These datasets are composite runoff data that combine simulated water balance model runoff estimates and monitored river streamflow (GRDC). CLM5.0 performs hydrological calibration in a Bayesian framework using a sequential Monte Carlo method (Lawrence et al., 2019). Five models (CLM4.5, DBH, MATSIRO, ORCHIDEE, and PCR-GLOBWB) adjust some parameters according to vegetation or soil properties, but they have no hydrologic calibration. Neither JULES-W1 nor LPJmL calibrate hydrology, although they do calibrate biophysical processes and crop yield, respectively. MPI-HM and H08 are not hydrologic calibrated. Generally, GHMs are hydrologic calibrated based on their main goal of quantitatively simulating the continental water cycle.

4. Review of the global water models included in the study

Global water models were developed from the earliest land surface models created by Manabe (1969), Freeze and Harlan (1969), and Deardorff (1978). These first land surface models simulated the terrestrial water cycle by considering vegetation processes, evaporation, soil moisture, and snow cover. Later on, Dooge (1982) identified the two major challenges of global hydrology: scaling and parameterization. Eagleson (1986) declared the necessity of global-scale hydrology. Inevitably, during the 1990s, the first global hydrological models were developed (Alcamo et al., 1997; Vörösmarty et al., 1998, Arnell, 1999). Over the years, many models have been developed and improved and many studies have been done to assess freshwater resources on the global scale (Bierkens, 2015).

In the present study, we analyze the state-of-the-art global water models included in the global water sector of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP: Frieler et al., 2017). GWMs simulate the terrestrial water cycle, on the global scale, and quantify water flows, water storage compartments, and human water use under past, current, and future climate and socioeconomic conditions. Some of these models also consider reservoir operations. In this study, GWMs do not simulate the ocean component of the global water cycle or water quality. They use input data at 0.5° × 0.5° spatial resolution to obtain their boundary conditions and parameters (Wada et al., 2017). Generally, these models are suitable for application over a minimum catchment size of 9,000 km^2 or at least four grid cells, at 0.5° × 0.5° spatial resolution (Döll et al., 2003; Hunger and Döll, 2008). For smaller catchments, the results are often not reasonable (e.g., Beck et al., 2016) and require some corrections

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(eventual post-process) due to inaccurate input data, spatial heterogeneity, and the lack representation of some hydrological processes, for example, capillary rise, artificial transfers, and pond development (Döll et al., 2003; Hunger and Döll, 2008).

Hattermann et al. (2017) highlighted the role of global and regional water models. Global water models assess the large-scale impacts of climate change and its variability, while regional water models assess the small-scale impacts that are specific to a particular river, catchment, or region. Gosling et al. (2017) underlined that the global and regional water models share many similarities regarding runoff simulation results and their conceptual approach to model development, although the GWM results vary more than regional water results.

Ultimately, GWMs have faced many challenges in selecting a good method to estimate water storage compartments, water flows, and human water use sectors. Some of these are presented in the following subsections.

4.1 Evaluation of global water model to observations

Many ISIMIP studies have evaluated the performance of GWMs for historical time intervals and have highlighted the importance of certain hydrological processes, in addition to many model shortcomings. For example, Wartenburger et al. (2018) concluded that the values of actual land evapotranspiration are affected by the methods used to estimate evapotranspiration, number of soil layers, model structure, and uncertainties in the climate input datasets. Zaherpour et al. (2018) showed that GWMs overestimated mean and extreme monthly runoff, mostly because the ISIMIP precipitation dataset had too-high values and due to the method used to generate surface runoff. They recommended improving the prediction of low runoff and the magnitude and timing of seasonal cycles, investigating methods to calibrate models, testing models with different parameter values, and examining the interconnected uncertainties (e.g., perturbed parameter ensembles: Gosling, 2013). Further, Veldkamp et al. (2018) identified that mean, high and low flows are improved by the parameterization of water abstractions and reservoir operations. However, these are also influenced by uncertainties regarding water abstraction sources, return flow sinks, and the timing of these issues. Masaki et al. (2017) reported that different simulated outflows from reservoirs depend on dam operation algorithms, with similar concepts in some cases, and on the simulated river inflows. Zhao et al. (2017) highlighted the influence of the routing scheme on streamflow timing and magnitude and recommended inclusion of floodplain storage and backwater effects in models.

Scanlon et al. (2019) highlighted that GWMs underestimated GRACE-derived seasonal water storages amplitudes in tropical and (semi-)arid basins and overestimated them in northern high-latitude basins. They suggested to increase the number of soil layers in the models, improve the simulation of snow physics by including processes that delay snowmelt, improve evapotranspiration schemes, and add surface water and groundwater storage compartments to some models.

GWMs were also evaluated a specific case: the 2003 European heatwave and drought (Schewe et al., 2019). The study showed that the models underestimated the streamflow on some European rivers, where no high anomalies were noticed, and underlined the need to further evaluate and improve the models for extreme conditions and to consider all optimistic and pessimistic results in an ensemble as hypotheses.

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335 Nevertheless, GWMs must be evaluated for historical periods before making future projections, in order to validate their performance and reduce uncertainties (Krysanova et al., 2018; Do et al., 2020).

4.2 Climate impact assessments with global water models

Historical performance evaluation studies provide context for further work by evaluating modeled projections of climate change on irrigation water requirements (Wada et al. 2013) and the impact on regional and global water scarcity (Schewe et
340 al., 2014) and on hydrological drought (Prudhomme et al., 2014). The first two studies, Wada et al. 2013 and Schewe et al., 2014, explained the high variation of projected impacts of climate change on the irrigation sector and river discharge through the differences extant in the model structures. A fundamental conclusion of these studies was that hydrological model uncertainty is higher than climate model uncertainty. Prudhomme et al. (2014) underlined that models project little or even no increase in drought frequency if they include the active response of vegetation to CO_2 and to climate change in their structure.
345 Reinecke et al. (2020) highlighted less severe decreases of groundwater recharge, and even increases in some regions, when the CO_2 fertilization effect (*active vegetation*) is considered. Grillakis (2019) found that agricultural droughts (soil moisture droughts) are expected to increase in frequency. Milly and Dunne (2017) concluded that hydrological models overestimated potential evapotranspiration, causing overestimation of actual evapotranspiration and an underestimation of the runoff, in comparison with climate models.
350 Nevertheless, studies on water scarcity and their results are affected by their methodology, definitions, and assumptions.

4.3 Uncertainties of the global water models

Multi-model intercomparison studies showed a significant variation in the model results. One explanation could be that global hydrological modeling imposes uncertainties from forcing data, model parameters, processes included or excluded, and numerical algorithms used. Additionally, each modeling group has a different model development concept and purpose.
355 Ultimately, hydrology is an *inexact science* influenced by *aleatory* (random) and *epistemic* (lack of knowledge) uncertainties (Beven, 2018). Therefore, many models combined in an ensemble approach collect many uncertainties and structural differences.

It has been found that uncertainties of evapotranspiration and snow water equivalent depend on model structures and their algorithms, while uncertainties of runoff depend on climate forcing, specifically, precipitation (Haddeland et al., 2011;
360 Hagemann et al., 2013).

Other uncertainties derive from meteorological data (Müller Schmied et al., 2016); model structure complexity (Döll et al., 2016); parameter estimation (Samaniego et al., 2017); model calibration (Müller Schmied et al., 2014); future scenarios of greenhouse gas emissions, land use management, water management, and socio-economic patterns (Wada et al., 2016a). Finally, many studies concluded that the uncertainty of the hydrological results is primarily determined by the selection of
365 hydrological model and it exceeds the uncertainty caused by selection of climate model or emission scenario (Wada et al.,

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2013; Schewe et al., 2014, Greve et al., 2018). Therefore, there is a need to better understand the models' structure complexity, their equations, and their approaches, and to improve the quality of the input data.

Some methodologies were also created on the catchment scale and they support the evaluation of multi-model structures and parameterizations, also considered as hypotheses on runoff generation, for example, analytical framework (Wagener et al., 2001); the rejectionist framework (Vaché and McDonnell, 2006); Framework for Understanding Structural Errors (FUSE, Clark et al., 2008); SUPERFLEX (Fenicia et al., 2011); Catchment Modelling Framework (CMF, Kraft, 2012); Unifying Multiple Modelling Alternatives (SUMMA, Clark et al., 2015 a and b).

Other methodologies used in the evaluation of parameter values might be found in the Model Parameter Estimation Experiment (MOPEX: Duan et al., 2006), multiple-try DREAM(ZS) algorithm (Laloy and Vrugt, 2012), Generalized Likelihood Uncertainty Estimation methodology (GLUE: Beven and Binley, 2014), perturbed parameter ensembles (Gosling, 2013), the Uncertainty Quantification Python Laboratory platform (UQ-PyL: Wang et al., 2016), Multiscale Parameter Regionalization (MPR, Samaniego et al., 2010 and 2017). Further, some studies have done multiple parameterizations of individual model compartments, to discover how these parameterizations influence the simulations: Essery et al., 2013 (testing 1701 snow models); Niu et al., 2011 (Noah-MP model); Pomeroy et al., 2007 (Cold Regions Hydrologic Model, CRHM); Kuppel et al., 2018 (Ecohydrologic model, EcH2O). Therefore, these methods might offer some solutions for reducing the high number of parameters and their values still found in global water models, and to apply more reasonable regionalization schemes in global hydrological research (Bierkens, 2015).

Other methods can also be found in frameworks proposed by Döll and Romero-Lankao, 2017 and Kundzewicz et al., 2018.

In the end, Arheimer et al., 2020 showed that the catchment models can be applied at a global scale because of the new global datasets, increased computational capacity, new methods to estimate parameters, and collaboration. Thus, GWMs may even become a part of the ESMs used to simulate the water cycle at a high resolution, including human water demand and use (Wood et al., 2011; Bierkens, 2015).

5 Similarities and differences among global water models

Similarities and differences among models are presented according to eight water stocks, five human water use sectors, and desalination.

5.1 Similarities and differences in simulating water storage compartments

Canopy water storage. The changes in canopy water storage depend on how much water evaporates (canopy evaporation) and how much water is intercepted by canopy. Thirteen models include canopy water storage in their structure, while three other models do not include it (H08, Mac-PDM.20, and MPI-HM: Table S3). Ten models compute canopy water storage by subtracting the throughfall amount and canopy evaporation from the total precipitation. Other three models (CLM4.5, CLM5.0, and MATSIRO) compute canopy water storage by subtracting the liquid or solid throughfall and canopy evaporation from the

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precipitation intercepted by the canopy storage. MATSIRO is the only model that has two canopy water compartments: one for rainfall interception and one for snowfall interception. It also computes in detail how much water is intercepted by canopies in stormy areas with high wind speeds and in calm areas with low wind speeds. In these areas, precipitation depends, mainly, on leaf area index (LAI) and water deficit in the canopy storage.

Three land surface models (CLM4.5, CLM5.0, and MATSIRO) divide total precipitation into precipitation intercepted by canopy, precipitation that penetrates the canopy and then reaches the ground (throughfall), and precipitation that falls directly on the ground (Tables S4–S6). Further, they also divide throughfall into liquid and solid phases.

Two models compute an interception scheme based on a leaf and stem area index, while seven models use only a leaf area index (Tables 7 and 8). Ten models compute this considering vegetation type (a plant functional type system) (Tables 7 and 8). MPI-HM used prescribed data taken from Land Surface Parameter dataset version 2 (Hagemann, 2002). PCR-GLOBWB uses HYDE3.2 (Klein Goldewijk, 2017), MIRCA (Portmann et al., 2010), and GlobCover datasets (ESA GlobCover Project, 2005). Generally, prescribed vegetation ignores the decisive interaction between vegetation and runoff as well as interactions between the atmosphere and Earth's surface.

Throughfall is estimated by 13 models (Table S5) depending on 1. total precipitation and relative canopy water content (JULES-W1); 2. difference between total precipitation and canopy storage deficit (mHM, WaterGAP2, WAYS); 3. ratio between rainfall or snowfall and total precipitation (CLM4.5, CLM5.0, MATSIRO); 4. total precipitation and minimum value of potential evapotranspiration (PET) or canopy storage (LPJmL); 5. canopy water content (PCR-GLOBWB); 6. a function of LAI then weighted by the canopy fraction in the grid cell (DBH and ORCHIDEE); 7. canopy water content and grid cell average precipitation (VIC); 8. total precipitation, canopy water content, and canopy evaporation (CWatM). Three models (H08, Mac-PDM.20, MPI-HM) do not estimate throughfall.

Four models (CLM4.5, CLM5.0, LPJmL, and ORCHIDEE; Tables 7 and 8) account for the CO_2 fertilization effect, in the LAI estimation, by using a photosynthesis scheme (*active vegetation* mentioned in section 2.1), and they have the ability to simulate the CO_2 effect on plant functioning. Generally, it was found that simulations depend on the number of PFTs prescribed or defined in the model and on the processes used to estimate plants' ability to adapt, acclimate, and grow in new environmental conditions (Sitch et al., 2008).

