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7 **PCR-GLOBWB 2: a 5 arc-minute global hydrological**
8 **and water resources model**

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28



29 **Abstract.**

30

31 We present PCR-GLOBWB 2, a global hydrology and water resources model. Compared to previous versions
32 of PCR-GLOBWB, this version fully integrates water use. Sector-specific water demand, groundwater and
33 surface water withdrawal, water consumption and return flows are dynamically calculated at every time step
34 and interact directly with the simulated hydrology. PCR-GLOBWB 2 has been fully rewritten in Python and
35 PCRaster-Python and has a modular structure, allowing easier replacement, maintenance, and development of
36 model components. PCR-GLOBWB 2 has been implemented at 5 arc-minute resolution, but a version
37 parameterized at 30 arc-minute resolution is also available. Both versions are available as open source codes
38 on https://github.com/UU-Hydro/PCR-GLOBWB_model. PCR-GLOBWB 2 has its own routines for
39 groundwater dynamics and surface water routing. These relatively simple routines can alternatively be
40 replaced by dynamically coupling PCR-GLOBWB 2 to a global two-layer groundwater model and 1D-2D-
41 hydrodynamic models, respectively. Here, we describe the main components of the model, compare results of
42 the 30 arc-minute and the 5 arc-minute versions and evaluate their model performance using GRDC discharge
43 data. Results show that model performance of the 5 arc-minute version is notably better than that of the 30 arc-
44 minute version. Furthermore, we compare simulated time series of total water storage (TWS) of the 5 arc-
45 minute model with those observed with GRACE, showing similar negative trends in areas of prevalent
46 groundwater depletion. Also, we find that simulated water withdrawal, by source and sector, matches
47 reasonably well with reported water withdrawal from AQUASTAT.

48



49 1 Introduction

50

51 The last decades saw the development of an increasing number of global hydrological models (GHMs), e.g.
52 VIC (Liang et al., 1994; Nijssen et al., 2001), WMB (Fekete et al., 2002), WaterGAP (Döll et al., 2003), H08
53 (Hanasaki et al., 2008a), MAC-PDM (Gosling and Arnell, 2011) (see Bierkens et al., 2014, Bierkens, 2015 and
54 Kauffeldt et al. 2016 for a more extensive list, also including land surface models). GHMs have become
55 essential tools to quantify and understand the global terrestrial water cycle, as they simulate the distributed
56 hydrological response to weather and climate variations at higher resolution (typically $0.5^{\circ} \times 0.5^{\circ}$) than used
57 previously in general circulation models (GCMs), with more sophisticated runoff generation processes and
58 river routing. As such, global hydrological models have been used for medium-range to seasonal flood
59 forecasting (Bierkens and van Beek, 2009; Alfieri et al., 2013; Candogan Yossef et al., 2013) as well as for a
60 myriad of water-related global change assessments. Examples are: the projection or estimation of future flood
61 and drought events (Sperna-Weiland et al., 2012; Dankers et al., 2013; Prudhomme et al., 2013, Wanders et al.
62 2015, Wanders and Wada, 2016), current and future flood hazard and risk (Pappenberger et al., 2012;
63 Hirabayashi et al., 2013; Ward et al., 2013; Winsemius et al., 2013; 2016), global groundwater depletion
64 (Wada et al., 2010; Gleeson et al., 2012), the contribution of terrestrial water stores to global sea level change
65 (Konikow, 2011; Wada et al., 2012; Pohkrel et al., 2013), current and future water scarcity under climate
66 change and increasing population growth (Hanasaki et al., 2008b; Wada et al., 2011a, 2011b; Schewe et al.,
67 2013; Haddeland et al., 2013; Wada and Bierkens, 2014), tele-connections between climate oscillations and
68 water availability (Wanders and Wada, 2015), the impact of land use change on global water resources (Rost
69 et al., 2008; Sterling et al., 2015; Bosmans et al., 2016) and trends in surface water temperature and cooling
70 water potential (van Beek et al., 2012; van Vliet et al., 2012). More recently, the output from global
71 hydrological models has been extended to study socioeconomic impacts, such as virtual water trade (Konar et
72 al., 2013; Dalin et al., 2017) and future agricultural production (Elliott et al., 2013). These applications show
73 that GHMs have become invaluable tools in support of global water management and policy assessments.

74

75 PCR-GLOBWB (PCRaster GLOBal Water Balance) (van Beek and Bierkens, 2009; van Beek et al. 2011) is
76 one of the recently developed GHMs. PCR-GLOBWB is a grid-based global hydrological model developed at
77 the Department of Physical Geography, Faculty of Geosciences, Utrecht University, the Netherlands. The
78 model, describing the terrestrial part of the hydrological cycle, was first introduced in a technical report by van
79 Beek and Bierkens (2009) and then formally published in a paper of Van Beek et al. (2011), focusing on
80 global water availability issues. PCR-GLOBWB was originally developed to solve the global daily surface
81 water balance with a spatial resolution of 30 arc-minutes (about 50 km by 50 km at the equator) and compare
82 the resulting fresh water availability with monthly sectoral water demand in order to assess global-scale water
83 scarcity (van Beek et al., 2011; Wada et al., 2011a,b). In this first version of PCR-GLOBWB (called PCR-
84 GLOBWB 1 hereafter), similar to other global-scale hydrological models, water demand and water availability
85 are treated independently, i.e. without direct feedback between human water use and other terrestrial water



86 fluxes (e.g. Döll and Siebert, 2002; Wisser et al., 2010). Since it was first introduced, PCR-GLOBWB has
87 been applied extensively in global water resources assessment studies. For instance, a recent search on Scopus
88 (accessed on 30 October 2017) on the key-word “PCR-GLOBWB” yielded 97 publications with collectively
89 over 2100 references. Since the first version, several new model features have been introduced such as a
90 comprehensive water demand and irrigation module (Wada et al., 2011b, 2014), a scheme for dynamic
91 allocation of sectoral water demand to available surface water and groundwater resources and the associated
92 calculation of return flow (de Graaf et al., 2014). These features essentially introduced a two-way interaction
93 between water demand, water withdrawal, water consumption and availability, particularly over irrigated areas
94 where water demand is large and return flow is significant. Nevertheless, all of these preceding studies using
95 PCR-GLOBWB were performed at a relatively coarse resolution of 30 arc-minutes, limiting their sub-regional
96 or local applications. Additionally, some added functionalities, such as the possibility to couple the land
97 surface component of PCR-GLOBWB to a global MODFLOW-based groundwater model (Sutanudjaja et al.,
98 2011; 2014; de Graaf et al., 2015; 2017) and an extension to simulate surface water temperature (Van Beek et
99 al., 2012), were incorporated in different versions based on the original PCR-GLOWB 1, leading to divergent
100 model code development.

101

102 The objective of this paper is to summarize and present the new version of the model, PCR-GLOBWB 2,
103 which consolidates all components that have been developed since the original version of the model was first
104 introduced (van Beek et al., 2011). The new version of the model, PCR-GLOBWB 2, simulates the water
105 balance at a finer spatial resolution of 5 arc-minutes and supersedes the original PCR-GLOBWB 1 that has a
106 resolution of 30 arc-minutes¹. The finer resolution of PCR-GLOBWB 2 allows a much better representation of
107 the effects of spatial heterogeneity in topography, soils, and vegetation on terrestrial hydrological dynamics
108 (Wood et al., 2011; Bierkens et al., 2014). Likewise, it provides a better resolution for visualization that allows
109 stakeholders and decision makers to assess model simulation output more easily and directly for the places
110 they are specifically interested in (Sheffield et al., 2010; Beven and Cloke, 2012). To evaluate the possible
111 improvements, this paper also presents the first validation results from the simulation of PCR-GLOBWB 2 at 5
112 arc-minute resolution and compares this with a 30 arc-minutes version. As discharge data are commonly used
113 in hydrological model performance evaluation, the simulated river discharge of PCR-GLOBWB 2 is compared
114 to in situ discharge observations from the Global Runoff Data Centre (GRDC, 2014).

115

116 The paper is organized as follows. Section 2 provides a global description of PCR-GLOBWB 2, including its
117 model structure and the new components and functionalities that have been added since PCR-GLOBWB 1. In
118 section 3 the global application of PCR-GLOBWB 2 is demonstrated and the results from a 58-year simulation
119 (1958-2015) are validated against observations of discharge, total water storage and reported withdrawal data.
120 Section 4 summarizes and concludes this paper and discusses possible future developments. Section 5 provides
121 information about availability of the model code and the underlying data.

¹ Note that Wada et al. (2016) made a preliminary version of the model that operates at 6 arc-minutes.



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123

124 2. PCR-GLOBWB 2 – Model description

125

126

127 2.1 General overview

128

129 PCR-GLOBWB 2 is a state-of-the-art grid-based global hydrology and water resources model. It is a
130 component-based model implementation in Python using open source PCRaster Python routines (Karssenberg
131 et al., 2010; <http://pcraster.geo.uu.nl/>). The code is distributed through Github. The computational grid covers
132 all continents except Greenland and Antarctica. Currently two versions are available: one with a spatial
133 resolution of 5 arc-minutes in latitude and longitude and one with a coarser resolution of 30 arc-minutes.
134 Typical time steps for hydrology and water use are one-day while sub-daily time stepping is used for
135 hydrodynamic river routing. For all dynamic processes involved, PCR-GLOBWB 2 uses a time-explicit scheme.
136 For each grid cell and each time step, PCR-GLOBWB 2 simulates moisture storage in two vertically stacked
137 upper soil layers (S_1+S_2 in Figure 1), as well as the water exchange between the soil, the atmosphere and the
138 underlying groundwater reservoir (S_3 in Figure 1). The exchange with the atmosphere comprises of
139 precipitation, evaporation from soils, open water, snow and soils and plant transpiration, while the model also
140 simulates snow accumulation and snowmelt. Sub-grid variability of land use, soils and topography is included
141 and influences the schemes for runoff-infiltration partitioning, interflow, groundwater recharge (from S_2 to S_3)
142 and capillary rise (from S_3 to S_2). Runoff, generated by snowmelt, surface runoff, interflow and baseflow, is
143 routed across the river network to the ocean or endorheic lakes and wetlands. Routing can either be simple
144 accumulation, simplified dynamic routing using a method of characteristics, or kinematic wave routing. In
145 case the kinematic wave routing is used, it is also possible to use a (simplified) floodplain inundation scheme
146 and to simulate the surface water temperature.

147

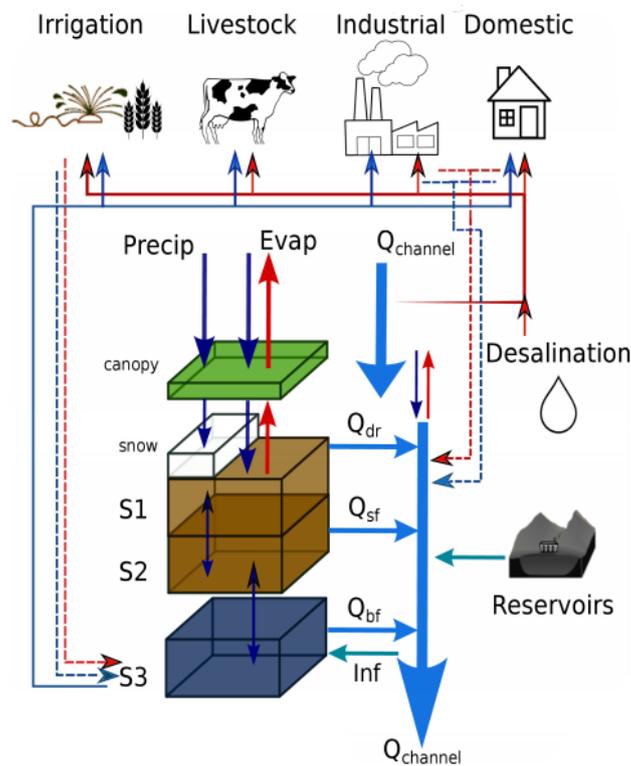
148 PCR-GLOBWB 2 includes a simple reservoir operation scheme that is applied to over roughly 6000 manmade
149 reservoirs from the Grand database (Lehner et al., 2011), which are progressively introduced according to
150 their construction year. Human water use is fully integrated within the hydrological model, meaning that at
151 each time step: 1) water demands are estimated for irrigation, livestock, industry and households; 2) these
152 demands are translated into actual withdrawals from groundwater, surface water (rivers, lakes and reservoirs)
153 and desalinization, subject to availability of these resources and maximum groundwater pumping capacity in
154 place; 3) consumptive water use and return flows are calculated per sector.

155

156 As an option PCR-GLOBWB 2 can be partially or fully coupled to a two-layer global groundwater model
157 based on MODFLOW (de Graaf et al, 2017). Recent work (Hoch et al., 2017a,b) also includes coupling PCR-
158 GLOBWB 2 to either Delft3D Flexible Mesh (Kernkamp et al., 2011) or LISFLOOD-FP (Bates et al., 2010)



159 which are model codes that can be used to solve the 1D-2D shallow water equations (or approximation
 160 thereof) for detailed inundation studies.
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165
 166 *Figure 1. Schematic overview of a PCR-GLOBWB 2 cell and its modelled states and fluxes. S_1 , S_2 (soil*
 167 *moisture storage), S_3 (groundwater storage), Q_{dr} (surface runoff – from rainfall and snowmelt), Q_{sf} (interflow*
 168 *or stormflow), Q_{bf} (baseflow or groundwater discharge), Inf (riverbed infiltration from to groundwater). The*
 169 *thin red lines indicate surface water withdrawal, the thin blue lines groundwater abstraction, the thin red*
 170 *dashed lines return flows from surface water use and the thin dashed blue lines return flows from groundwater*
 171 *use surface. For each sector: withdrawal - return flow = consumption. Water consumption adds to total*
 172 *evaporation.*
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 174



175

176 **2.2 Model structure and flexibility**

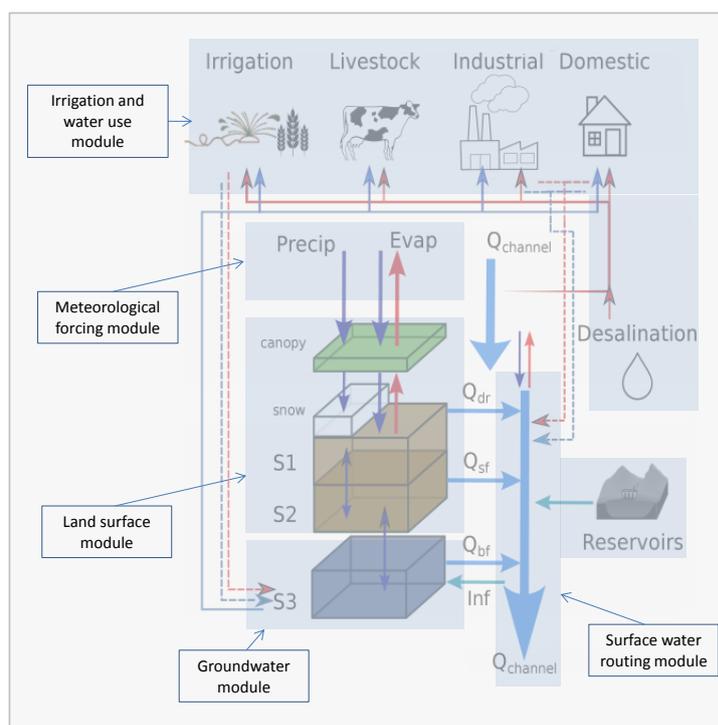
177

178 PCR-GLOBWB 2 has a flexible modular structure in which the exchange of water between a series of
 179 interconnected stores is easily performed (Figure 1). The modular structure of PCR-GLOBWB 2, both in terms
 180 of model concepts and implementation (separate modules are called from a main program), makes it easy to
 181 modify or replace components according to specific objectives of the model application, to introduce new
 182 modules or components within the modelling system and to couple it to existing codes.

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187 *Figure 2. The five modules that make up PCR-GLOBWB 2 portrayed on the model components of Figure 1.*

188

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190

191 There are currently five main hydrological modules in PCR-GLOBWB 2 as illustrated in Figure 2 and briefly
 192 described in Section 2.3: Meteorological forcing; Land surface; Groundwater; Surface water routing; Irrigation
 193 and water use. For an extensive description of the underlying equations and methods used in each of these
 194 modules we refer to the following sources:



195

- 196 • Meteorological forcing module: van Beek (2008) <http://vanbeek.geo.uu.nl/supinfo/vanbeek2008.pdf>
- 197 • Land surface module, groundwater module and surface water routing module: van Beek and Bierkens
- 198 (2009) <http://vanbeek.geo.uu.nl/supinfo/vanbeekbierkens2009.pdf> ; van Beek et al. (2011)
- 199 <http://dx.doi.org/10.1029/2010WR009791>
- 200 • Irrigation and water use module:
 - 201 ○ Calculation of water demand: Wada et al., (2014) <https://doi.org/10.5194/esd-5-15-2014>
 - 202 ○ Calculation of water withdrawal, consumption and return flows: de Graaf et al. (2014)
 - 203 <https://doi.org/10.1016/j.advwatres.2013.12.002>; Wada et al. (2014) [https://doi.org/10.5194/esd-](https://doi.org/10.5194/esd-5-15-2014)
 - 204 [5-15-2014](https://doi.org/10.5194/piahs-372-83-2015); Erkens and Sutanudjaja (2015) <https://doi.org/10.5194/piahs-372-83-2015>

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206

207 Furthermore: for details about coupling to MOFLOW we refer to:

- 208 • One-way coupling: Sutanudjaja et al. (2011) <https://doi.org/10.5194/hess-15-2913-2011>; De Graaf et
- 209 al. (2017) <https://doi.org/10.1016/j.advwatres.2017.01.011>
- 210 • Two-way coupling: Sutanudjaja et al. (2014) <http://dx.doi.org/10.1002/2013WR013807>

211

212

213 **2.3 Description of the modules**

214

215 Hereafter, we briefly describe the main features of the five modules. Additionally, a (non-exhaustive) list of

216 the model state and flux variables is provided in Table A1, whereas Table A2 lists the model inputs and

217 parameters, including their sources.