Snow water storage accumulates snow below freezing and loses snow by melting and surface and/or snowdrift sublimation. GHMs use the degree-day method to compute snow accumulation and snowmelt, while LSMs use the energy balance method (Tables 7 and 8). Among GHMs, H08 is the only one that applies the energy balance method to compute snow accumulation and melt. Additionally, three models (CLM4.5, CLM5.0, and CWatM) include glacier storage. CLM4.5 and CLM5.0 use a physically based snow module to calculate snow accumulation and melt; therefore, they include multiple snow layers where compaction, melt, refreezing, firn, and other snow related processes take place.

Four models (CLM4.5, CLM5.0, MPI-HM, and VIC) have two water storage compartments for snow: for estimation of frozen water and for liquid water content (Table S8). WaterGAP2 calculates snow accumulation and melting in 100 subgrid cells using a degree-day algorithm (Schulze and Döll, 2004; Müller Schmied et al., 2014), while CWatM calculated using 3 to 10

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elevation zones per grid. Five models (CLM5.0, DBH, JULES-W1, MATSIRO, and VIC) estimate snow held on the canopy, while ten models do not estimate it (Table S9). Further, seven models differentially estimate snow under the canopy (Table S10). Five models do not estimate sublimation: Mac-PDM.20, mHM, MPI-HM, PCR-GLOBWB, and WAYS (Table S11). MATSIRO is the only model that distinguishes between sublimation on snow-covered ground and snow-free ground. Snow layers vary between 1 (most of the GHMs) and 12 (CLM5.0; Tables 7 and 8).

Soil water storage keeps and loses water from flows above and below the ground's surface. Hydrologically, this includes an unsaturated zone.

Soil hydrologic processes. Overall, 10 models consider initial infiltration as inflow of the soil storage, while 3 models (H08, JULES-W1 and WAYS) consider throughfall (Table S14). Mac-PDM.20 considers total precipitation as inflow of soil storage (Table S14). All models compute surface runoff (Table S20), soil evaporation (Table S24), and infiltration (Table S25), while six models compute interflow (Table S26). Six models compute Hortonian overland flow (Table S21) and six models compute saturation excess overland flow (Table S22). H08 computes runoff properties varying according to the climate zone (Table 7). CLM4.5 includes an empirical soil evaporation resistance parameterization, while CLM5.0 includes a mechanistically based parameterization where the soil evaporation is controlled by a dry surface layer. Therefore, CLM5.0 has the ability to model the seasonality of soil evaporation and soil water storage in (semi-)arid regions. It also explicitly simulates spatial variation in soil thickness (0.4 to 8.5 m) and columnar water holding capacity, unlike CLM4.5 (Lawrence et al., 2019). These models have a large number of soil layers, each having moisture storage potential depending on the soil texture. They use the same approach to calculate surface runoff and have the ability to compute liquid runoff and solid runoff from snow capping. Both models consider subsurface runoff as a product of an exponential function of the water table depth and a single coefficient (Niu et al., 2005). VIC uses the variable infiltration curve (Zhao et al., 1980) to account for the spatial heterogeneity of runoff generation, and assumes that surface runoff from the upper two soil layers is generated by those areas where precipitation exceeds the storage capacity of the soil. The mHM model has one more bucket between the soil storage and groundwater storage named "unsaturated storage" representing the source for interflow and groundwater recharge.

LPJmL was adjusted, and the water from the uppermost soil layers is considered to contribute to surface runoff if excess of storage is calculated according to the infiltration or percolation rates, which depend on soil type. LPJmL routes, what was previously lateral runoff, from "layer 0" (first 20 cm), as surface runoff.

In JULES-W1, water that reaches the soil surface is split between water that infiltrates into the soil and surface runoff. Infiltration takes place at a rate equal to saturated hydraulic conductivity multiplied by an infiltration enhancement factor, which is dependent on the presence and type of vegetation. If a soil layer becomes saturated, the water in excess of saturation is put into the layer below. JULES-W1 also uses a "zero-layer" scheme that does not use explicit model layers to represent snow, instead adapting the topsoil level to represent lying snow processes (Best et al., 2011). WAYS simulates the water storage and flows in soil only for the entire root zone (Table 8). In the DBH model, runoff is generated directly when soil layer is saturated, or is generated when rainfall intensity is larger than the infiltration rate estimated with the Green–Ampt method (Tang et al., 2006).

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Two models (CWatM and MPI-HM) have an additional water storage compartment to compute the runoff concentration in a grid cell that has a lag time before entering the river storage compartment (Table S19). Consequently, this storage serves to create a delay between runoff and streamflow, and accounts for the average distance that runoff, generated at a specific point within a grid cell, has to travel before reaching the river. This storage collects water from rivulets and creeks or concentrates runoff in rivulets and creeks before it enters the river storage, because the rivulets and creeks are smaller than the size of a single grid cell and have different water retention properties from the main river channel within the grid cell. Therefore, this compartment does not act as a floodplain, to delay floods, or as overland flow, to express too much water in the soil. In its original structure, MPI-HM named this compartment "overland flow", but we decided to rename it "rivulet storage" to avoid confusion among readers.

Some GWMs compute vertical water movement in unsaturated soils by applying the Richards equation (Richards, 1931; e.g., CLM4.5, CLM5.0, CWatM, JULES-W1, MATSIRO, ORCHIDEE, VIC). However, the Richards equation might be not relevant for the models that have one soil layer. LPJmL uses a percolation scheme to estimate vertical water movement that applies the storage routine technique developed by Arnold et al. (1990) and simulates free water in the soil bucket. DBH uses the Green–Ampt equation to compute infiltration in unsaturated soils.

Two models (CWatM, LPJmL) compute percolation (infiltration below the root zone; Table S27). Five models compute capillary rise (CLM4.5, CLM5.0, CWatM, MATSIRO, and PCR-GLOBWB), with CWatM and PCR-GLOBWB using the same approach (Table S28).

Soil column configuration. Number of soil layers ranges between 1 (H08, MPI-HM, and WaterGAP2) and 25 (20 soil layers + 5 bedrock layers: CLM5.0), while total soil depth is between 1 m (H08) and 49.6 m (CLM5.0; Tables 7 and 8). ORCHIDEE uses a relatively deeper soil column to account for soil thermic. LPJmL has five hydrologically and thermal active soil layers plus one thermal active soil layer. MPI-HM defines soil storage in terms of the maximum water column, varying between 0 and 5 m; therefore this cannot be translated into soil depth directly. Five models (CLM4.5, CLM5.0, CWatM, MATSIRO, and VIC) compute frozen soil (Table S13).

Groundwater storage, beneath the soil water storage compartment, receives water from seepage and groundwater recharge. It loses water through capillary rise, groundwater runoff, and abstraction for human water use. Hydrologically, it includes the saturated zone or phreatic zone. Eleven models include groundwater storage in their structure, and most of them have only one groundwater layer (Tables 9, 10, S29). In ISIMIP2b, two models (JULES-W1 and LPJmL) consider the water excess from the bottom soil layer as *seepage* and relate this variable with *groundwater runoff* and *groundwater recharge* because they do not have a groundwater compartment.

CLM4.5 simulates an unconfined aquifer parameterization as a groundwater component, below the saturated soil storage and with a prescribed maximum value (5000 mm), while CLM5.0 simulates an impermeable bedrock with five layers and therefore assumes no groundwater flow as bottom boundary conditions. In CLM4.5, the unconfined aquifer interacts with the saturated soil storage through the water table, whether it is within or below this storage. When the water table is below the soil storage, the aquifer recharge is estimated by applying Darcy's law across the water table (Lawrence et al., 2019).

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MATSIRO has a dynamic groundwater scheme (Koirala et al., 2014; Pokhrel et al., 2015) in which the number of soil layers in the saturated zone (i.e., groundwater) varies in time depending on water table location between 1 and 13 (Table 7). The two-way interaction between the unsaturated zone (for which vertical moisture movement is resolved by solving the Richards equation) and the underlying aquifer is simulated through moisture flux exchange at the water table. This flux exchange is determined as the algebraic sum of downward gravity drainage from the unsaturated soil layer overlying the water table and the upward capillary flux (Koirala et al., 2014; Pokhrel et al., 2015). The water balance of the saturated zone is resolved by considering recharge to the groundwater aquifer and groundwater runoff that is determined by using a two-parameter, statistical-dynamical formulation considering soil hydraulic properties and basin geomorphology (Yeh and Eltahir, 2005). The variation in the water table is also determined by the aquifer specific yield.

In Mac-PDM.20, it is assumed that all water in excess of field capacity drains in one day to the deep store, which for ISIMIP2b is used to represent groundwater recharge (R_{gwr}). The total runoff (q_{tot}) is the sum of direct runoff (q_s) plus delayed runoff from the deep soil and groundwater (q_{sb}). This delayed runoff (q_{sb}) is assumed to be a non-linear function of the amount of water held in the groundwater and deep soil store (Table S31). Thus, like with MPI-HM, the purpose of the delayed runoff (or baseflow) is predominantly to cause a delay in river discharge and not to simulate groundwater in detail.

H08 separates groundwater into renewable and one nonrenewable layers (Hanasaki et al., 2008). WaterGAP2 is the only model that simulates the groundwater recharge from surface water bodies in semiarid and arid grid cells (Döll et al., 2014).

Fourteen models compute groundwater recharge, three using the same approach (H08, WaterGAP2, and WAYS: Döll and Fiedler, 2008; Table S30), while twelve models compute groundwater runoff (Table S31).

Lake storage fills with water through flows above and below the ground and stores water for a certain residence time. It loses water through discharge to other storages, evaporation, groundwater recharge, and water abstraction for human water use. Ten models do not include lakes (Tables 9 and 10). Five models compute evaporation from lakes, three of them based on a PET approach (Table S33), while four models compute outflow from lakes (Table S34). CLM4.5 and CLM5.0 compute the lake storage as virtual storage where the difference between precipitation and evaporation is balanced automatically by their outflow, named *lake runoff*. CLM4.5 uses constant lake depth, while CLM5.0 uses spatially variable lake depth, and freezing and thawing are included in the lake body (Vanderkelen et al., 2020).

LPJmL treats natural lakes and rivers in a similar way in terms of inputs and output. Lake inputs to a river can also include upstream river inputs to the lake. LPJmL also keeps track of a lake fraction in the river input. WaterGAP2 and CWatM have two types of lake storage: “local lake storage”, gets water from runoff resulting within the cell, and “global lake storage”, gets water from runoff resulting within the cell and the upstream cell (Döll et al., 2012). For ISIMIP2b, MPI-HM has used the prescribed wetlands and lakes extent, taken from the Land Surface Parameter dataset 2 (Hagemann, 2002).

Reservoir storage fills with water behind dams through flows above and below the ground and stores water for a residence time. It loses water through discharge to other storages, evaporation, groundwater recharge, and water abstraction for human water use. Ten models (CLM4.5, CLM5.0, DBH, JULES-W1, Mac-PDM.20, mHM, MPI-HM, ORCHIDEE, VIC, and WAYS) do not include reservoir storage for ISIMIP2b (Tables 9, 10, S35). Further, only WaterGAP2 simulates explicitly the

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reservoirs, lakes, and wetlands (Tables 9 and 10). Six models compute outflow from reservoirs (Table S37), while evaporation from reservoirs is computed by four models (Table S38).

In general, most of the models use the Global Reservoir and Dam database (GRanD: Lehner et al., 2011), but with a different number of active managed reservoirs, used for reservoir operation during simulations. Three models (LPJmL, WaterGAP2 and PCR-GLOBWB) merge more than one reservoir per grid cell into one reservoir, if required.

Four models (CWatM, H08, MATSIRO, and WaterGAP2) use two water compartments, global and local reservoirs, to represent the reservoirs, following the reservoir algorithm developed by H08. However, there are some differences on how the scheme was implemented in the models, mainly, because of model structure, but the approach is essentially the same. These four models use the same approach in selecting active managed reservoirs for reservoir operation, but they use different thresholds. WaterGAP2 considers 1109 active managed reservoirs and handles reservoirs below 0.5 km^3 storage capacity as local lakes. MATSIRO considers only 728 out of 6862 reservoirs for reservoir operation. In MATSIRO, global reservoirs have more than 1 km^3 total storage capacity and "local reservoirs" or "ponds" have less than 1 km^3 (around 6134 reservoirs; Hanasaki et al., 2006; Pokhrel et al., 2012a and b). H08 considers 963 active managed reservoirs (global reservoirs) and 5824 local reservoirs; therefore, global reservoirs regulate river flow, while local reservoirs do not. Global reservoirs have 4773 km^3 of total storage capacity, while local reservoirs have 1300 km^3 of total storage capacity. In H08, when multiple local reservoirs are present in a grid cell, their capacity is added together. CWatM considers 3663 active managed reservoirs, while PCR-GLOBWB considers 6177. LPJmL includes 4134 reservoirs that become active after the first year of operation. In LPJmL, reservoirs are not managed according to an operation scheme, they are modeled as lakes with a maximum storage amount and the water over this amount is released as reservoir outflow; irrigation water can also be taken from the reservoir.

Five models (CWatM, H08, LPJmL, MATSIRO, and WaterGAP2) use a retrospective reservoir algorithm, while one model (PCR-GLOBWB) uses a prospective reservoir algorithm. The retrospective reservoir algorithm uses river flows and water demand, which were processed in a previous step, while the prospective reservoir algorithm uses predicted river flows and water demand (van Beek et al., 2011).