218

219

220 **2.3.1 Meteorological forcing module**

221

222 Meteorological forcing of PCR-GLOBWB 2 uses time series of spatial fields of precipitation, temperature and

223 reference evaporation. Reference potential evaporation can be prescribed or calculated within the model, and is

224 used in the land surface module to calculate crop-specific potential evaporation based on crop factors of the

225 various land cover types according to the FAO guidelines (Allen et al., 1998). There are two options for

226 calculating reference potential evaporation: 1) using Hamon (1963) in case only daily mean temperature is

227 available; 2) using Penman-Monteith following the FAO guidelines (Allen et al., 1998) if net radiation, wind

228 speed and vapour pressure deficit are additionally available. See van Beek et al. (2008) for details. The

229 resulting crop specific potential evaporation is subsequently used to compute the actual evaporation for

230 different land cover types in each cell. Apart from the calculation of evaporation, temperature is also used to

231 partition precipitation into snow and rain and to drive snowmelt.



232

233

234 **2.3.2. Land surface module**

235

236 This core module of PCR-GLOBWB 2 covers the land-atmosphere exchange, the vertical flow between soil
237 compartments and the eventual groundwater recharge, snow and interception storage and the runoff generation
238 mechanisms. Information is organized per land cover type and the fraction it occupies within a cell. The
239 number of land cover types is configurable; the standard parameterization of PCR-GLOBWB 2 carries: tall
240 natural vegetation, short natural vegetation, irrigated crops (non-paddy) and paddy-irrigation (i.e., wet rice).
241 For each land cover type, separate soil conditions can be specified. It should be noted that the soil and
242 vegetation conditions are in any case fully spatially distributed. Thus, vegetation properties (e.g., crop factor,
243 Leaf Area Index) and soil properties (depth, saturated hydraulic conductivity, etc.) vary not only between land
244 cover types, but may also vary from cell-to-cell (e.g., per climate zone). In the standard parameterization
245 vegetation properties vary over the year using a monthly climatology of phenology and crop calendars (i.e. for
246 the crop factor and LAI). The application of irrigation water for paddy and non-paddy irrigation is done by the
247 irrigation and water use module. It is based on the FAO guidelines of Allen et al. (1998) and is dependent on
248 the actual soil water storage (S_1 , S_2) or paddy-open water storages. All fluxes, from and to the land surface
249 module in Figure 2, are thus calculated separately per land cover type. The resulting vertical fluxes for each
250 land cover type are: interception evaporation, bare soil evaporation, snow sublimation, vegetation-specific
251 transpiration. In the soil column, vertical fluxes are based on Darcian flow and interact with the underlying
252 groundwater store, S_3 . Surface runoff (Q_{dr} , from precipitation and snowmelt) consists of infiltration excess
253 runoff and saturation excess runoff following a sub-grid approach that mimics variable source areas, i.e. the
254 improved Arno Scheme (Todini, 1996; Hagemann and Gates, 2003). Interflow or stormflow (Q_{sf}), mostly
255 occurring in regolith soils on hillslopes, is also handled with a sub-grid approach based on a runoff
256 parameterization by Sloan and Moore (1984). All fluxes are computed per land cover type and balanced with
257 the available storage to arrive at the net flux that is used to update the storages for the next time step. Also, to
258 report the overall fluxes per cell, and to pass these to other modules, the land cover specific fluxes are
259 subsequently averaged (weighted by land cover type fractions).

260

261 For the standard parameterization of the land surface module the following data sets are combined (see Table
262 A2): the cell fractions of various non-irrigation land cover types are based on the map of Global Land Cover
263 Characteristics Data (GLCC) Base Version 2.0 (Loveland et al., 2000) with the land cover classification
264 following Olson (1994a; b) and the parameter sets from Hagemann et al. (1999) and Hagemann (2002).
265 Irrigation land cover types (i.e. paddy and non-paddy), including their crop calendars and growing season
266 lengths, are parameterized based on the data set of MIRCA2000 (Portmann et al., 2010) and the Global Crop
267 Water Model of Siebert and Döll (2010). We refer to van Beek et al. (2011) for detailed descriptions.

268



269 2.3.3. Groundwater module

270

271 The groundwater module calculates groundwater storage dynamics subject to recharge and capillary rise
272 (calculated by the land surface module), groundwater discharge (Q_{bf} ; in case of a positive groundwater
273 storage) and riverbed infiltration (Inf). Groundwater discharge (assumed the same as groundwater baseflow
274 here) depends on a linear storage-outflow relationship ($Q_{bf} = S_3/J$) where the proportionality constant J is
275 calculated following drainage theory of Kraijenhoff-van de Leur (1958) based on drainage network density
276 and aquifer properties. Riverbed infiltration occurs only in case Q_{bf} becomes 0 by groundwater withdrawal,
277 and only in areas where under natural conditions (without groundwater withdrawal) significant groundwater
278 discharge occurs. Under persistent groundwater withdrawal (calculated with the Irrigation and Water use
279 module) that is larger than the sum of recharge and riverbed infiltration, the groundwater storage S_3 is allowed
280 to become negative. In this case, the part of the withdrawn groundwater in excess of the input (recharge and
281 riverbed infiltration) is seen as non-renewable groundwater withdrawal leading to groundwater depletion
282 (permanent loss of groundwater from storage). In case withdrawal becomes smaller than the input, the
283 remaining input is used to first fill the negative storage to zero, before baseflow Q_{bf} commences again.
284 Alternatively, an initial estimate of a fossil, i.e. a non-actively replenished, groundwater store can be imposed
285 that provides a similar functionality.

286

287 It is possible to use a full-fledged groundwater flow model based on MODFLOW: Harbaugh et al., 2000)
288 coupled to PCR-GLOBWB 2 in order to calculate groundwater heads and flow paths. This can be done as a
289 one-way coupling where PCR-GLOWB 2 is first run with the standard groundwater module (reservoir S_3 with
290 only vertical fluxes) to yield time series of net groundwater recharge (recharge – capillary rise) and surface
291 water levels. These fluxes/inputs are subsequently used to force the groundwater flow model (see e.g.
292 Sutanudjaja et al., 2011; de Graaf et al., 2017). Another possibility is to use a two-way coupling where the
293 groundwater module of PCR-GLOBWB 2 is replaced by the groundwater flow model. In this case, at each
294 time step fluxes are exchanged between the groundwater model and the land surface module, and the
295 groundwater model and the surface water routing module (Sutanudjaja et al. 2014).

296

297

298 2.3.4 Surface water routing module

299

300 Following an 8-point steepest gradient algorithm across the terrain surface (local drainage direction or LDD),
301 all cells of the modelled domain are connected to a strictly convergent drainage network that together make up
302 the river basins and sub-basins of the model domain. The lowermost cell is either connected to the ocean or to
303 an endorheic basin. Per cell, the sum of the three daily runoff fluxes (Figure 1) is aggregated and routed along
304 the drainage network. Routing can be done in three ways of increasing complexity: 1) accumulation of the
305 fluxes over the drainage network, typically aggregated over longer time steps (e.g. month or year) that are



306 larger than the travel times of water along the longest river length; 2) a travel-time characteristic solution
307 (Karssenberget al., 2007). Here, for each cell flow velocity is calculated in advance based on bankfull
308 discharge and Manning's equation (assuming the energy slope to be equal to the bed slope). Next, this
309 velocity is used to move the volume of water in the channel of a cell the corresponding distance within one
310 time step along the drainage network. This method works reasonably well for relatively steep rivers in humid
311 climates where the friction slope is close to the bed slope and the rivers are equally filled with water
312 throughout the year; 3) the kinematic wave approximation of the Saint Venant equations with flow described
313 by Manning's equation. Also, here, it is assumed that friction slope and bed slope are equal, which makes it
314 valid for rivers without backwater effects. The kinematic wave is solved using a time-explicit variable sub-
315 time stepping scheme based on the minimum Courant number. Of these methods, the kinematic wave solution
316 simulates the propagation of the flood wave more realistically while the others provide an expedient means to
317 approximate discharge over longer periods.

318

319 Using the kinematic wave method, it is possible to model floodplain inundation which occurs if the discharge
320 exceeds the bankfull capacity of a channel. The excess discharge volume is spread over the entire cell from the
321 lowest part of the cell (based on a higher resolution sub-grid DEM) yielding a flooded area with an
322 approximated flood depth. In case of flooding, the simulated river flow is impacted by adjusting the wetted
323 area and wetted perimeter and calculating a weighted Manning coefficient from the individual Manning
324 coefficients of the floodplains and the channel.

325

326 Lakes and reservoirs are part of the drainage network. Lakes and reservoirs can extend over multiple cells, in
327 which case the storage is subdivided by area such as to ensure that lake and reservoir levels are the same
328 across their extent. The active storage of lakes and the actual storage of reservoirs are dynamically updated; for
329 the lake outflow a standard storage-outflow relationship is used based on a rectangular cross-section over a
330 broad-crested weir, while reservoirs follow a release strategy. This strategy is, by default, aimed at passing the
331 average discharge, while maintaining levels between a minimum and maximum storage, but more elaborate
332 strategies that take account of downstream water demand are possible (e.g. Van Beek et al., 2011). Lakes and
333 reservoir areas change based on global volume-area relationships. All surface water areas, i.e. the river
334 channel, inundated floodplains, lakes and reservoirs, are subject to open water evaporation calculated from
335 reference potential evaporation multiplied with a factor depending on water type and water depth. Moreover,
336 surface waters are subject to surface water withdrawal calculated with the Irrigation and Water Use module.