Wetlands storage fills and empties with water similarly to lake and reservoir compartments. Two models (MPI-HM and WaterGAP2) compute wetland compartment, evaporation, and outflow from land (Tables S39–S42). WaterGAP2 has two types of wetland storage: “local wetland storage”, which obtains water from runoff resulting within the cell, and “global wetland storage”, which obtains water from runoff resulting within the cell and the upstream cell (Döll et al., 2012).

River storage fills with water through flows above and below the ground. It loses water through streamflow, evaporation, channel transmission, and water abstraction for human water use. Five models (DBH, JULES-W1, Mac-PDM2.0, VIC, WAYS) do not include river storage for ISIMIP2b simulations, because of computational and resource constraints, nor do they compute streamflow (Tables 9, 10, S43, and S46). Four models (LPJmL, MATSIRO, MPI-HM, WaterGAP2) use a linear reservoir cascade approach to compute the water balance of the river storage (Tables 9 and 10). Furthermore, MATSIRO uses Total Runoff Integrating Pathways (TRIP) for river routing through a channel. Three models (CWatM, H08, and LPJmL) consider the minimum release for environmental flow. CWatM adopts a kinematic wave approach, approximation of the Saint-

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Venant equation (Chow et al., 1998), linked with dynamic reservoir and lake operation. Further, CWatM computes runoff concentrated in creeks and rivulets, with a lag time before entering the river storage, by using a triangular weighting function (Burek et al., 2020). ORCHIDEE includes a river transport module that involves the Simulated Topological Network (STN-30p). PCR-GLOBWB uses a travel time routing (characteristic distance) linked with dynamic reservoir operation. For runoff and streamflow simulation, CLM4.5 uses a river transport model (RTM), while CLM5.0 uses a new physically based runoff routing model, called the Model for Scale Adaptive River Transport (MOSART; Oleson et al., 2013, Lawrence et al., 2019). The mHM model uses a mesoscale routing model with an adaptive time step according with the spatially varying celerity (Thober et al., 2019). Only MPI-HM and ORCHIDEE include a routing model with a wetlands and floodplain scheme, in which wetlands act as floodplains. Furthermore, ORCHIDEE includes swamps.

Six models (CLM5.0, CWatM, MPI-HM, ORCHIDEE, PCR-GLOBWB, WaterGAP2) apply the Manning–Strickler equation to estimate river flow velocity and use various values for it. CLM4.5 uses a standard river flow velocity of 0.35 m s^{-1}, while H08 and MATSIRO use 0.5 m s^{-1} (Tables 9 and 10). LPJmL considers a standard river flow velocity of 1 m s^{-1}. MPI-HM uses the Manning–Strickler equation only for flow velocity computation in wetlands, while, for rivers, it computes a slope-dependent flow velocity following the approach by Sausen et al. (1994).

Inflow from upstream grid cell surface water bodies represents the sum of inflow water from neighboring upstream grid cells for CLM4.5, CLM5.0, CWatM, mHM, and WaterGAP2 (Table S45). Additionally, CWatM and WaterGAP2 route this water also through lakes and reservoirs before it reaches its final point. H08 computes it as being the product between a 0.5 m s^{-1} flow velocity and river storage from upstream grid cells. LPJmL considers it as being the outflow of river storage reduced by evaporation from lakes and reservoirs, while MPI-HM considers it as being the sum of outflow from rivulet storage, groundwater runoff, and streamflow from the upstream grid cells, then reduced by inflow from the wetland of an upstream grid cell. MATSIRO considers it as being the sum of inflow water from the neighboring upstream grid cell multiplied by outflow of river from an upstream grid cell. ORCHIDEE calculates it as being the sum of stream river storage of upstream grid cells divided by topographic index of the retention time and a reduction factor of stream river storage. PCR-GLOBWB takes into account the outflow from river storage, time of process duration, length of river sections, and the coefficient friction of the reservoir weir.

Evaporation from rivers is computed only by three models, CWatM, LPJmL, and PCR-GLOBWB, based on a PET approach (Table S47).

5.2 Similarities and differences in simulating human water use sectors

Some GWMs simulate water extracted from surface water compartments and/or a groundwater compartment that is used for human activities. Human water abstraction represents the sum of the water consumed by humans, evaporative and speculative water losses (named *water consumption*), and water returned to the groundwater or surface water compartments (named *return flow*, being the part of the water not consumed). Generally, three models extract water for human activities from groundwater

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or surface water bodies (H08, PCR-GLOBWB, and WaterGAP2). Seven models (DBH, JULES-W1, Mac-PDM.20, mHM, ORCHIDEE, VIC, and WAYS) do not include any human water use sectors in their structures (Table 6).

Irrigation sector. Irrigation water demand (potential irrigation water abstraction) is computed by three models (Table S52). Groundwater abstraction and its consumption for the irrigation sector is simulated by five models (CWatM, H08, MATSIRO, MPI-HM, and WaterGAP2: Tables S53 and S54), while three models explicitly compute the return flow (Table S55). Irrigation surface water abstraction is calculated by nine models (Table S56, Tables S100–S101). CWatM includes a "normal irrigation scheme", to mimic rainfall when the plants need it, and a paddy rice irrigation scheme, to mimic the flooding of the rice area (Table S56).

The main water source for the irrigation sector is *river* for nine models (CLM4.5, CLM5.0, CWatM, H08, LPJmL, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2), and then the secondary source is *groundwater* for six models (CWatM, H08, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2). Five models take water from lakes for the irrigation sector and four models take water from reservoirs. Only two models take water for irrigation from the ocean (Figure 1). Return flows from irrigation sector recharge the soil (seven models), groundwater (seven models), and rivers (six models), while the return flows from domestic and manufacturing recharge lakes (three models), reservoirs (two models), and rivers (five models; Figure 2).

Domestic, livestock, and industry sectors. Generally, four models (H08, MATSIRO, PCR-GLOBWB, and WaterGAP2) simulate water abstraction, water consumption, and return flow for the domestic (household: Tables S59–S64) and manufacturing sectors (Tables S69–S74). MATSIRO and LPJmL used prescribed data for water demand of the domestic and industry sectors, offered by the ISIMIP2b framework, representing annual sums divided evenly over all days. These input datasets provide water consumption, but not return flow from these sectors. Consumption water can return to the atmosphere as evapotranspiration. LPJmL used prescribed data for domestic and industrial water consumption data and assumed that only the consumed water amount is withdrawn. MATSIRO used prescribed data for domestic and industrial water demand and it computed itself the water abstraction and consumption for these sectors, by applying a simple approach. ISIMIP2b does not offer prescribed data for livestock sector. MATSIRO combines manufacturing and electricity sectors in one sector, the industry sector. PCR-GLOBWB computes amount of water abstracted and consumed for livestock sector, taken from groundwater and surface water bodies (Tables S65–S68), while WaterGAP2 computes only the amount of water taken from surface water bodies (Tables S67–S68). WaterGAP2 is the only model that computes amount of water abstracted and consumed for electricity sector (Tables S75–S76).

Total groundwater abstraction (Table S77) is computed differently by MATSIRO, MPI-HM, and WaterGAP2. MATSIRO and WaterGAP2 take similar approaches: groundwater abstraction for the irrigation sector is reduced by the sum of groundwater abstraction for the domestic and industry sectors. MPI-HM considers the total as being equal only to groundwater abstraction for the irrigation sector, as other sectors are not included in the model.

Total lake abstraction (Table S78) is computed differently by LPJmL, MPI-HM, PCR-GLOBWB, and WaterGAP2. LPJmL sums the gross irrigation requirement and household, industry, and livestock demand in the grid cell, with gross irrigation requirement and household, industry, and livestock demand in the downstream grid cell. MPI-HM considers lake abstraction

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equal to surface water abstraction for the irrigation sector, while PCR-GLOBWB sums water abstraction demand for the industry, irrigation, domestic (household), and livestock sectors. WaterGAP2 computes it as the sum of water abstraction for the irrigation, livestock, domestic, manufacturing, and electricity sectors taken from surface water bodies. The net surface water abstraction is satisfied in WaterGAP2 in the following order: 1) river, 2) global lakes and reservoirs, and 3) local lakes.

Total reservoir abstraction (Table S79) is computed differently by H08, LPJmL, MATSIRO, PCR-GLOBWB, and WaterGAP2. H08 considers it as being sum of monthly water abstraction for the irrigation, industry, and domestic sectors. LPJmL adds up the gross irrigation requirement and household, industry, and livestock demand at the grid cell with the gross irrigation requirement and household, industry, and livestock demand at the downstream grid cell (similar to lake abstraction). MATSIRO adds up water abstraction from reservoir for the domestic, industry, and irrigation sectors, while PCR-GLOBWB adds water abstraction demand for the industry, irrigation, domestic (household), and livestock sectors (similar to lake abstraction). WaterGAP2 sums up water abstraction for the irrigation, livestock, domestic, manufacturing, and electricity sectors taken from surface water bodies. The net surface water abstraction is satisfied in WaterGAP2 in the following order: 1) rivers, 2) global lakes and reservoirs and 3) local lakes.

Total river abstraction (Table S80) is computed by CLM5.0 and WaterGAP2. WaterGAP2 considers it as the sum of water abstraction for the irrigation, livestock, domestic, manufacturing, and electricity sectors taken from surface water bodies. The net surface water abstraction is satisfied in WaterGAP2 in the following order: 1) rivers, 2) global lakes and reservoirs and 3) local lakes (similar to lake and reservoir is equal to surface water bodies).

5.3 Similarities and differences in simulating desalination

Seawater abstraction, consumption, and return flows (Tables S81–S83) are computed only by H08 (Hanasaki et al., 2018). Seawater abstraction represents the sum of seawater abstraction for the municipal and industry sectors. Three conditions must be met in order to use desalination: i) GDP > USD 14,000 person year^{-1} in terms of purchasing power parity (PPP); ii) humidity index below 8%; iii) within three grid cells of the seashore. It is assumed that seawater desalination is not used for irrigation and that all demand for municipal and industrial water is abstracted by desalination if available. In the context that desalination is not used for irrigation, seawater consumption represents seawater abstraction weighted by the ratio of consumption to withdrawal, which is equal to 0.1 and 0.15 for industrial and municipal water use. Return flow from seawater abstraction represents seawater abstraction weighted by the non-used fraction (0.1 and 0.15 for industrial and municipal water use) and proportion lost during delivery (set to zero).

5.4 Examples of how parameterization can differ between GWMs

Different equations used by GWMs led to different model results, for example, different evapotranspiration methods led to significant differences in runoff estimation (Gosling and Arnell, 2011b; Kingston et al., 2009). The equations include parameters that are used to calibrate GWMs. The application of different parameter values can lead to different results between

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models (as can the employment of different model structures). For example, we present how global water models simulate the groundwater recharge and the maximum value of canopy storage differently.

Groundwater recharge (Table S30) is computed by 14 models. JULES-W1 and LPJmL do not include in their structure groundwater storage and seepage (the water that seeps from the last soil layer), which was reported as groundwater recharge and groundwater runoff for ISIMIP2b. CLM4.5 and CLM5.0 use the same approach to compute groundwater recharge, by using the concept of soil matrix potential and considering the hydraulic conductivity of the layer containing the water table. CWatM and PCR-GLOBWB use the same approach by reducing percolation with capillary rise, but CWatM also considers preferential flow as inflow. DBH estimates it depending on potential soil water content multiplied by the soil depth layer and maximized by soil hydraulic conductivity. Three models (H08, WaterGAP2, and WAYS) consider it as being the minimum value between maximum groundwater recharge and total runoff from land, weighted by a relief-related factor, a soil texture-related factor, a hydrogeology-related factor, and a permafrost- and/or glacier-related factor (Döll and Fiedler, 2008). Further, WaterGAP2 sets (semi-)arid grid cells, sandy texture, and grid cells with throughfall equal or below 12.5 (mm day^{-1}) to 0. MATSIRO estimated groundwater recharge as being the variation of unfrozen soil moisture over time. MPI-HM equals groundwater recharge to percolation. ORCHIDEE estimates it depending on relative soil water content, but it is capped down to 0 and maximized by groundwater runoff.

Maximum value of canopy storage (Table S7). Another example is that the models estimate differently the maximum value of canopy storage and leaf area index (LAI) values. WaterGAP2 and WAYS estimate the maximum value of canopy storage by multiplying 0.3 mm with LAI. Further, WAYS estimates seasonal LAI depending on the growing-season index, day length, and the actual root zone water storage. The root zone soil moisture stress parameter is fixed at 0.07, while WaterGAP2 estimates LAI based on a simple growth model and based on land cover characteristics (Table S7). VIC multiplies 0.2 mm by the monthly LAI. Additional, VIC takes into account aerodynamic and architectural resistances. CWatM equals maximum value of canopy storage with LAI that varies every 10 days depending on land use classes.

5.5 How many water flows, water storage compartments, and human water use sectors are included in the GWMs?

One way of showing the number of equations and/or parameterization schemes that comprise a model is to count the number of water flows, storage compartments, and use sectors existent in each model participating in ISIMIP2b. Generally, GHMs have a high number of water storage compartments because their main purpose is to simulate the water cycle. LSMs and DGVMs have a relatively smaller number of process (in this count), but each process is simulated in a more sophisticated way or has a physically based representation. LSMs exclude some hydrological processes because they are not relevant for their research purpose, spatial resolution, or cannot be parametrized in a general manner, adding some uncertainty.

In this study, WaterGAP2 includes the highest number of water storage compartments (11; see Figure 3), while JULES-W1, Mac-PDM.20, and VIC have the lowest, three water compartments (Figure 3). Others include CWatM, with ten compartments, then MATSIRO (seven compartments), followed by seven models (CLM4.5, CLM5.0, H08, LPJmL, mHM, MPI-HM, and PCR-GLOBWB) with six compartments. Seven models do not simulate water used by humans for economic purposes such as

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irrigation, domestic, livestock, manufacturing, electricity, and desalination (Figure 4). Four models (CWatM, MATSIRO, H08, and LPJmL) combine the manufacturing and electricity sectors in one sector: the industry sector. WaterGAP2 simulates five human water use sectors. Three models (H08, PCR-GLOBWB, and CWatM) simulate four human water use sectors and one model (MATSIRO) simulates three. Four models (CLM4.5, CLM5.0, LPJmL, and MPI-HM) simulate only water used by humans for the irrigation sector. WaterGAP2 has the highest number of water flows (22) to simulate water use, while MPI-HM has the lowest number (2; Figure 4).

6 Challenges and potential in global hydrological modeling

6.1 Challenges in making this intercomparison study

We encountered many challenges in harmonizing terminology among the 16 global water models, as well as among climate, global hydrological, and vegetation communities. It was challenging to intercompare the global water models using their different style in describing the model structure, defining the variables, and writing the model equations. Therefore, we decided to create a standard writing style for model equations, presented in subsection 3.2, and to decide upon clear definitions of the analyzed variables.

We discovered that, in some models, *groundwater runoff* and *baseflow* are used synonymously and define the water that leaves groundwater storage. We also found that *baseflow* and *subsurface runoff* are used synonymously, and define the amount of water estimated for the third soil layer (VIC). Hence, we decided to use *subsurface runoff* synonymously with *interflow* and to define it as the amount of water that leaves the soil layer laterally. In this paper, *baseflow* is considered to be the low part of the streamflow that is supplied by groundwater, drainage from lakes, wetlands, glaciers, and interflow during long periods when no precipitation or snowmelt occurs. Ultimately, we have excluded the variable *baseflow* from the analysis because it is not simulated by GWMs in ISIMIP2b.

MPI-HM includes additional storage, called *baseflow storage*, that collects the drainage leaving through the bottom of the soil storage and applies a substantial time lag before passing it on to the river storage. In ISIMIP2b, the drainage computed by MPI-HM was submitted as subsurface runoff, but considering that this baseflow storage acts similarly to a groundwater storage, drainage could be used as groundwater recharge in ISIMIP3a/b. Consequently, its outflow could be submitted as groundwater runoff. However, the purpose of this baseflow storage is predominantly to cause a delay in river discharge and not to simulate groundwater in detail.

We also found out that the words *drainage* (MPI-HM), *aquifer recharge* (CLM4.5), and *groundwater recharge* (GHMs) are used synonymously to define the amount of water that reaches the groundwater storage. In this case, we decided to use only *groundwater recharge*, because of its hydrological meaning.

We define *percolation* as the amount of water that infiltrates beyond the root zone and *seepage* as the amount of water that leaks at the bottom of the soil storage. We relate *seepage* with *groundwater recharge* and *groundwater runoff* for the models that do not include a groundwater storage, supposing that this water would reach groundwater storage if it would exist.

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Another discovery was that *throughfall* and *drip* in some models were considered synonyms and they were used to describe precipitation that falls to the ground through canopy spaces (CLM4.5, CLM5.0, MATSIRO). In this case, we decided to separate these words and to define *throughfall* as being precipitation that falls to the ground through canopy spaces and *drip* as being precipitation that leaks at the edge of canopy.

We conclude that within hydrology and among communities there is great confusion regarding the terminology used, including the variables and their definitions. Therefore, we need to communicate, interact, and engage to clarify the meaning of the words and processes, and to facilitate easier communication, understanding, and analysis.

6.2 Challenges in global hydrological modeling

Simulating the terrestrial water cycle on the global scale involves many challenges. These various challenges were identified by reviewing articles published by the climate, global hydrological, and vegetation communities (Table 11). The challenges have been classified according to the 23 unsolved problems in hydrology (UPH), identified by Blöschl et al., 2019, to harmonize the efforts of the global and catchment hydrological communities. These challenges can generally be overcome through the development of new datasets, innovative and creative collaboration among communities, and investment in technical infrastructure.

6.3 Recommendations for multi-model intercomparison projects

Multi-model intercomparison projects (MIPs) are based on communication and collaboration. Ideally, through collaboration, communities will fill in existing knowledge gaps, improve the quality of the input data and the processes in the models, and implement the missing processes in the models.

Wagener et al., 2020 well described the hydrological knowledge gaps as *hydrologic lions*, similar to the knowledge gaps of medieval maps represented as lions. They proposed focusing hydrological research on openly shared perceptual models, inclusion of metadata for each hydrologic study (e.g., location and time period covered by a study), and effective knowledge accumulation. In addition to these statements, we also propose focusing on effective collaboration that starts with effective *wish lists*, including specific research questions, goals to answer these questions, methods to achieve the goals, datasets to be used, and tasks to be done.

We encourage communities to write and convey clear, simple, and understandable texts for large audiences. We consider that *simplicity* improves communication, and communication starts with a common language, the same words having the same meaning for the sender and the receiver. Theoretically this is possible, but in practice, there are some discrepancies among scientists (highlighted in subsection 2.2), as well as between scientists and stakeholders, as revealed by Sultan et al. (2020). They underlined that scientists and stakeholders use vocabulary differently in climate impact science.

The review of GWMs, presented in section 4, highlights the need to design hydrological inter-model comparison studies by nominating models or research questions according to some specific criteria, for example, (i) specific model compartments (Nazemi & Wheater, 2015; Wada et al., 2017), (ii) specific evaluation metrics (Gupta et al., 2009; Veldkamp et al., 2018;

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Zaherpour et al., 2018), (iii) locations of specific hydrological indicators, regions, or rivers (Masaki et al., 2017; Veldkamp et al., 2018). These studies still emphasized the need to improve the quality of the input data, upgrade the hydrological processes in the models' structure, integrate missing hydrological processes, and further reduce uncertainties.

We recommend, for the benefit of the multi-model intercomparison projects, to 1. maintain very good documentation of the model code; 2. always start research with a list, for example, with water storage compartments, flows, and human water use sectors included in the model structures; 3. have clear definitions of the variables, water storage compartments, flows, and human use sectors, describing exactly their role in the model; 4. have synonyms for variables, helping to show similarities and differences among models; 5. collect all ideas, recommendations, and improvements received from everyone (in our case, they were required to complete our study); 6. collaborate and communicate with peers, which was very useful in our study for identifying synonyms among communities; 7. describe *your model* or *a model* through *your eyes* and *other's people eyes*; 8. invest much time and patience and be meticulous about extracting equations of water storage, flow, and human water use sectors from the model code.

Our future research will include describing the GWMs analyzed in this study, through a standard visualization of the water cycle that will show the water storage compartments, water flows, and human water use sectors included in the ISIMIP2b model structures. These diagrams would be connected with the tables presented in the supplement of the present paper (Tables S1–S83).

We affirm that model intercomparison projects need to organize workshops on model parameterization including some *parameterization* experiments and some evaluation studies on the equations applied to compute water storage compartments, water flows, and human water use sectors, as well as considering model outputs. We also note that this review and description study had a positive impact on the modeling groups, motivating them to re-think and re-analyze model structures, equations, and descriptions.

6.4 Potential future research in global hydrological modeling

In this study, we analyzed the GWMs version used for ISIMIP2b. Hence, in their original structure, these models include some water stocks, water flows, and human water use sectors that have not been used for ISIMIP2b. In this section, we present potential future research for the 16 analyzed modeling groups (Tables S102 and S103).

Some GWMs, such as gridded models, have the ability to operate at various spatial–temporal scales: CWatM, CLM4.5, CLM5.0 (3 h time step at around 11 km).

Numerous developments are ongoing within the CLM team and can be followed on the model's GitHub page (https://github.com/ESCOMP/CTSM). Active developments include the improvement of the irrigation scheme (Thiery et al., 2017; 2020), the representation of land cover and land management (Meier et al., 2018; Hirsch et al., 2017; 2018), and the implementation of reservoirs (Hauser et al., 2019).

CWatM developed, in addition ISIMIP2b, a groundwater scheme with linkages to MODFLOW for 5 arcmin and 30 arcsec spatial resolution. The CWatM modeling group plans to develop a reservoir storage including different operation schemes

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(e.g., energy, irrigation), to increase the temporal resolution (at 1 h), to apply a global calibration also for ungauged catchments, such as using the Budyko framework (Greve et al. 2020), applying both the day-degree method and energy balance method to estimate snow accumulation and melt, and applying several methods to estimate evaporation based on changing CO_2 concentration.

DBH plans to include human water uses (industrial and domestic sectors), either by developing a new module or using the simulations from other models (e.g., WFaS dataset), to calibrate the model in the new ISIMIP3 simulation round, and to improve the input/output module to read and write netcdf files.

The H08 modeling team used an approximate Bayesian computation technique to calibrate four parameters that are transferred to other regions containing no observations, mainly, based on Köppen–Geiger regions. The modeling group also increased the spatial resolution to 5 min and improved the representation of crops used for biofuel in the model.

The JULES-W1 modeling group plans to make a technical update that will enable the river routing module to estimate discharge.

The LPJmL group developed an improved energy balance module and soil hydrological scheme that can estimate permafrost dynamics (Schaphoff et al., 2013) and made the model source code freely available on GitHub (https://github.com/PIK-LPJmL/LPJmL; Schaphoff et al., 2018), hoping to engage a broader scientific community in LPJmL model development and applications.

The Mac-PDM.20 modeling group plans to develop a water use module.

MATSIRO modeling group has implemented a land-use change process, terrestrial biogeochemical processes, and an additional crop growth process into MATSIRO to develop a new modeling framework. As key interactions are taken into account and all processes are coupled, important boundary conditions for hydrological simulations can be dynamically simulated internally. This hydrological simulation modeling framework has been coupled with MIROC GCM and has been used as an Earth system model. In addition, the group recently proposed new schemes for lateral groundwater flow, water temperature, and sediment transportation.

Ongoing efforts to improve the realism of hydrologic processes in the mHM include the development of the multiscale lake module (mLM), a comprehensible framework for reservoir regulation as well as natural processes in lakes. Near-future developments will focus on a glacial module, to better account for processes in cold regions, as well as coupling it to a groundwater model that will replace the current linear groundwater reservoir.

The MPI-HM modeling group plans to increase the spatial resolution of regional versions. The group currently implemented canopy storage in the latest model version and is developing experiments to integrate reservoir storage.

The ORCHIDEE group is focusing on calibration, soil storage, groundwater storage, river storage, reservoir storage and wetland storage (MacBean et al., 2019; Verbeke et al., 2019; Yin et al., 2020; Schrapffer et al., 2020; Mizuochi et al., 2020).

The PCR-GLOBWB modeling group plans to increase the temporal and spatial resolution of the input data, to increase the temporal resolution (3 h) for energy balance calculations and the global spatial resolution (1 km), to improve the soil

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representation by including the Richards equation, to add more snow elevation layers, to include additional fast runoff component for improving daily discharge simulations, and to improve the reservoir operating scheme (Sutanudjaja et al., 2018).

The VIC modeling group developed different irrigation practices (Shah et al., 2019a and b) and included a reservoir (Dang et al., 2019 and 2020) as well as a groundwater scheme in the model structure.

The WaterGAP2 modeling group plans to update the GRanD dataset used by the model, to include water temperature calculations, to couple the new developed groundwater model (Reinecke et al., 2019), and to update the non-irrigation water use datasets.

The WAYS modeling group plans to develop a new human water use module to consider agricultural, industrial, and domestic water use in the water cycle.

7. Conclusions

Global water models are used to simulate the climate–water–human system. However, recent evaluation studies show that there is a need to better simulate this system by including other hydrological processes, data on physical infrastructure, societal behavior, cultural behavior, water diversions, and virtual water, as well as by identifying its teleconnections on the global scale (Zaherpour et al., 2018; Veldkamp et al., 2018; Wada et al., 2017). These studies also underline the need to better explain various model results.

We undertook the present study mainly to find similarities and differences among global water models that will facilitate interpretation of various results, as well as those of further intercomparison studies. We developed a standard equation writing style to achieve this goal. We found that there are some similarities among the models when applying similar equations for the same hydrological processes; however, model structures are different and various values have been used for parameters or variables or some equations have been adjusted. For example, 10 models (CWatM, DBH, JULES-W1, LPJmL, mHM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS) simulate the canopy water storage in a similar way, while 3 models (H08, Mac-PDM.20, and MPI-HM) do not include this compartment. MATSIRO is the only one that has two canopy water compartments: one for rainfall interception and one for snowfall interception. Three models (CLM4.5, CLM5.0, MATSIRO) differentiate between solid and liquid throughfall. Eight global water models (CWatM, LPJmL, Mac-PDM.20, mHM, MPI-HM, PCR-GLOBWB, WaterGAP2, WAYS) use the degree-day method to compute snow accumulation and melt, while six models use the energy balance method (DBH, H08, JULES-W1, ORCHIDEE, MATSIRO, VIC).