337

338 If the kinematic wave approach is used, it can be also augmented with an energy routing scheme to simulate
339 surface water temperature (Van Beek et al., 2012). Finally, it should be noted that it is possible to run the
340 routing routine from PCR-GLOBWB 2 as a stand-alone routine, which allows it to be fed with the specific
341 discharge from other land surface models.

342



343 The routing methods that are available in PCR-GLOBWB 2 will yield significant errors for wide lowland
344 rivers where backwater effects are important. In this case, it is possible to replace the surface water module for
345 part of the modelling domain with hydrodynamic models solving the shallow water equations (Hoch et al.,
346 2017a). Hoch et al. (2017b) developed a generic coupler for this purpose that enables coupling to multiple
347 hydrodynamic modelling codes (<https://doi.org/10.5281/zenodo.597107>).

348

349 Although any data set can be used to define the drainage network and locate the lakes and reservoirs, the
350 standard parameterization of PCR-GLOBWB 2 that runs globally uses the drainage network derived from
351 HydroSHEDS (Lehner et al., 2008) combined with GTOPO30 (Gesch et al., 1999) and Hydro1k (Verdin and
352 Greenlee, 1996; USGS EROS Data Center, 2006); lakes taken from GLWD1 (Lehner and Döll, 2004) and
353 reservoirs obtained from Grand (Lehner et al., 2011).

354

355

356 **2.3.5 Irrigation and water use module**

357

358 In PCR-GLOWB 1 water demand was calculated separately from the hydrology and water availability
359 calculated as a post-processing step by subtracting upstream demand (Wada et al., 2011a,b). In PCR-
360 GLOBWB 2 water use (withdrawal and consumption) is fully integrated. Hereafter, the main features of the
361 irrigation and water use module are described in the following order: water demand, water withdrawal, water
362 consumption and return flows.

363

364 Water demand

365 *Irrigation water demand* is calculated based on the crop composition (which changes per month and includes
366 multi-cropping) and the irrigated area per cell. As stated above, these are obtained from MIRCA2000
367 (Portmann et al., 2010) and the Global Crop Water Model (Siebert and Döll, 2010). In the standard PCR-
368 GLOBWB 2 parameterization the irrigated areas change over time. In want of detailed data, fractions of paddy
369 and non-paddy irrigation, as well as the crop composition per month stay fixed (as obtained from
370 MIRCA2000), while the total irrigated area per cell changes over time and is based on the FAOSTAT (FAO,
371 2012) reported irrigated areas. Irrigation water demand is computed using the FAO guidelines (Doorenbos and
372 Pruit, 1977; Allen et al., 1998): in case of non-paddy irrigation, water is applied whenever soil moisture falls
373 below a pre-set value and then the soil column is replenished up to field capacity. In case of paddy irrigation,
374 the water level is kept at a water depth of 5 cm above the surface until the late crop development stage (~ 20
375 days) before the harvest. After that, no irrigation is applied anymore such that the water level is allowed to
376 drop to zero under infiltration and evaporation (Wada et al., 2014). The net irrigation demand is augmented to
377 account for limited irrigation efficiency and losses. In the standard parameterization of PCR-GLOBWB the
378 irrigation water demand is increased by 40% to obtain gross irrigation water demand (meaning an irrigation
379 efficiency of $(1/1.4) \times 100 = 71\%$.) However, it is possible to use spatio-temporal varying irrigation
380 efficiencies if needed, which is the case for all other variables.



381

382 *Non-irrigation water demand* covers three sectors; industry, households and livestock. For each of these
383 sectors, the gross demand and net demand are prescribed to the model and calculated using separate scripts.
384 The calculation of net non-irrigation water demand, which varies with time, follows methods developed by
385 Wada et al (2014). We refer to Wada et al. (2014) for an extensive description. Trends in water demand are
386 prescribed on an annual basis as a function of population, electricity demand and gross domestic product
387 (GDP) per capita. In addition, domestic water demand exhibits a seasonal variation on the basis of
388 temperature. Domestic and industrial gross water demand is calculated from net water demand using a
389 country-specific recycling ratio RC (based on development stage or GDP per capita and additionally access to
390 domestic water demand): $gross = net/(1-RC)$. This takes into account that much of the domestic and industrial
391 water is not consumed but returned as surface water. For livestock, the return flow is assumed to be zero,
392 meaning all water is consumed.

393

394 *Water withdrawal*

395 The water withdrawal estimation is based on the work by de Graaf et al. (2014) and Wada et al. (2014). In
396 PCR-GLOBWB 2 water withdrawal is set equal to gross water demand (summed over all the sectors) unless
397 sufficient water is not available. In that case, water withdrawal is scaled down to the available water and then
398 allocated proportionally to gross water demand per sector. Thus, no allocation preference is available in the
399 standard parameterization of PCR-GLOBWB 2, but it would be rather straightforward to change this.

400

401 Water can be abstracted from three sources: surface water, groundwater (fossil and non-fossil) and desalinated
402 water. The latter is prescribed (Wada et al., 2011a), while the fractions of the other two sources are determined
403 as function of their relative abundance. Groundwater and surface water availability are determined based on
404 two-year running means of groundwater recharge and river discharge respectively, thus keeping track of the
405 prevalence of local resources and their temporal change (de Graaf et al., 2014). These fractions determine on a
406 monthly basis from which source water is abstracted. Surface water withdrawal is ceased if river discharge
407 falls below 10% of the long-term average yearly discharge under naturalized flow conditions (determined by
408 running the model without withdrawal). If, for some reason, the surface water amount is insufficient, the
409 model falls back on groundwater to meet the resulting gap. Groundwater is first abstracted from the renewable
410 groundwater storage, and if not this is not present, non-renewable groundwater is abstracted. The amount of
411 groundwater that can be abstracted is, however, capped by the groundwater pumping capacity which is based
412 on data by IGRAC GGIS database. The described dynamic allocation scheme is not always in line with local
413 preferences or the infrastructure. However, there is a possibility to use literature fractions of groundwater
414 withdrawal and surface water withdrawal. For urban areas, we rely on the data set of McDonald et al. (2014)
415 that states whether a surface water distribution infrastructure is available. If this is the case, industrial and
416 domestic water withdrawals are mainly taken from surface water before abstracting groundwater. If surface
417 water infrastructure is limited, groundwater source is prioritized (see e.g. Erkens and Sutanudjaja, 2015). For



418 urban areas that are not in the McDonald (2014) data set, we give preference to the dynamic allocation
419 scheme. For irrigation, we use the ratios supplied by Siebert et al. (2010) in regions where they are said to be
420 reliable. In regions where they are not fully reliable, we take the average ratio provided by Siebert et al. (2010)
421 and the one provided by the dynamic allocation scheme. For regions where the data of Siebert (2010) are not
422 reliable (i.e., extrapolated data), we give preference to the dynamic allocation scheme.

423

424 Moreover, we cannot assume that all the water demand is supplied from surface water and groundwater
425 resources in the same cell. Ideally, the local water redistribution network should be used to define a surface
426 water service area. Unfortunately, this information is not available at the global scale. Therefore, in our current
427 parameterization of PCR-GLOBWB 2, we pool water availability of desalinated and surface water over zones
428 of approximately 1 arc-degree around each 5 arc-minute cell that are truncated by country and basin borders if
429 applicable. For groundwater, 0.5 arc-degree zones are used. The downside of the current scheme is that a cell
430 does not always have access to its nearest water resource if this lies outside its prescribed service area.

431 Available surface water for abstraction is stored in channels, lakes and reservoirs within each cell and service
432 area. Groundwater availability is also limited by the pumping capacity in the service area.

433

434 Water consumption and return flows

435 In case of irrigation, all the withdrawn water is applied to the soil (non-paddy) or the water level on the field
436 (paddy). Part of that water is lost by transpiration and part by soil and open water evaporation. Transpiration
437 and evaporation together make up the irrigation water consumption. The remaining part of irrigated water is
438 lost by percolation and contributes to groundwater recharge as return flow. Irrigation efficiency (not including
439 conveyance losses) could also be calculated after the fact by the difference between withdrawal and
440 transpiration. In case of domestic and industrial water use, water consumption depends on the recycling ratio
441 RC and equals $\text{withdrawal} \times (1 - \text{RC})$, while $\text{withdrawal} \times \text{RC}$ constitutes return flow. All return flow is added to
442 the surface water. For livestock, the consumption is set equal to the withdrawal and no return flow is assumed.

443

444

445 **2.4 Differences between PCR-GLOBWB 1 and 2**

446

447 PCR-GLOBWB 2 has the following new capabilities compared to PCR-GLOBWB 1 (cf. Van Beek et al.,
448 2011; Wada et al, 2011):

- 449 • the model was completely rewritten in PCRaster Python and now has a modular structure;
- 450 • the inputs and outputs are in the form of NetCDF files and output can be reported for daily monthly and
451 yearly time steps;
- 452 • parameterizations are available at 30 arc-minute and 5 arc-minute resolution;
- 453 • water use (demand, withdrawal, consumption and return flow) is fully integrated;
- 454 • distinction is made between paddy and non-paddy irrigation and irrigation follows FAO guidelines;



- 455 • three different options for surface water routing are available and a surface water temperature module is
456 fully integrated with the routing scheme;
- 457 • it is possible to run surface water routines separately with specific discharge from other sources (e.g. other
458 land surface models);
- 459 • PCR-GLOBWB 2 can be coupled to a two-layer transient groundwater model (Sutanudjaja et al., 2014;
460 De Graaf et al., 2017) and to the hydrodynamic models Delft3D Flexible Mesh (Kernkamp et al., 2011) or
461 LISFLOOD-FP (Bates et al., 2010, see Hoch et al., 2017b).

462

463

464 **2.5 Model code**

465

466 The original PCR-GLOBWB version 1 (van Beek et al., 2011) was written in the PCRaster scripting language.
467 PCRaster (Wesseling et al., 1996) is a high-level programming language that started as a dynamic raster-based
468 Geographical Information System (GIS) and is tailored to spatiotemporal modelling for environmental and
469 earth science applications. The generic nature of PCRaster with its many tailor-made built-in hydrological
470 functions and its syntax that reads like pseudo-code, generally results in short and readable model codes, short
471 development times and limited programming errors. Karssen et al. (2010) developed a PCRaster Python
472 package such that PCRaster functions, implemented in C++, can also be called via Python
473 (<http://www.python.org/>). Using PCRaster Python also makes it possible for students and beginner modellers
474 to contribute to the model quickly, while it allows experts to be more productive and focus on the science
475 rather than on the programming language syntax. Realising the aforementioned advantages, PCR-GLOBWB,
476 particularly starting from this version 2, has been rewritten in the Python scripting language.

477

478 To run the model a so-called initialization file or configuration file is used (with extension .ini). In this file the
479 following aspects are defined: the spatial and temporal domain, the time step, the settings of the different
480 modules (e.g. which surface water routing, human water use or not etc.) and the locations and names of the
481 parameter files and forcing files. As mentioned above, PCR-GLOBWB 2 uses NetCDF files for most input
482 and all output, thus making it easier to exchange data with other scientists and use existing tools to analyse its
483 output.

484

485 PCR-GLOBWB 2 generally runs under Linux. It is also possible to run it under Windows, but Windows
486 memory constraints limit domain size and time steps simulated. In order to run PCR-GLOBWB the following
487 additional software needs to be installed: PCRaster version 4, Python versions 2.7 with Python packages
488 numPy and netCDF4 and gdal version 1.8 or higher.

489



490 **3. Model demonstration and evaluation**

491

492 To test and evaluate the performance of PCR-GLOBWB 2, we ran the model at both 30 arc-minute and 5 arc-
493 minute resolution over the period 1958-2015. We compared the results of both simulations with discharge data
494 from the GRDC Global Runoff Data Centre (GRDC, 2014), with total basin water storage estimates
495 from GRACE (Gravity Recovery and Climate Experiment; Wiese, 2015) and with water withdrawal
496 data from the FAO AQUASTAT database (FAO, 2016).

497

498

499 **3.1 Model run setup**

500

501 **3.1.1 Parameterization**

502

503 We used the standard parameterization (parameters, forcing and their sources in Table A2) of PCR-
504 GLOBWB 2 at 30 arc-minute and 5 arc-minute spatial resolutions to simulate global hydrology at daily
505 resolution over 1958-2015. Outputs were reported as monthly averages. Note that parameterizations
506 were derived directly following their source data sets using hydrological concepts described in Van
507 Beek and Bierkens (2009). We stress that no calibration was performed. We ran the model with human
508 water use options on and used the travel-time characteristic solution routing option.

509

510 **3.1.2 Forcing**

511

512 The forcing data set is based on time series of monthly precipitation, temperature and reference
513 evaporation from the CRU TS 3.2 data set of Harris et al. (2014) downscaled to daily values with
514 ERA40 (1958-1978; Uppala et al., 2005) and ERA-Interim (1979-2015; Dee et al., 2011). CRU is
515 specified at 30 arc-minute spatial resolution and directly usable. We used ERA40 and ERA-I results
516 that had been resampled by ECMWFs resampling scheme from their original resolutions (~1.2° and
517 ~0.7°) to 30 arc-minutes first. Precipitation was temporally downscaled by first applying a threshold of
518 0.1 mm/day to the ERA daily time series to estimate the number of rain days for ERA. The amount of
519 rainfall below this threshold was proportionally allocated to the rain days. Next, the daily rainfall totals
520 were scaled in order to reproduce the CRU monthly precipitation total using multiplicative scaling.
521 Equally, monthly reference potential evaporation, computed with Penman-Monteith from the CRU data
522 set was scaled using multiplicative scaling and downscaled to daily data proportional to Hamon (1967)
523 evaporation calculated from daily ERA temperatures. For the air temperature, an additive scaling factor
524 was used. To better simulate snow-dynamics for the 5-arc-minute model, the temperature values from
525 CRU were further spatially downscaled to 5 arc-minutes using a temperature lapse-rate derived from
526 the higher-resolution CRU V1.0 climatology (New et al., 2002). For areas where the number of stations



527 underlying the CRU data set was found to be small, preference was given to using directly the
528 meteorological data from ERA. The method used to create the forcing data set is described more
529 extensively in Van Beek (2008).

530

531 **3.1.3 Spin-up**

532

533 The large groundwater response times for certain regions (e.g. Niger and Amazon) requires substantial
534 spin-up for the groundwater volumes to be in equilibrium with the current climate. To reach this
535 equilibrium, the model was spun-up using the average climatological forcing over the years 1958–2000
536 back-to-back for 150 years to reach a dynamic steady state. This spin-up was executed under
537 naturalized condition which means no reservoirs and no human water use.

538

539 **3.1.4 Computation time and parallelization**

540

541 The models were run on Cartesius, the Dutch national supercomputer
542 (<https://userinfo.surfsara.nl/systems/cartesius>). Without parallelization, the wall clock time for a one-
543 year global simulation run of the 30 arc-minute model was about one hour. This entails that a one-year
544 global simulation run with the 5 arc-minute model, might result in wall clock times at least 36 hours.
545 Hence, to speed-up computation, the 5 arc-minute model domain was divided into 53 groups of river
546 basins such that it could be run as 53 separate processes. With this simple parallelization technique, the
547 wall clock time for a one-year simulation run of the 5 arc-minute model reduced to about one hour
548 again. Note that these computation times were obtained for simulations with the travel-time characteristic
549 routing option. Calculation times would have been significantly longer if the kinematic wave routing had been
550 used (e.g. about 6 hours for a one-year 5 arc-minutes global run including parallelization).

551

552

553

554 **3.2 Data used for comparison**

555

556 **3.2.1 River discharge**

557

558 We used discharge stations from GRDC (2014) to compare simulated discharge from PCR-GLOBWB
559 2 with monthly reported discharge. From all the globally available stations in the database, we selected
560 a subset of stations using the following criteria: 1) allowing a not more than 15% difference in
561 catchment area between PCR-GLOBWB 2 and the area reported with the GRDC discharge station; 2)
562 not more than 1 cell distance between the station location and the nearby location of a main river in
563 PCR-GLOBWB 2; 3) at least 1 year of discharge data. This yielded 5363 stations for the 5 arc-minute



564 simulation, 3910 stations for the 30 arc-minute simulation and 3597 stations fulfilling the criteria for
565 both resolutions. As we jointly compared the performance of both simulations, we used the set of 3597
566 locations throughout. The average time series length of these stations is equal to 36 years.

567

568 **3.2.2 Total water storage**

569

570 We compared total water storage (TWS) as simulated by PCR-GLOBWB 2 with the TWS estimated
571 from GRACE (Gravity Recovery and Climate Experiment) gravity anomalies. We used the GRACE
572 JPL Mascon product PL-RL05M (Wiese, 2015; Watkins et al., 2015; Wiese et al., 2016). Scanlon et al.
573 (2016) suggest that recent developments in mascon (mass concentration) solutions for GRACE have
574 significantly increased the spatial localization and amplitude of recovered terrestrial TWS signals. They
575 also claim that one of the advantages of using the mascon solutions relative to traditional SH (spherical
576 harmonic) solutions is that it makes it much easier for non-geodesists to apply GRACE data to
577 hydrologic problems. Note that although the data of PL-RL05M are represented on a 30 arc-minutes
578 lat-lon grid, they represent the 3x3 arc-degree equal-area zones, which is the actual resolution of JPL-
579 RL05M. We compared trends on a pixel-by-pixel basis. Given the coarse resolution of GRACE
580 products of about 300 km by 300 km we compared cross-correlations only for major river basins with
581 an area of 900,000 km² and up.

582

583 **3.2.3 Water withdrawal**

584

585 The water withdrawal for a large number of countries is taken from FAO's AQUASTAT database
586 (FAO, 2016) This data is on average reported in every 5 years. We compared simulated water
587 withdrawal per sector and per water source (surface water and groundwater) with reported values per
588 country and per reporting period, whenever available.