Four models (CLM4.5, CLM5.0, JULES-W1, and MATSIRO) use TOPOMODEL for the runoff generation scheme, while three models (CWatM, MPI-HM, and PCR-GLOBWB) use the ARNO model with or without adjustments. Other methods used for runoff generation scheme include Green-Ampt (DBH), Probability Distributed Moisture (Mac-PDM.20), HBV with or without adjustments (mHM and WaterGAP2), XIANJIANG (VIC), bucket (WAYS), Arnold-Bucket (LPJmL), and a leaky bucket (H08).

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Three models (H08, WaterGAP2, and WAYS) compute *groundwater recharge* using the same approach described by Döll and Fiedler, 2008. Four models (CWatM, PCR-GLOBWB, WaterGAP2, and WAYS) use the same approach to simulate the *groundwater runoff* by considering it as a part of groundwater storage which is weighted by a groundwater discharge coefficient.

Ten models do not include a lake compartment, while fourteen models do not include a wetland compartment. Four models (CWatM, H08, MATSIRO, and WaterGAP2) include a "global lakes" compartment and "local lakes" compartment in their structure. Furthermore, CWatM, MATSIRO, and WaterGAP2 use the reservoir algorithm developed by H08 modeling group, but with some adjustments. WaterGAP2 also includes a "global wetlands compartment" and "local wetlands compartment". Five models (CWatM, H08, LPJmL, MATSIRO, and WaterGAP2) use a retrospective reservoir algorithm, while one model (PCR-GLOBWB) uses a prospective reservoir algorithm.

Seven models do not simulate human water use sectors (DBH, JULES-W1, Mac-PDM.20, mHM, ORCHIDEE, VIC, and WAYS). Nine models simulate water abstraction for the irrigation sector from surface water bodies (CLM4.5, CLM5.0, CWatM, H08, LPJmL, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2). Additionally, H08, MATSIRO, PCR-GLOBWB, and WaterGAP2 simulate water abstraction for the domestic (household) and manufacturing sectors. Furthermore, WaterGAP2 divides the industry sector in manufacturing and electricity.

Ultimately, in this study and for ISIMIP2b, WaterGAP2 has used the highest number of water storage compartments (11 compartments), while JULES-W1, Mac-PDM.20, and VIC have used the lowest number (3 compartments). CWatM uses 10 compartments, while seven models use six compartments (CLM4.5, CLM5.0, LPJmL, H08, mHM, MPI-HM, and PCR-GLOBWB). Two models (CLM4.5 and CLM5.0) have used similar approaches, in most of the cases, because one model (CLM5.0) represents the new extended version of the other (CLM4.5). WaterGAP2 simulates five human water use sectors, while four models (CLM4.5, CLM5.0, LPJmL, and MPI-HM) simulate only water used by humans for the irrigation sector.

We highlight the need to undertake experiments on individual water compartments in order to analyze the equations used and the results obtained. We also underline the need to make multi-model intercomparison projects: firstly, because they enhance collaboration and communication between modeling groups, communities, countries and cultures; secondly, through communication and collaboration, these projects enhance creativity and open opportunities to finding new ways to improve the models. The present study was possible through the international ISIMIP framework.

By improving these models, we can make better decisions on how to use water more efficiently. Therefore, we need to have global water models that develop scenarios regarding how the Earth's water cycle will develop and how it will be affected by climate change. We consider the simulations provided by the ISIMIP2b global water models to represent good hypotheses of our water future and based on them we can make decisions.

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Supplement

Tables with equations of each water storage, water flow, human water use sectors, datasets used by global water models, models' structures, future research perspectives.

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Code availability

Information on the availability of source code for the models featured in this article can be found in the Table 12.

Author contributions

CET proposed, designed, and led the conceptualization of ISIMIP2b models' intercomparison based on their water cycle simulation and of a standard writing style of their equations. Initial idea was proposed by HMS, respectively, to compare the ISIMIP2b models based on their equations and a standard diagram. CET, WT, GL, PB, OR, TS, TT, FH, SR, HMS provided LaTeX support to write equations on the overleaf platform. HMS, WT, GL, PB, XL, JESB, LPS, MG, YS, OR, TS, JC, NW, HLS, TT, and GM checked the code and provided models' equations for each water storage and water flow. CET, HMS, WT, GL, PB, XL, JESB, LPS, MG, YS, OR, TS, JC, NW, HLS, TT, GM, AK, YP, LS, YW, VM, JL, and PD checked the consistency and correctness of the equations. HMS, WT, GL, PB, XL, JESB, LPS, MG, YS, OR, TS, JC, NW, HLS, GM run simulations for ISIMIP2b project. SNG and HMS coordinated the ISIMIP2b model simulations of the global water sector. CET conducted the analysis, visualization, and wrote the original draft. All authors reviewed, commented, and contributed to the final draft.

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Competing interests

The authors declare that they have no conflict of interest.

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Table 1: Canopy compartment and its water flows included in ISIMIP2b Global Water Models

Canopy water storage (S_{ca}) (Tables S3 – S7): CLM4.5, CLM5.0, CWatM, DBH, JULES-W1, LPJmL, mHM, MATSIRO, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS.
Inflows: - total precipitation (P) (sum of rainfall and snowfall, as input data): CWatM, DBH, JULES-W, LPJmL, mHM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS. - rainfall (P_{ra}) (as input data): CLM4.5, CLM5.0, MATSIRO. - snowfall (P_{sn}) (as input data): CLM4.5, CLM5.0, MATSIRO. - precipitation intercepted by canopy storage: CLM4.5, CLM5.0, CWatM, DBH, Mac-PDM.20, MATSIRO, mHM, WaterGAP2, WAYS. **Outflows:** - evaporation of the water intercepted by canopy or interception loss or canopy evaporation (E_{ca}): CLM4.5, CLM5.0, CWatM, DBH, JULES-W1, LPJmL, mHM, MATSIRO, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS. -precipitation falls directly to the ground: CLM4.5, CLM5.0, H08, VIC. - throughfall (P_{th}): CLM4.5, CLM5.0, CWatM, DBH, JULES-W1, LPJmL, MATSIRO mHM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS.

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Table 2: Snow and soil compartments and their water flows included in ISIMIP2b Global Water Models

Snow storage (S_{sn}) (Tables S8 – S13): CLM4.5, CLM5.0, CWatM, DBH, H08, JULES-W1, LPJmL, Mac-PDM.20, mHM, MATSIRO, MPI-HM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS. - snow held on the canopy (S_{soc}): CLM5.0, DBH, JULES-W1, MATSIRO, VIC. - snow under the canopy (S_{suc}): CLM5.0, DBH, JULES-W1, MATSIRO, ORCHIDEE, VIC.
Inflows: -total precipitation (P_{tot}): DBH, CWatM, JULES-W1, WaterGAP2. - snowfall (P_{sn}): CLM4.5, CLM5.0, H08, Mac-PDM.20, MATSIRO, mHM, MPI-HM, PCR-GLOBWB, WAYS. -throughfall (P_{th}): LPJmL. -snowfall and rainfall: ORCHIDEE, VIC. **Outflows:** - sublimation (E_{sn}): CLM4.5, CLM5.0, CWatM, DBH, H08, JULES-W1, LPJmL, MATSIRO, ORCHIDEE, VIC, WaterGAP2. - snowmelt (M): CLM4.5, CLM5.0, CWatM, DBH, H08, JULES-W1, LPJmL, Mac-PDM.20, mHM, MATSIRO, MPI-HM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS.
Soil storage (S_{so}) (Tables S14 – S25): CLM4.5, CLM5.0, CWatM, DBH, H08, JULES-W1, LPJmL, Mac-PDM.20, mHM, MATSIRO, MPI-HM, ORCHIDEE, PCR-GLOBWB, VIC, WaterGAP2, WAYS.
Inflows: **-total precipitation (P_{tot}):** Mac-PDM.20 - infiltration (R_{in}): CWatM, DBH, H08, LPJmL, mHM, MPI-HM, ORCHIDEE, PCR-GLOBWB, WaterGAP2,. -throughfall (P_{th}): JULES-W1, WAYS. -snowmelt (M): JULES-W1, Mac-PDM.20, WAYS. - capillary rise (R_{cr}): CWatM. **Outflows:** - transpiration (T): CLM4.5, CLM5.0, CWatM, DBH, LPJmL, MPI-HM, PCR-GLOBWB. - evaporation from soil (E_{so}): CWatM, DBH, H08, JULES-W1, LPJmL, Mac-PDM.20, mHM, MPI-HM, ORCHIDEE, PCR-GLOBWB, WaterGAP2, WAYS. - surface runoff (Rsu): JULES-W1, Mac-PDM.20, ORCHIDEE. - interflow (R_{if}): CWatM, JULES-W1, LPJmL, PCR-GLOBWB. - groundwater recharge (R_{gwr}): CWatM, DBH, MATSIRO, PCR-GLOBWB.

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Table 3: Groundwater, lake, reservoir, and wetland compartments and their water flows included in ISIMIP2b Global Water Models

Groundwater storage (Sgw) (Table S26-S28): CLM4.5, CLM5.0, CWatM, H08, Mac-PDM.20, mHM, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2, WAYS.
Inflows: - groundwater recharge (R_{gwr}): CLM4.5, CLM5.0, H08, Mac-PDM.20, mHM, MPI-HM, WaterGAP2, WAYS. -percolation (R_{pe}): CWatM, PCR-GLOBWB. -preferential flow (Q_{pf}): CWatM. **Outflows:** - capillary rise (R_{cr}): CWatM, PCR-GLOBWB. - groundwater runoff (R_{gw}): CLM4.5, CLM5.0, CWatM, H08, Mac-PDM.20, mHM, MPI-HM, PCR-GLOBWB, WaterGAP2, WAYS. - groundwater withdrawal for human water use (A_{gw}): PCR-GLOBWB, WaterGAP2. -total human water abstraction (A_{tot}): H08.
Lake (S_{la}) (Tables S29-S31): CLM4.5, CLM5.0, CWatM, LPJmL, PCR-GLOBWB, WaterGAP2.
Inflows: - precipitation (P_{tot}): LPJmL, WaterGAP2 - inflow from upstream surface water bodies (Q_{iu}): LPJmL, WaterGAP2 - groundwater runoff (R_{gw}): WaterGAP2 - return flow from human water use (A_{rf}): WaterGAP2 - water abstraction for human purposes: LPJmL **Outflows:** - evaporation from lake (E_{la}): LPJmL, PCR-GLOBWB, WaterGAP2 - outflow from lake (Q_{la}): LPJmL, PCR-GLOBWB, WaterGAP2 - groundwater recharge (R_{gwr}): WaterGAP2 - water abstraction for human water use from lake (A_{la}): WaterGAP2, LPJmL
Reservoir storage (S_{re}) (Tables S32-S35): DBH, H08, LPJmL, MATSIRO, PCR-GLOBWB, WaterGAP2.
Inflows: - precipitation (P_{tot}): WaterGAP2, LPJmL - inflow from upstream surface water bodies (Q_{iu}): CWatM, PCR-GLOBWB, WaterGAP2. - total runoff (R_{tot}): H08, MATSIRO - groundwater recharge below surface water bodies (R_{gwr}^{swb}): WaterGAP2 - return flow from human water use (A_{rf}): LPJmL, MATSIRO, PCR-GLOBWB, WaterGAP2 **Outflows:** - evaporation from reservoir (E_{re}): WaterGAP2, CLM4.5, CLM5.0, LPJmL, VIC. - outflow from reservoir (Q_{re}): DBH, H08, LPJmL, MATSIRO, PCR-GLOBWB, WaterGAP2. - groundwater recharge (R_{gwr}): WaterGAP2. - water abstraction for human water use from reservoir (A_{re}): LPJmL, H08, MATSIRO, PCR-GLOBWB, WaterGAP2.
Wetland storage (S_{we}) (Tables S36-S39): MPI-HM, WaterGAP2.
Inflows: - precipitation (P): MPI-HM, WaterGAP2 - inflow from upstream surface water bodies (Q_{iu}): MPI-HM, WaterGAP2 **Outflows:** - groundwater recharge (R_{gwr}): WaterGAP2 - evaporation from wetland (E_{we}): MPI-HM, WaterGAP2 - outflow from wetland (Q_{we}): MPI-HM, WaterGAP2

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Table 4: River compartment and its water flows included in the ISIMIP2b Global water Models

River storage (S_{ri}) (Tables S40-S45): CLM4.5, CLM5.0, CWatM, DBH, H08, LPJmL, mHM, MATSIRO, MPI-HM, ORCHIDEE, PCR-GLOBWB, WaterGAP2, WAYS.
Inflows:
- inflow from upstream surface water bodies (Q_{iu}): CLM4.5, CLM5.0, CWatM, H08, LPJmL, mHM, MATSIRO, PCR-GLOBWB, WaterGAP2.
-total runoff (R_{tot}): mHM
- surface runoff or overland flow or fast runoff (R_{su}): CLM4.5, CLM5.0, CWatM, ORCHIDEE, PCR-GLOBWB, WaterGAP2.
- interflow (R_{if}): CWatM, PCR-GLOBWB
- groundwater runoff (R_{gw}): CLM4.5, CLM5.0, CWatM, H08, mHM, MATSIRO, MPI-HM, ORCHIDEE, PCR-GLOBWB, WaterGAP2.
- return flow from human water use (A_{rf}): WaterGAP2 .
- streamflow (Q_{ri}): H08, MPI-HM
Outflows:
- streamflow or outflow or river discharge (Q_{ri}): CLM4.5, CLM5.0, LPJmL, mHM, MPI-HM, WaterGAP2
- inflow upstream of a grid cell (Q_{iu}): H08
- mean total annual inflow in a lake ($Q_{iu,la}$): LPJmL
- outflow downstream of a grid cell (Q_{od}): CWatM, PCR-GLOBWB
- water abstraction for irrigation (A_{irr}): LPJmL,
- water abstraction for irrigation from surface water bodies (A_{irr}^{sw}): CWatM, PCR-GLOBWB
- water abstraction for domestic sector from surface water bodies (A_{dom}^{sw}): CWatM, PCR-GLOBWB
- water abstraction for livestock from surface water bodies (A_{liv}^{sw}): CWatM, PCR-GLOBWB
- water abstraction for manufacturing from surface water bodies (A_{man}^{sw}): CWatM, PCR-GLOBWB
- water abstraction for human water use from river (A_{ri}): WaterGAP2, H08, MATSIRO
- water abstraction for irrigation sector (A_{irr}): LPJmL

1425

Table 5: Human water use sectors estimated by ISIMIP2b GWMs

Human water use sectors (A) (Tables S40-S80):
Irrigation (A_{irr}): CLM4.5, CLM5.0, CWatM, H08, LPJmL, MATSIRO, MPI-HM, PCR-GLOBWB, WaterGAP2.
Domestic (A_{dom}): MATSIRO, PCR-GLOBWB, WaterGAP2, CWatM
Manufacturing (A_{man}): MATSIRO, PCR-GLOBWB, WaterGAP2, CWatM
Electricity (A_{ele}): PCR-GLOBWB, WaterGAP2, CWatM
Livestock (A_{liv}): CWatM, PCR-GLOBWB, WaterGAP2.

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Table 6: Key characteristics of the Global Water Models

Model	Model Type	Temporal resolution	Discretization Type	Calibration / Ability to calibrate / Details	Human water use sectors
CLM4.5	LSM	6 hours	grid, subgrid for vegetation, surface runoff, and evapotranspiration	no / no, adjustment of some parameters according to vegetation or soil properties / not available	sim A_{irr}
CLM5.0	LSM	6 hours	grid, subgrid for vegetation, surface runoff, and evapotranspiration	no / yes / calibration performed in a Bayesian framework based on sequential Monte Carlo	sim A_{irr}
CWatM	GHM	1 day	grid, subgrid for land cover, snow	yes, calibrated for 12 catchment / monthly or daily discharge / hydrological calibration uses DEAP (Burek et al., 2020)	sim: A_{irr}, A_{dom}, A_{nd}, A_{liv}
DBH	LSM	1 day	grid	no / no hydrological calibration, adjustment of some parameters according to vegetation or soil properties / most parameters derived from satellite data.	not included
H08	GHM	1 day	grid	no / can be calibrated but generally done at the regional scale / the model can be applied at the global or regional scale	sim A_{irr} and A^{ocean}, A_{dom}, A_{ind}, A^{ocean}
JULES-W1	LSM	1 day	grid	biophysical processes are calibrated / no hydrologic calibration / ×	not included
LPJmL	DGVM	1 day	grid	yield calibration to match FAO stats / no hydrological calibration	sim A_{irr}, ISIMIP2b prescribed A_{dom} and A_{ind}
Mac-PDM.20	GHM	1 day	grid	no / yes / calibration uses a 100,000 GLUE ensemble with WATCH Forcing Data (Smith, 2016)	not included
MATSIRO	LSM	1 hour	grid	no / yes / adjustment of some parameters according to vegetation or soil properties, no calibration capability in TRIP model for routing discharge.	sim A_{irr}, ISIMIP2b prescribed A_{dom} and A_{ind}
mHM	GHM	1 day	grid	yes / yes / calibration is performed against observed daily discharge GRDC stations, gridded fields of TWS and gridded ET from FLUXNET with the ERA5 climate forcing	not included
MPI-HM	GHM	1 day	grid, subgrid for surface runoff and evapotranspiration	no / × / ×	sim A_{irr}
ORCHIDEE	LSM	30 min	grid	no / yes / adjustment of some parameters	not included
PCR-GLOBWB	GHM	1 day	grid, subgrid for vegetation, land cover	no / yes / adjustment of some parameters	sim: A_{irr}, A_{dom}, A_{ind}, A_{liv}, A_{ocean}
VIC	GHM	1 day	grid, subgrid for vegetation and elevation	no calibration for ISIMIP2b	not included
WaterGAP2	GHM	1 day	grid, subgrid for snow	yes / mean annual discharge / Beta function, 1319 GRDC stations	sim: A_{irr}, A_{dom}, A_{man}, A_{elec}, A_{liv}
WAYS	GHM	1 day	grid	yes / yes / calibrated against the ISLSCP, Initiative II UNH or GRDC composite monthly runoff data (Fekete et al., 2011) from 1986 to 1995 at a 0.5°resolution	not included

Legend: × = no details; DEAP = Distributed Evolutionary Algorithms in Python; DGVM = dynamic global vegetation model; EB = energy balance; GHM = global hydrological model; GRDC = Global Runoff Data Centre; ISLSCP = International Satellite Land Surface Climatology Project; LSM = land surface model; sim = simulated by the model; UNH = University of New Hampshire; A_{irr} = water abstractions for irrigation; A_{dom} = water abstractions for domestic; A_{man} = water abstractions for manufacturing; A_{ele} = water abstractions for cooling of thermal power plants; A_{ind} = water abstractions for industry (sum of A_{man} and A_{ele}); A_{liv} = water abstractions for livestock; TRIP = Total Runoff Integrating Pathways; **Bold** = LSMs; *Italic* = GHMs; Underline = DGVMs.

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Table 7: Representation of the water storages and water flows included in the Global Water Models – PART I

Model	Interception scheme	Vegetation scheme Partition / Photosynthesis scheme	(Potential) evapotranspiration scheme	Soil scheme Number of soil layers	Soil scheme Soil layer depth SLD [m]	TSD [m]	Snow scheme Snow accumulation and snowmelt	$Snow_{acc}$
CLM4.5	*f*(LAI, SAI)	tile approach with 24 PFTs (including 10 crop types) / ×; CO_2	Monin-Obukhov Similarity Theory computes only AET	15	depth at layer interface: 0.0175, 0.0451, 0.0906, 0.1655, 0.2891, 0.4929, 0.8289, 1.3828, 2.2961, 3.8019, 6.2845, 10.3775, 17.1259, 28.2520, 42.1032.	42.1	physically based snow module	5 layers
CLM5.0	*f*(LAI, SAI)	naturally vegetated surfaces are comprised of up to 14 possible plant functional types (PFTs) / dynamic global vegetation model (DGVM); CO_2	Monin-Obukhov Similarity Theory computes only AET	25, *f*(depth to bedrock)	depth at layer interface: 0.020; 0.060; 0.120; 0.200; 0.320; 0.480; 0.680; 0.920; 1.200; 1.520; 1.880; 2.280; 2.720; 3.260; 3.900; 4.640; 5.480; 6.420; 7.460; 8.600; 10.990; 15.666; 23.301; 34.441; 49.556.	49.6	physically based snow module	maximum 12 layers, depends on snow depth
CWatM	*f*(veg)	subgrid	Penman-Monteith	3	0.05,0.05-0.3, 0.3-1.7 depends on HWSD data	2.0	Degree-day Method	7 layers
DBH	*f*(LAI)	prescribed, 10 vegetation types (PFTs) with fixed vegetation characteristics / ×	Energy balance model with Monin-Obukhov similarity theory computes only AET	3	from 1.5 to 3.5m; top layer = 0.020m; root layer = 1.0 to 1.5m.	3.5	Energy Balance Method	1 layer
H08	×	tile approach / ×	Bulk, Bulk transfer coefficient set to 0.003	1 / RCZ	1	1	Energy Balance Method	1
JULES-W1	*f*(LAI)	5 static vegetation types (PFTs) with fixed plant characteristic / ×	Penman-Monteith	4	0.10; 0.25; 0.65; 2.00	3.0	Energy Balance Method	zero-layer scheme
LPJmL	*f*(LAI)	9 PFTs *f*(L, W, S) / DVPNV; CO_2	Priestley-Taylor modified for transpiration	5+1	0.20; 0.30; 0.50; 1; 1m. 1 thermally active soil of 10m	13	Degree-day Method with precipitation factor	1 layer
Mac-PDM.20	*f*(veg)	prescribed, 16 PFTs with fixed vegetation characteristics / ×	Penman-Monteith	1	none	none	Degree-day Method	1 layer
MATSIRO	*f*(LAI)	11 static vegetation types with fixed characteristics (PFTs) / ×	Monin-Obukhov Similarity Theory, to compute only actual evapotranspiration	13	0.05; 0.2; 0.75; 1; 1; 1; 1; 1; 1; 1; 1; 1; 90m.	100	Energy Balance Method	3 layers

Legend: AET = actual evapotranspiration; CO_2 = CO_2 fertilization effect; DGVM = dynamic global vegetation model; DVPNV = dynamic vegetation composition on potential natural vegetation areas; *f*(LAI) = function of leaf area index; *f*(LAI, SAI) = function of leaf area index (LAI) and stem area index (SAI); *f*(veg) = function of vegetation type; HWSD = Harmonized World Soil Database (FAO et al., 2012: http://www.fao.org/soils-portal/soil-survey/soil-maps-and-databases/harmonized-world-soil-database-v12/en/); L= light; PFTs = Plant functional types; RCZ = runoff properties varies with climate zones; SLD = soil layers depth from top to bottom; TSD = total soil layer depth; $Snow_{acc}$ = snow accumulation; S = space; W = water; × = not included in the model; **Bold** = LSMs; *Italic* = GHMs; Underline = DGVMs.

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Table 8: Representation of the water storages and water flows included in the Global Water Models – PART II

Model	Interception scheme	Vegetation scheme Partition / Photosynthesis scheme	(Potential) evapotranspiration scheme	Number of soil layers	Soil scheme Soil layer depth SLD [m]	TSD [m]	Snow scheme Snow accumulation and snowmelt	$Snow_{acc}$
mHM	*f*(veg)	3 major vegetation classes: (forest, impervious, pervious) for parameter regionalization + long-term dynamics based on LAI-based on GIMMS	Hargreaves-Samani	6	soil layers correspond to SoilGrids250 vertical discretizaion, i.e.: 0-5cm, 5-15cm, 15-30cm,30-50cm, 50-100cm,100-200cm	2.0	Degree-day Method	1 layer
MPI-HM	×	prescribed, Land Surface Parameter dataset 2 / ×	Penman-Monteith reference Evapotranspiration	1, *f*(FC)	none	none	Degree-day Method	1 layer
ORCHIDEE	*f*(LAI)	tile approach with 17 vegetation types (PFTs); CO_2	Penman & Monteith (Monteith, 1965) based on the correction term developed by Chris Milly (1992)	11	0.001; 0.003; 0.006; 0.012; 0.023; 0.047; 0.094; 0.188; 0.375; 0.750; 0.500.	2	Energy Balance Method	3 layers
PCR-GLOBWB	*f*(veg)	natural vegetation (short and tall vegetation) and agriculture (rainfed, rice irrigated and non-rice irrigated) prescribed annually by HYDE dataset and MIRCA, GLOBCOVER / ×	Hamon	2	variable up from 0 to 0.3 (first layer) and variable from 0.3 to 1.5 (second layer)	1.5	Degree-day Method	1 layer
VIC	*f*(veg)	any number of vegetation types with fixed characteristics can be represented (PFTs) / ×	Penman-Monteith	3	variable, first layer is fixed to 0.1-0.3m, second and third layers are calibrated	6.15	Energy Balance Method	variable
WaterGAP2	*f*(LAI)	LAI development model based on T and P / ×	Priestley-Taylor with varying alpha-values for arid and humid areas	1	from 0.1 to 4m	4	Degree-day Method	SG
WAYS	*f*(LAI)	14 static vegetation types (PFTs) with fixed characteristics / ×	Penman-Monteith	1/the complete root zone	variable, derived separately from remote sensing data	variable	Degree-day Method	1

Legend: AET = actual evapotranspiration; CO_2 = CO_2 fertilization effect; *f*(LAI) = function of leaf area index; *f*(veg) = function of vegetation type; *f*(FC) = function of field capacity; P = precipitation; PFTs = Plant functional types; SG = subgrid; SLD = soil layers depth from top to bottom; TSD = total soil layer depth; $Snow_{acc}$ = snow accumulation; T = subgrid temperature (daily average) (0° C); × = not included in the model; **Bold** = LSMs; *Italic* = GHMs.