589

590

591

592

593 **3.3 The global water balance simulated at 30 and 5 arc-minutes**

594

595 We calculated the main global water balance components from the 30 arc-minute and 5 arc-minute
596 simulations over the period 2000-2015. The results in Table 1 show that there are some differences
597 between the two model runs, but values are in the same order of magnitude. The small difference in
598 precipitation is due to the fact that the area of the land cells is slightly different at the two resolutions.
599 Differences in evaporation and runoff show that the runoff and evaporation parameterization of PCR-
600 GLOBWB 2 is not entirely scale-consistent. Differences in evaporation may also be causing the



601 differences in irrigation water demand which in turn may explain the differences in water withdrawal.
 602 Recently, Samaniego et al. (2017) applied their multiscale parameter regionalization (MPR) technique
 603 to PCR-GLOBWB 2 for the Rhine basin, showing that scale-consistent flux-preserving
 604 parameterisation is possible. However, a global application of this method to all PCR-GLOWB 2
 605 parameters is not possible yet. Nonetheless, when comparing the results of both model runs with data
 606 reported in the literature, it shows that the global water balance components are similar to recent
 607 assessments (e.g. by Rodell et al., 2015) and groundwater withdrawal and total withdrawal estimates
 608 match those of previous studies (see Table 2).

609

610 From Table 1, it can also be seen that there is a negative change in total terrestrial water storage in both
 611 model runs. Table 1 shows that this can only be partly explained by groundwater depletion, which is
 612 localized to certain regions (see also Sect. 3.4.2). Further analysis shows that this change can also be
 613 attributed to the trends in precipitation forcing used, particularly over the tropics.

614

615

616

617

618 *Table 1. Global Water balance components and human water withdrawal (in km³/year) over the period*
 619 *2000-2015 as obtained from the 30 arc-minutes and the 5 arc-minute simulations. The numbers are*
 620 *shown to high significance to show the water balance closure. This does not mean that we pretend to*
 621 *know e.g. global discharge with a km³ accuracy (actual accuracy of the large fluxes is more in the*
 622 *order of 10³ km³)*

		30 arc-min (km ³ /year)	5 arc-min (km ³ /year)
Global water balance	Precipitation	107452	107495
	Desalinated water use	3	2
	Runoff	42393	43978
	Evaporation*	65754	63974
	Change in total water storage	-693	-455
Groundwater budget	Groundwater recharge	27756	25521
	Groundwater withdrawal	737	632
	Non-renewable groundwater withdrawal (groundwater depletion)	173	171
	Renewable groundwater withdrawal	564	460
Withdrawal by sector	Agricultural water withdrawal (irrigation + livestock)	2735	2309
	Domestic water withdrawal	380	314
	Industrial water withdrawal	798	707
Withdrawal by source	Total water withdrawal	3912	3330
	Surface water withdrawal	3172	2697
	Desalinated water use	3	2
	Groundwater withdrawal	737	632

623 * Includes consumptive water use for livestock, domestic and industrial sectors

624

625 *Table 2. Groundwater withdrawal (a) and total water withdrawal (b) as compared to other studies***a) Groundwater withdrawal**

Source	Year	Value (km ³ /year)
Döll et al. (2012)	1998-2002	571
Döll et al. (2014) (their Table 2).	2003-2009	690-888
Döll et al. (2014) (their Table 6).	2000-2009	665
Pokhrel et al. (2015)	1998-2002	570 (±61)
Wada et al. (2010) (from the IGRAC database)	2000	734 (±87)
This study (5 arc-minutes)	2000-2015	632

b) Total water withdrawal

Source	Year	Value (km ³ /year)
Döll et al. (2012)	1998-2002	4340
Döll et al. (2014) (their Table 2)	2003-2009	3000-3700
FAO (2016)	2010	3583
Oki and Kanae (2006): 3800 km ³ /year (contemporary)	2006	3800
Vörösmarty et al. (2005)	1995-2000	3560
This study (5 arcminutes)	2000-2015	3330

626

627

628

629

630 **3.4 Evaluation of the 30 and 5 arc-minute simulations**

631

632 **3.4.1 Discharge**

633

634 When evaluating the simulated discharge with discharge observations from GRDC we calculated three
635 different measures: 1) the cross-correlation coefficient between simulated and observed GRDC time
636 series, which is a measure of reproducing correct timing of high and low discharge. A correlation
637 coefficient of 1 is perfect timing; 2) the Kling-Gupta efficiency coefficient or KGE (Gupta et al., 2009)
638 which equally measures bias, differences in amplitude and differences in timing. The KGE varies
639 between 1 and minus infinity, where 1 means a perfect fit in terms of bias, amplitude and timing; 3)
640 anomaly cross-correlation, i.e. the cross-correlation between time series after the seasonal signal
641 (climatology) has been removed. This statistic measures the ability of the model to correctly simulate
642 timing of seasonal and the inter-annual anomalies from the yearly climatology. It shows if the model is
643 capable of capturing hydrological extremes and is not only driven by the climatology. An anomaly
644 correlation of 1 indicates perfect characterization of the extremes and values below 0 indicates a lack
645 thereof.

646

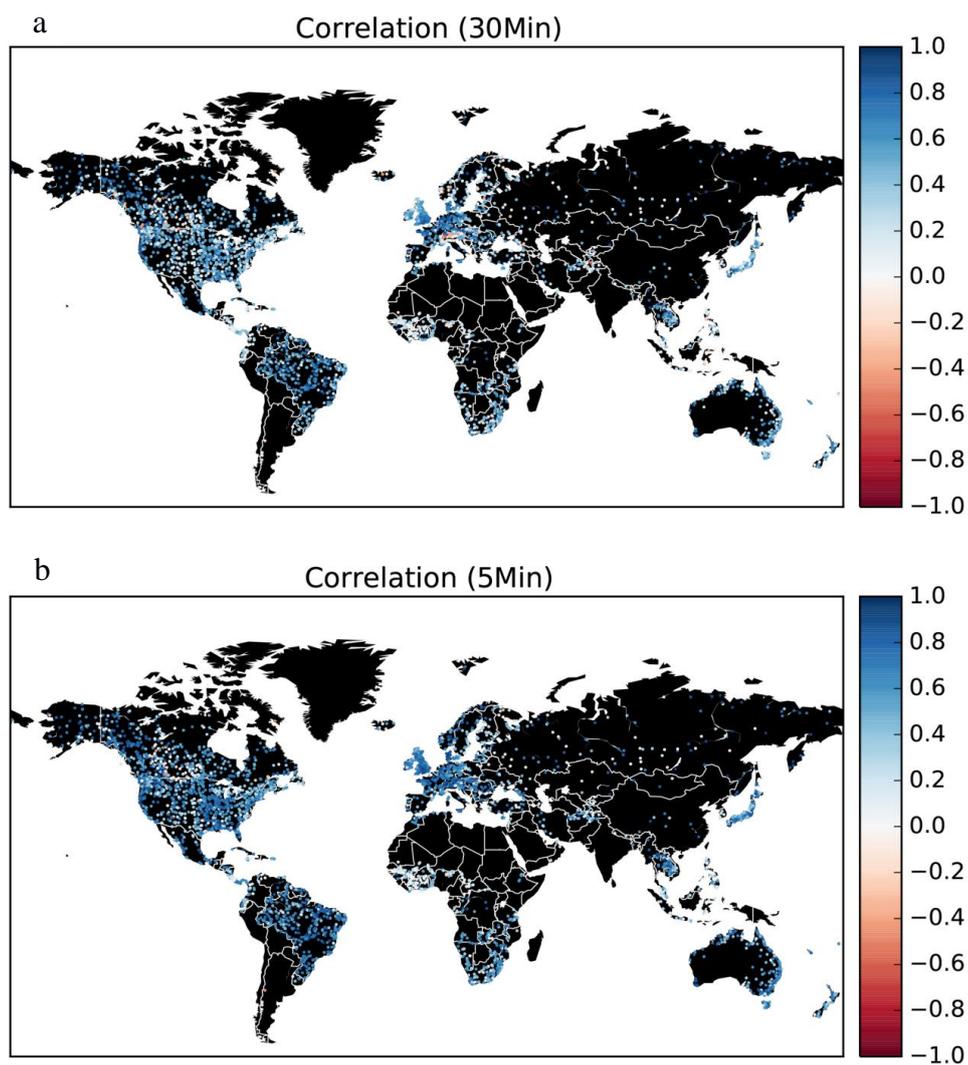
647 Figure 3 shows maps of the cross-correlation coefficients for the GRDC stations considered and Figure
648 4 shows histograms of cross-correlation and KGE values. Both figures show that the validation results
649 of the 5 arc-minute simulation are notably better than those of the 30 arc-minute simulation. For the 30



650 arc-minute model the number of catchments with $KGE > 0$, 0.3 and 0.6 are equal to 48%, 26% and 7%
651 of the total catchments respectively. For the 5 arc-minute model these values are respectively equal to
652 63%, 40% and 12% of the total catchments. Note that for both runs the standard parameterization was
653 used. Possible explanations for the better performance of the 5 arc-minute run are: a better delineation
654 of the outline of the basins, particularly the smaller ones, a better characterization of basin relief and the
655 drainage network, more accurate sub-grid parameterization of soil and land cover due to a smaller
656 scale-gap that needs to be overcome, better estimates of the basin storage and better snow dynamics
657 due to the downscaling of temperature to 5 arc-minute resolution. The KGE values are less favourable
658 than the cross-correlation coefficients. This is mostly due to biases in runoff caused by to incorrect
659 meteorological forcing.

660

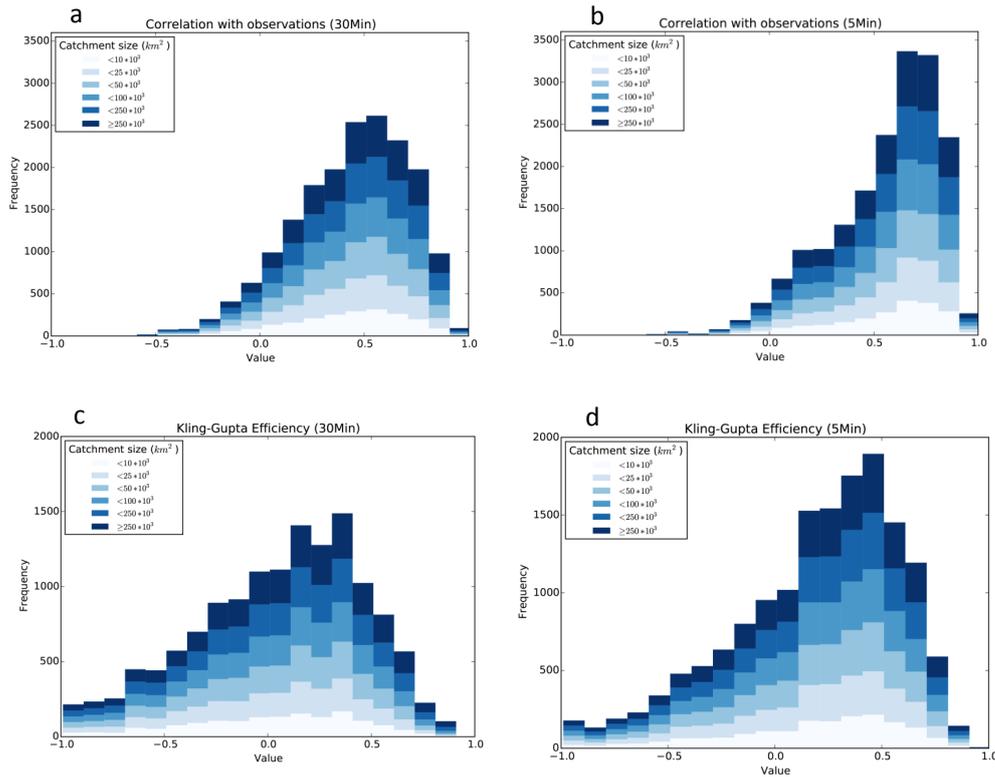
661 The maps of cross-correlations (Figure 3) show the best results in Europe and North America where the
662 meteorological forcing is generally more accurate as a result of more data used in the re-analysis
663 products and higher station availability in the CRU data set. Also, monsoon-dominated basins are well
664 simulated due to the strong seasonal nature of both forcing and related discharge. The improvement of
665 the 5 arc-minute simulation over the 30 arc-minute simulation in Europe is mostly seen in the Alps and
666 the Norwegian mountains. This reflects the fact that topography and thus snow dynamics is better
667 represented at higher resolution. The least accurate results are obtained for some of the African rivers,
668 in particular the Niger where the groundwater recession constants are probably over-estimated and
669 inland delta evaporation is under-estimated, and for some rivers in the Rocky Mountains, which may be
670 the result of errors in snow dynamics. Although results are generally better, the spatial distribution of
671 results is similar to those found by Van Beek et al. (2011) for PCR-GLOBWB 1. The histograms of
672 validation results in Figure 4 do not show a strong relationship between catchment size and validation
673 statistics. This suggests that the improvements of model results equally apply to all catchment sizes
674 when moving from a coarser to higher resolution.



675

676 *Figure 3 Maps of cross-correlation between simulated and observed discharge time series for 3597 GRDC*

677 *discharge stations; a. results for the 30 arc-minute simulation; b. results for 5 arc-minute simulation.*



678 *Figure 4. Histograms of validation statistics showing the cross-correlation and Kling-Gupta efficiency (KGE)*
679 *values for the simulated discharge for the 30 arc-minutes and the 5 arc-minute simulations based on 3597*
680 *GRDC discharge stations; a. cross-correlation 30 arc-minute simulation; b. cross-correlation 5 arc-minute*
681 *simulation; c. KGE 30 arc-minute simulation; d. KGE 5 arc-minute simulation; note: the percentage*
682 *catchments with KGE < -1 are 21% and 12% for 30 and 5 arc-minutes respectively.*

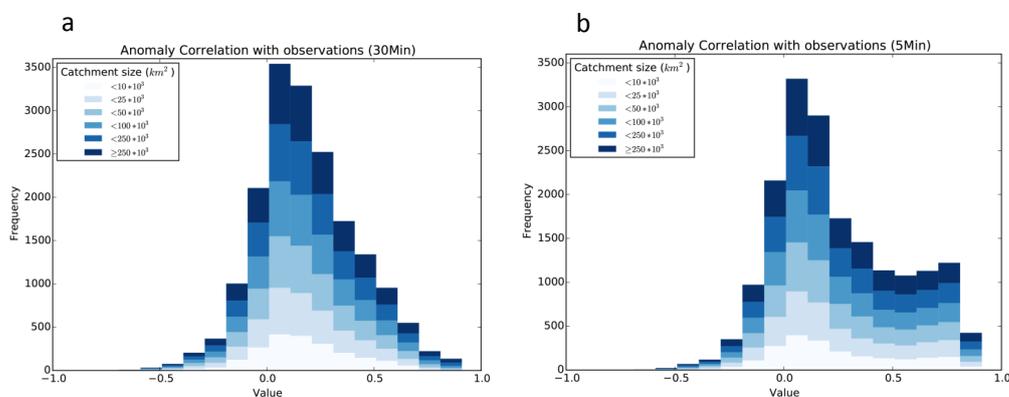
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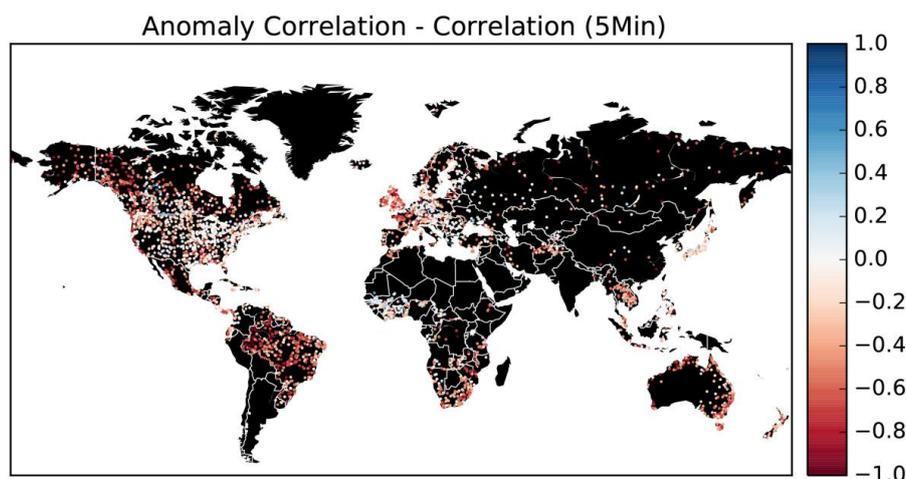
685 The histograms of the anomaly cross-correlation are shown in Figure 5 The anomaly cross-correlations are
686 generally lower than the cross-correlations, showing that seasonality explains part of the skill in many regions
687 where seasonal variation is dominant when compared to intra-annual or inter-annual variability. Clearly, the 5
688 arc-minute results are much better than those of the half-degree simulation, indicating a higher skill with
689 regard to capturing extremes and anomalies. Figure 6 shows a map of the difference between the anomaly
690 cross-correlation and the cross-correlation for the 5 arc-minute case. This map shows that there are some
691 regions where the anomaly cross-correlation is better than the cross-correlation (blue colours), e.g. snow-
692 dominated regions in Canada and the Niger basin. These are catchments where the model has difficulty



693 reproducing the correct seasonality as a result of errors in snow dynamics (Canada) or groundwater dynamics
694 (Niger). Also, in case of the Niger River, not representing the inner delta flooding and resulting high
695 evaporation may be the cause of poor seasonal timing of discharge.
696



697
698 *Figure 5. Histograms of validation statistics showing the anomaly cross-correlation for the simulated*
699 *discharge for the 30 arc-minutes and the 5 arcminute simulations based on 3597 GRDC discharge stations; a.*
700 *anomaly cross-correlation half arc-degree simulation; b. anomaly cross-correlation 5 arcminute simulation.*
701



702
703 *Figure 6. Map showing for the 5 arc-minutes run the difference between the cross-correlation and the*
704 *anomaly cross-correlation between simulated and observed discharge time series for 3597 GRDC discharge*
705 *stations; negative values mean that the cross correlation is higher than the anomaly cross-correlation.*
706