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Table 9: Representation of the water storages and water fluxes included in the Global Water Models – PART III

Model	Groundwater scheme / groundwater layer	Runoff generation scheme surface runoff / subsurface runoff	River scheme / River routing[1] / flow velocity[2] / floodplain scheme / Details	Reservoir scheme / reservoir operation / Number / Details	Lakes scheme / Details	Wetlands scheme / Details
CLM4.5	✓ / 1	TOPMODEL[Beven and Kirkby,1979] / R_{ho}, R_{sat} / *f*(gw)	✓/ River Transport Model (RTM) / 0.35 m s^{-1} RtM / × / diagnostic tool, conserves water globally	×	virtual storage / constant lake depth	×
CLM5.0	✓ / 1	TOPMODEL[Beven and Kirkby,1979] / R_{ho}, R_{sat} / *f*(gw)	✓/ MOSART / based on Manning's equation / ×/ MOSART based on kinematic wave method	×	virtual storage / spatially variable depth	×
CWatM	✓ / 1	ARNO [Dümenil and Todini, 1992] / R_{sat} / *f*(soil and gw)	✓/ Kinematic wave, approximation of the Saint-Venant equation[Chow et al., 1998] / variable Manning-Strickler equation / × / linear storage	✓/ ✓ / 3663, HydroLakes[3]/ retrospective: following H08: Hanasaki et al. (2018) and Wisser et al. (2010).	✓ / Modified Puls	×
DBH	× / ×	Green-Ampt method/ R_{ho} / ×	×/ ×/ ×/ × / × /.	×/ ×/ ×	×	×
H08	✓ / 1 renewable and 1 nonrenewable gw layer	leaky Bucket[Manabe,1969] / R_{sat} / *f*(soil) RCZ	✓/ based on 30' flow drainage direction map (DDM30) / 0.5 m s^{-1} / × / Rfd	✓ / ✓/ 963 global reservoirs and 5824 local reservoirs / retrospective: Hanasaki et al., 2006	×	×
JULES-W1	seepage as gw recharge and gw runoff / ×	TOPMODEL[Beven and Kirkby,1979] / R_{ho}, R_{sat} / *f*(gw)	× / × / × / × / ×	×	×	×
LPJmL	seepage as gw recharge and gw runoff / ×	Bucket[Arnold et al., 1990]/ R_{sat} / *f*(soil)	✓ / continuity equation derived from linear reservoir model / 1 m s^{-1} / × / linear storage buffer; Rfd	✓ / ✓ / 4134, GRanD / retrospective: Biemans et al., 2011	✓	×
Mac-PDM.20	× / 1	Probability Distributed Moisture (PDM)[Moore and Clarke,1981] / Rsat / f(gw)	× / × / × / × / ×	×	×	×
MATSIRO	✓ Dgws / ~13	TOPMODEL[Beven and Kirkby,1979] / R_{ho}, R_{sat} / *f*(soil)	✓ / linear reservoir, TRIP / 0.5 m s^{-1} / × / × TRIP	✓ / ✓ / 728 global reservoirs and 6134 'local reservoirs' / following H08, retrospective: Pokhrel et al., 2012	×	×

Legend: ✓= included in the model; × = not included in the model for ISIMIP2b simualtions; Dgws = dynamic groundwater scheme; GRanD = Global Reservoir and Dam database according to Lehner et al., 2011; gw = groundwater; R_{su} = surface runoff; R_{sat} = R_{su} modelled as saturation excess overland flow; R_{ho} = R_{su} modelled as infiltration excess or hortonian overland flow; *f*(gw) = subsurface flow or interflow modelled as a function of groundwater; *f*(soil) = subsurface flow or interflow modelled as a function of soil moisture (soil); Rfd = the model routes runoff along flow direction; RtM = routing model; TRIP = Total Runoff Integrating Pathways; **Bold** = LSMs; *Italic* = GHMs; Underline = DGVMs.
Notes: **1:** Data source: www.isimip.org. **2:** Zhao et al., 2017. **3: CWatM**, HydroLakes database: Messager et al., 2016; Lehner et al., 2011.

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Table 10: Representation of the water storages and water fluxes included in the Global Water Models – PART IV

Model	Groundwater scheme / groundwater layer	Runoff generation scheme surface runoff / subsurface runoff	River scheme / River routing[1] / flow velocity[2] / floodplain scheme / Details	Reservoir scheme / reservoir operation / Number / Details	Lakes scheme / Details	Wetlands scheme / Details
mHM	× / 1	HBV[Bergström,1976] + VIC 3Layers / R_{sat} / f(soil)	✓ / mesoscale Routing Model with adaptive timestep, spatially varying celerity[3] / × / ×/ ×	×	×	×
MPI-HM	× / 1	ARNO[Dümenil and Todini, 1992] / R_{sat} / *f*(soil)	✓ / linear reservoir cascade / variable, Manning-Strickler Equation / ✓ / RtMwefp	×	lake storage is part of the wetland storage	
ORCHIDEE	×/ ×	SECHIBA[Ducoudré et al., 1993] / R_{ho} / *f*(soil)	✓/ STN-30p river network / variable, Manning-Strickler Equation / ✓ / wetlands act as floodplains	×	×	× / wetlands act as floodplains
PCR-GLOBWB	✓ / 1	ARNO[Dümenil and Todini, 1992] / R_{sat} / *f*(soil and gw)	✓/ travel time routing (characteristic distance) linked with dynamic reservoir operation / variable based on channel dimension and Manning-Strickler Equation / ✓ / ×	✓ / ✓ / 6862: GRanD / prospective: Wada et al., 2014	×	×
VIC	× / × / seepage as gw recharge and gw runoff / ×	XIANJIANG [Zhao, 1980] / R_{sat} / *f*(soil)	×/ ×/ × / × / ×	×	×	×
WaterGAP2	✓ / 1	HBV[Bergström,1976] / R_{sat}, Beta function / ×	✓ / linear reservoir cascade / variable, Manning-Strickler Equation / × / ×	✓ / ✓ / 11097: GRanD / retrospective, following H08: Döll et al, 2009	✓ / local and global lakes[4]	✓/ local and global wetlands[5]
WAYS	✓ / 1	Bucket[Manabe,1969]/ Beta function[3] / f(soil)	× / × / × / × / ×	×	×	×

Legend: ✓= included in the model; × = not included in the model for ISIMIP2b simualtions; GRanD = Global Reservoir and Dam database according to Lehner et al., 2011; gw = groundwater; R_{su} = surface runoff; R_{sat} = R_{su} modelled as saturation excess overland flow; R_{ho} = R_{su} modelled as infiltration excess or hortonian overland flow; *f*(gw) = subsurface flow or interflow modelled as a function of groundwater; *f*(soil) = subsurface flow or interflow modelled as a function of soil moisture (soil); RtMwefp = routing model with wetlands (we) and floodplain (fp) scheme; **Bold** = LSMs; *Italic* = GHMs.
Notes: **1:** Data source: www.isimip.org. **2:** Zhao et al., 2017. **3:** Thober et al, 2019; **4 and 5: WaterGAP2**, Döll et al., 2012.

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Table 11 Challenges of global hydrological modelling overlapping with unsolved problems in hydrology

	Challenges of hydrological modelling
Time variability and change (Blöschl et al., 2019)	**Challenges of simulating terrestrial water cycle on the global scale, identified through the present study**
1. Is the hydrological cycle regionally accelerating/decelerating under climate and environmental change, and are there tipping points (irreversible changes)? 2. How will cold region runoff and groundwater change in a warmer climate (e.g. with glacier melt and permafrost thaw)? 3. What are the mechanisms by which climate change and water use alter ephemeral rivers and groundwater in (semi-) arid regions?	**a.** couple the climate and hydrological models, having climate feedback from the hydrological models (Ning et al., 2019); **b.** add glacial meltwater runoff (Schewe et al., 2019; Huss and Hock, 2018, Zekollari et al., 2019; Cáceres et al., 2020); **c.** couple the climate, lands use, hydrology, and human components including their feedbacks and interactions (Nazemi &Wheater, 2015; Pokhrel et al., 2016; Wada et al., 2017; Thiery et al., 2017; 2020); **d.** land-use dynamics scheme (Sood and Smakhtin, 2015)
Measurements and data (Blöschl et al., 2019)	**Challenges of simulating terrestrial water cycle on the global scale, identified through the present study**
16. How can we use innovative technologies to measure surface and subsurface properties, states, and fluxes at a range of spatial and temporal scales? 18. How can we extract information from available data on human and water systems in order to inform the building process of socio-hydrological models and conceptualizations?	**e.** perform the GWMs at a high resolution of 1 km than 55 km (Wood et al., 2011; Bierkens 2015; Beven et al., 2015; Wada et al., 2016b; Burek et al., 2020); **f.** improve the quality of the input data, GRACE products (Murray et al., 2012; Scanlon et al., 2018); **g.** make single-model sensitivity analyses (Gosling and Arnell, 2011; Müller Schmied et al. 2014; Pianosi et al., 2015; Cuntz et al., 2016); **h.** make multi-parameterization of the single models or model compartments; **j.** improve the simulation of the human impact on freshwater resources (Bierkens, 2015; Nazemi&Wheater, 2015; Döll et al., 2016; Wada et al., 2017; Masaki et al., 2017; Veldkamp et al., 2018); **i.** distinguish between the groundwater source and surface water source for water abstractions and identify how the return flows recharge groundwater (Döll et al., 2016; Veldkamp et al., 2018; Scanlon et al., 2019).
Modelling methods (Blöschl et al., 2019)	**Challenges of simulating terrestrial water cycle on the global scale, identified through the present study**
19. How can hydrological models be adapted to be able to extrapolate to changing conditions, including changing vegetation dynamics? 20. How can we disentangle and reduce model structural/parameter/input uncertainty in hydrological prediction?	**k.** understand different model biases (errors) and their influence on the simulations identify and explain the strengths and weaknesses of individual models (fire community: Rabin et al., 2017); **l.** assess the influence of the models' structure on simulations, go deep into equations, to improve the equations, and to create new equations; **m.** improve the processes representation of the models, for example, incorporation of a dynamic groundwater scheme (Pokhrel et al., 2016; Scanlon et al., 2019); **n.** add other processes in the models such as transmission losses, capillary rise, evaporation from small ephemeral ponds, dynamic response of vegetation to the climate change and CO_2 concentrations; improve the capture of the spatial pattern, intra and inter-annual variabilities; explain the reasons for different output results and use several types of data (e. g., GRACE, GPS, well observations, MODIS, Envisat) for multi-criteria validation (of the models' outputs), model calibration (models' parameters), data assimilation (Döll et al., 2003; Döll et al., 2015; Döll et al., 2016; Vanderkelen et al., 2020); **o.** improve parameterizations by using parameter transfer method, multiscale parameter regionalization (Samaniego et al., 2010), or by using stepwise parameter estimation (Arheimer et al., 2020); **p.** add floodplain storage and wetland evaporation; to develop or open new data sets on "interbasin transfers, regional water distribution network, river cross-sectional dimensions, and hydrogeological subsurface properties" (Bierkens, 2015, page 4942); **q.** weight individual models based upon their performance (Zaherpour et al., 2019) **r.** identify hidden parameters in the code (Mendosa et al., 2015)
Interfaces with society (Blöschl et al., 2019)	**Challenges of simulating terrestrial water cycle on the global scale, identified through the present study**
21. How can the (un)certainty in hydrological predictions be communicated to decision makers and the general public? 22. What are the synergies and tradeoffs between societal goals related to water management (e.g. water–environment–energy–food–health)? 23. What is the role of water in migration, urbanisation and the dynamics of human civilisations, and what are the implications for contemporary water management?	**s.** evaluate the models' performance, for example, following the steps proposed by Krysanova et al., 2018 or to create new feasible steps for GWMs taking into account their shortcomings (Zaherpour et al., 2018 and 2019) or evaluating them for several scales and gauge stations (Samaniego et al., 2017); **t.** compare with the outputs of the high-resolution continental scale models (for example, Parflow) (Scanlon et al., 2018); **u.** complement the global studies with regional studies (Gosling et al., 2011; Gosling et al., 2017; Hatterman et al., 2017); **v.** connect the GWMs with socio-economic and energy models (Calvin et al., 2013; Burek et al., 2020); **x.** identify and explain the strengths and weaknesses of multi-model ensembles, individual model compartments (Clark et al., 2011; Niu et al., 2011; Essery et al., 2013);

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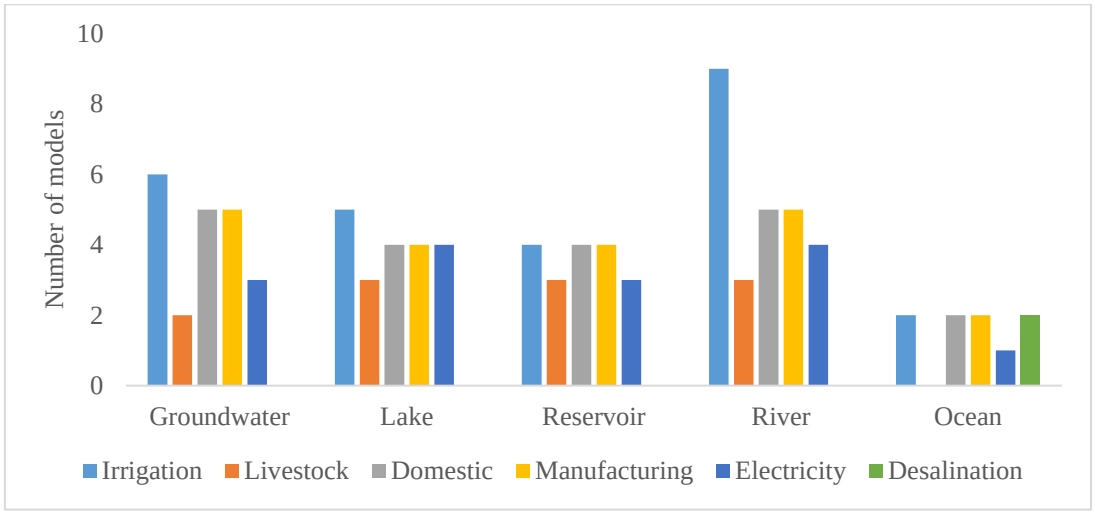

Figure 1: Number of global water models that consider water source for human water use sectors

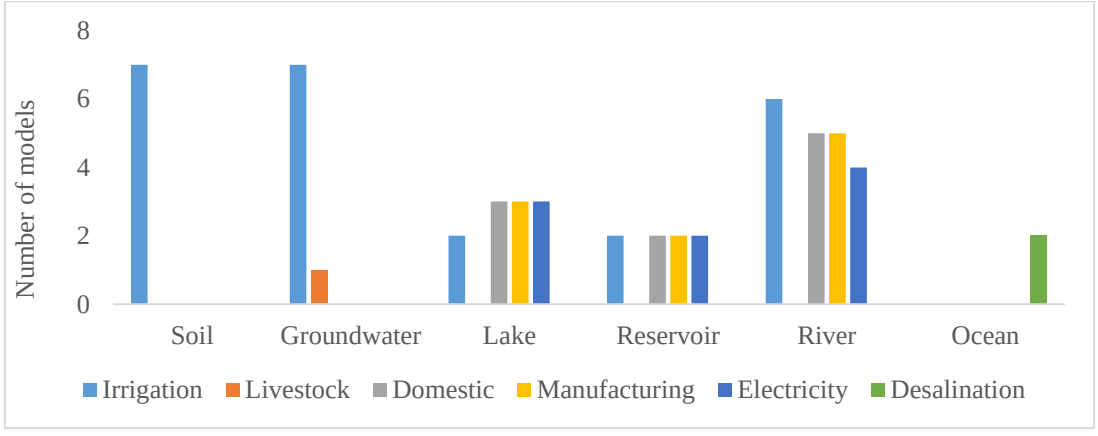

Figure 2: Number of global water models that consider return flow destination

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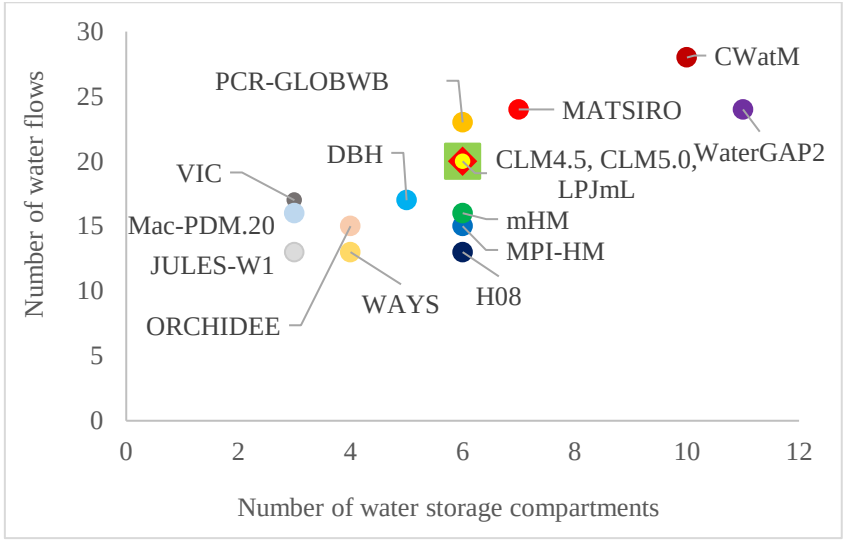

Figure 3: Number of water storage compartments and water flows included in the global water models.

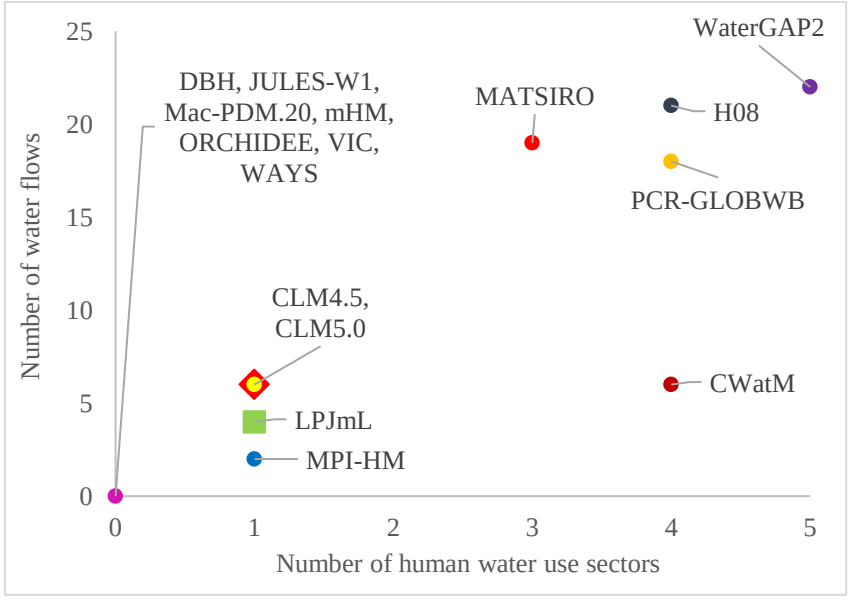

Figure 4: Number of human water use sectors and related water flows included in the global water models.

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Table 12: Code availability of the ISIMIP2b Global water models

Model Abbreviation	Code availability	References
CLM4.5	CLM4.5 is under active development by the University Corporation for Atmospheric Research (UCAR) - National Center for Atmospheric Research (NCAR; https://ncar.ucar.edu). The model version is licensed under CC BY 4.0. The exact version of the model, used to produce the results of this paper, is archived on Zenodo (Thiery, 2020).	Oleson and Lawrence, 2013
CLM5.0	CLM5.0 is under active development by the University Corporation for Atmospheric Research - National Center for Atmospheric Research and hosted at the National Center for Atmospheric Research (NCAR; https://ncar.ucar.edu/). The version of model is licensed under CC BY 4.0. The exact version of the model, used to produce the results of this paper, is archived on Zenodo (CTSM Development Team, 2020).	Lawrence et al., 2019
CWatM	CWatM is under active development funded by the International Institute for Applied Systems Analysis (IIASA, Austria; http://www.iiasa.ac.at/cwatm). CWatM is open source and available online via GNU General Public License v3. The code can be used on different platforms (Unix, Linux, Window, Mac) and is provided through a GitHub repository https://github.com/cwatm/cwatm. The version of the model used to produce the results in this paper are stored as version 1.04 in the GitHub repository (https://github.com/CWatM/CWatM.) and at Zenodo (Burek et al., 2019).	Burek et al., 2020 Burek et al., 2019
DBH	DBH is under active development funded by the Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, Beijing, China (http://english.igsnrr.cas.cn/). The exact version of the model (global version 1), used to produce the results of this paper, is not open source. It is only available by request to the editors / reviewers in charge of this paper.	Tang et al., 2006; Liu et al., 2016
H08	H08 is under active development by the National Institute for Environmental Studies, Japan (Japan; http://www.nies.go.jp/index-e.html; http://h08.nies.go.jp). H08 is open source and available online via http://h08.nies.go.jp. The version of model is licensed under the terms and conditions: https://h08.nies.go.jp/h08/files/licence_en.pdf. The version of model is licensed under CC BY 4.0. The exact version of the model (model version 20190101), used to produce the results of this paper, is archived on Zenodo (Hanasaki, 2020).	Hanasaki et al., 2006; Hanasaki et al., 2008a,b; Hanasaki et al., 2018.
JULES-W1	JULES (the Joint UK Land Environment Simulator) is a community land surface model under continuous development by a wide community of UK researchers, coordinated by UKMO and CEH. The exact version of the model (version 4.7) used in these simulations is available from the Met Office Science Repository Service (registration required) at https://code.metoffice.gov.uk/trac/jules. To access the code a freely available non-commercial research license is required (https://jules-lsm.github.io/).	Best et al., 2011; Clark et al., 2011
LPJmL	LPJmL is under active development funded by the Potsdam Institute for Climate Research (Germany; https://www.pik-potsdam.de/en/home). The exact version of the model (model version 3.5), used to produce the results of this paper, is not open source. It is only available by request to the editors / reviewers in charge of this paper.	Gerten, 2004; Bondeau et al., 2007; Rost et al., 2008; Biemans et al., 2011
Mac-PDM.20	Mac-PDM.20 is under active development by the University of Nottingham (UK; https://www.nottingham.ac.uk/) and the University of Reading (UK; https://www.reading.ac.uk/). The version of the model (version 20), used in ISIMIP2b and in this paper, is not open source as it under active development. It is only available by request to the editors / reviewers in charge of this paper.	Gosling and Arnell, 2011; Smith, 2016
MATSIRO	MATSIRO is under active development funded by the University of Tokyo (Japan; https://www.u-tokyo.ac.jp/en/index.html) and National Institute for Environmental Studies (Japan; http://www.nies.go.jp/index-e.html). The exact version of the model (model version MIROC-INTEG1), used to produce the results of this paper, is not open source. It is only available by request to the editors / reviewers in charge of this paper.	Takata et al., 2003; Pokhrel et al., 2012; 2015
mHM	mHM is under active development funded by the Helmholtz Centre for Environmental Research – UFZ (Germany; https://www.ufz.de/index.php?en=33573; https://git.ufz.de/mhm). The version of model is licensed under GNU General Public License v3: https://git.ufz.de/mhm/mhm/-/blob/develop/LICENSE. The exact version of the model (model version 5.10), used to produce the results of this paper, is archived on Zenodo (Samaniego et al., 2017).	Samaniego, 2017 ; Samaniego et al., 2010; Kumar et al., 2013; Thober et al., 2019
MPI-HM	MPI-HM was developed at the Max Planck Institute for Meteorology (Germany; https://mpimet.mpg.de/en/homepage). The exact version of the model (model version 1.2), used to produce the results of this paper, is not open source. It is only available by request to the editors / reviewers in charge of this paper.	Stacke and Hagemann, 2012
ORCHIDEE	ORCHIDEE is under active development funded by the Institute Pierre Simon Laplace (France; https://www.ipsl.fr/en/; http://forge.ipsl.jussieu.fr/orchidee/wiki/Branches/ORCHIDEE-MICT-	Guimberteau et al., 2014; Guimberteau et al., 2018

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	IMBALANCE-P/MergeNews). The source code for ORCHIDEE- MICT version 8.4.1 is available online, but its access is restricted. Consequently, one is required to communicate with the corresponding author for a username and password. The source code can be found at the following address: https://forge.ipsl.jussieu.fr/orchidee/browser/branches/ ORCHIDEE-MICT/tags/ORCHIDEE_MICT_8.4.1 The exact version of the model (model version v8.4.1), used to produce the results of this paper, is not open source. It is only available by request to the editors / reviewers in charge of this paper.	
PCR-GLOBWB	PCR-GLOBWB is under active development funded by the Utrecht University (The Netherlands; https://www.uu.nl/en/research/department-of-physical-geography). PCR-GLOBWB is open source and available online via: https://github.com/UU-Hydro/PCR-GLOBWB_model.The version of model is licensed under GNU General Public License v3. The exact version of the model (model version 2.0), used to produce the results of this paper, is archived on Zenodo: https://doi.org/10.5281/zenodo.1045338 (Sutanudjaja et al., 2017).	Van Beek et al., 2011; Wada et al., 2011; Wada et al., 2014; Sutanudjaja et al., 2018
VIC	VIC is under active development funded by the University of Washington, (USA; https://vic.readthedocs.io/en/master/). It was applied by the Indian Institute of Technology Gandhinagar, Gandhinagar (India; http://www.iitgn.ac.in/). VIC is open source and available online via https://github.com/UW-Hydro/VIC. The version of model is licensed under GNU General Public License v2.0. The exact version of the model (model version 4.1.2.g), used to produce the results of this paper, is archived on Zenodo (Shah and Vimal, 2020).	Gao et al., 2009
WaterGAP2	WaterGAP2 is under active development funded by the Goethe University Frankfurt (https://www.goethe-university-frankfurt.de/en?legacy_request=1; https://www.uni-frankfurt.de/45218063/WaterGAP) and Kassel University (https://www.uni-kassel.de/uni/) (Germany). The exact version of the model (model version 2.2c), used to produce the results of this paper, is not open source due to licensing issues. It is only available by request to the editors / reviewers.	Döll et al., 2012, 2014; Portmann et al., 2010; Müller Schmied et al., 2014, 2016; Verzano et al., 2012; Flörke et al., 2013
WAYS	WAYS is under active development funded by the Southern University of Science and Technology – SUSTech (China: https://www.sustech.edu.cn). The version of model is licensed under Creative Commons Attribution 4.0 International. The exact version of the model used to produce the results used in this paper is archived on Zenodo (Mao and Liu, 2019).	Mao and Liu, 2019