707

708

709 **3.4.2 Total water storage**

710

711 Figure 7 compares the trends in 5 arc-minute simulated total water storage (TWS) with those from GRACE,
712 estimated as the average change in m/year over the period 2003-2015. Generally, the PCR-GLOBWB 2
713 simulation is able to capture major groundwater depleted regions as suggested by GRACE, such as those in the
714 Central Valley aquifer, the High Plains aquifer, the North China Plain aquifer, as well as parts of the Middle
715 East, Pakistan and India. For these regions, the absolute rates of TWS change (i.e. TWS declines) of PCR-
716 GLOBWB 2 are generally larger, while the spatial pattern in the GRACE map tends to be smoother. This is
717 mainly due to the lower resolution and spatial averaging used in the GRACE product, as well as the fact that
718 the current PCR-GLOBWB 2 simulation does not include lateral groundwater flow between cells. In the polar
719 regions where GRACE estimates mass loss due to melting glaciers and ice sheets, PCR-GLOBWB 2 simulates
720 accumulation as a result of lack of a glacier parameterization. Finally, there are some clear differences over the
721 Amazon and some parts of Africa. A possible explanation are errors in meteorological forcing data, which is
722 not very accurate in these parts, but also problems with the over-estimation of PCR-GLOBWB's groundwater
723 response times in these regions which therefore fail to be sufficiently sensitive to recent changes in terrestrial
724 precipitation.

725

726 Further analyses were conducted at the basin-scale resolution, where both TWS time series of PCR-GLOBWB
727 2 and GRACE *JPL-RL05M* were averaged over a river basins areas map derived from the 5 arc-minute PCR-
728 GLOBWB drainage network. We identified all river basins with sizes larger than 900,000 km², which is
729 similar to the GRACE resolution. Smaller river basins were merged to the nearest river basins or grouped
730 together. For the remaining map of large basins, the cross-correlations between PCR-GLOBWB 2 and
731 GRACE basin-average monthly and annual TWS time series were calculated. Monthly cross-correlation
732 provides information about PCR-GLOBWB's ability to correctly time TWS seasonal variability (with a value
733 equal to 1 for perfect timing), while the cross-correlation for annual time series measures inter-annual
734 variability.

735

736 The results in Figure 8 show that PCR-GLOBWB 2 is able to capture GRACE's TWS seasonality for most
737 basins around the world, with the exception of some cold regions in high latitudes (e.g. the Yukon River basin,
738 Iceland). This shortcoming is most likely due to the lack of a proper representation of glacier and ice processes
739 in PCR-GLOBWB 2. As expected, the cross-correlation values for inter-annual time series are generally lower
740 than the ones for monthly time series. There are some areas with negative correlation values, such as the
741 Amazon, Niger and Nile river basins. Apart from the uncertainty in the GRACE signal, these deficiencies may
742 be related to errors in model forcing and structural errors such as errors in the groundwater response time and
743 the effects of wetlands that have not been represented sufficiently well.



744

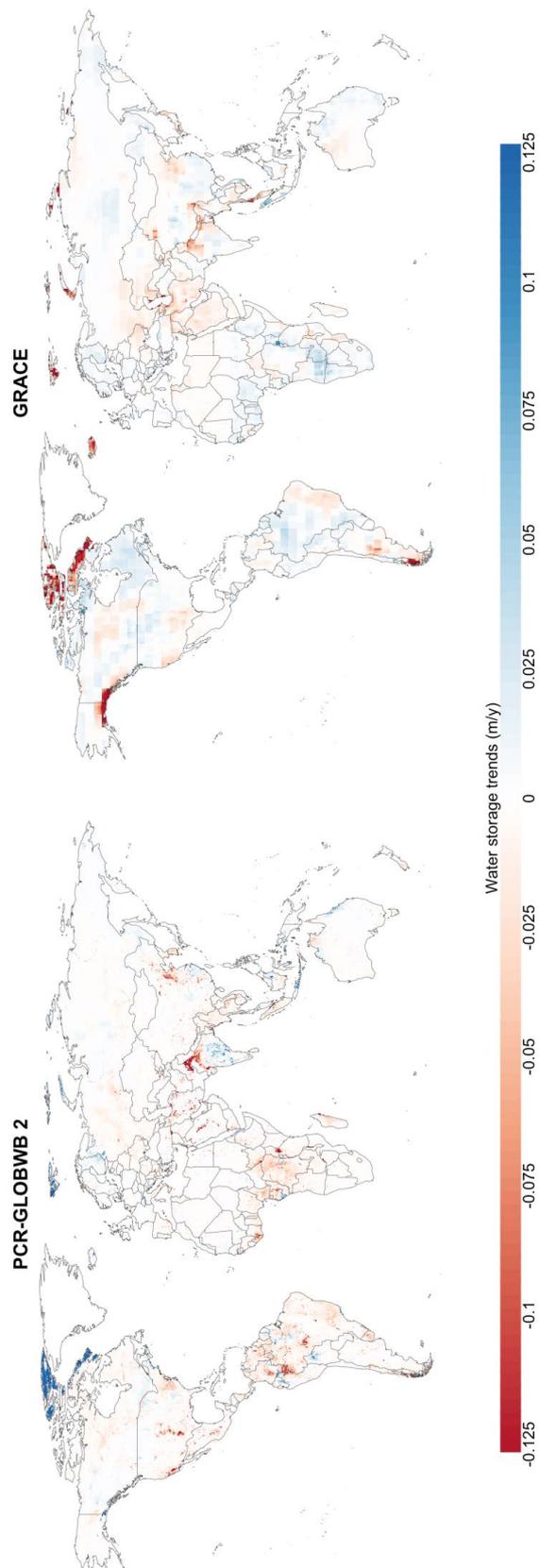


Figure 7. Comparison of PCR-GLOBWB 2 total water storage trends (m/year) with those estimated with GRACE over the period 2003-2015. a. TWS trends simulated with PCR-GLOBWB 2 at 5 arc-minute resolution (~10 km at the equator). Negative values indicate declining TWS (e.g. groundwater depleted regions). b. TWS trends obtained based on the GRACE JPL PL-RL05M Mascon product. The GRACE data were resampled to the resolution of 30 arc-minutes, but they actually represent the 3 x 3 arc-degree (~300 km x 300 km) area, which is the native resolution of the GRACE signal.



745

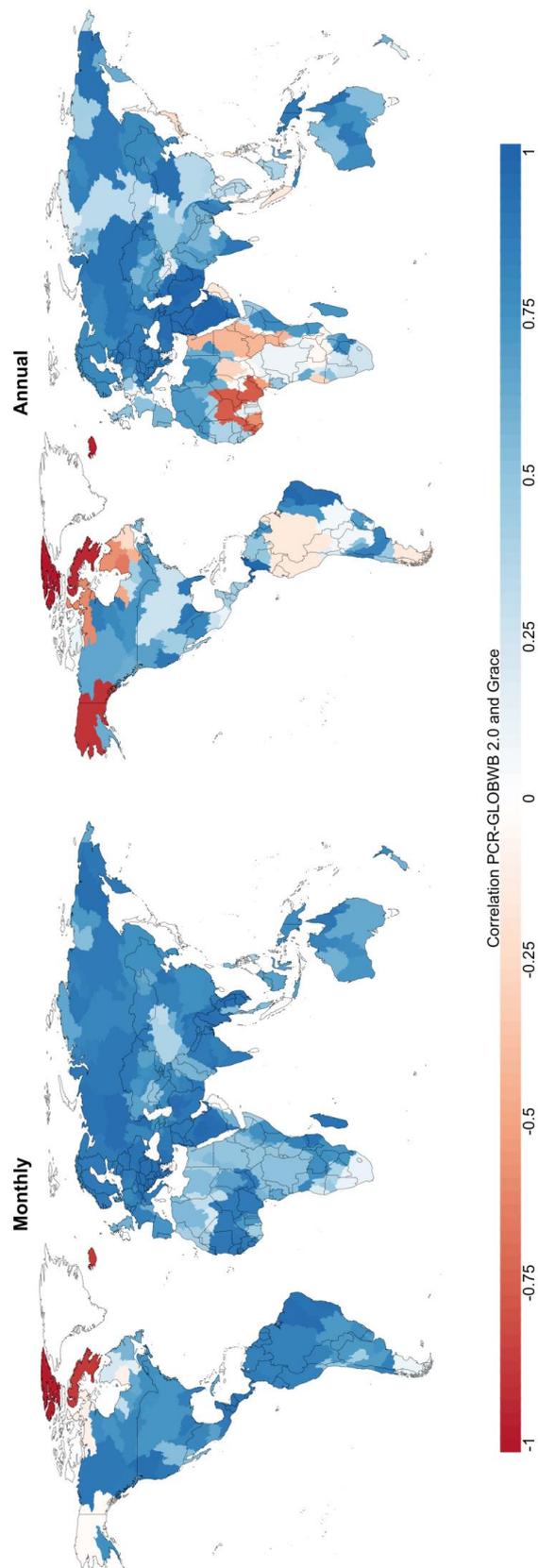
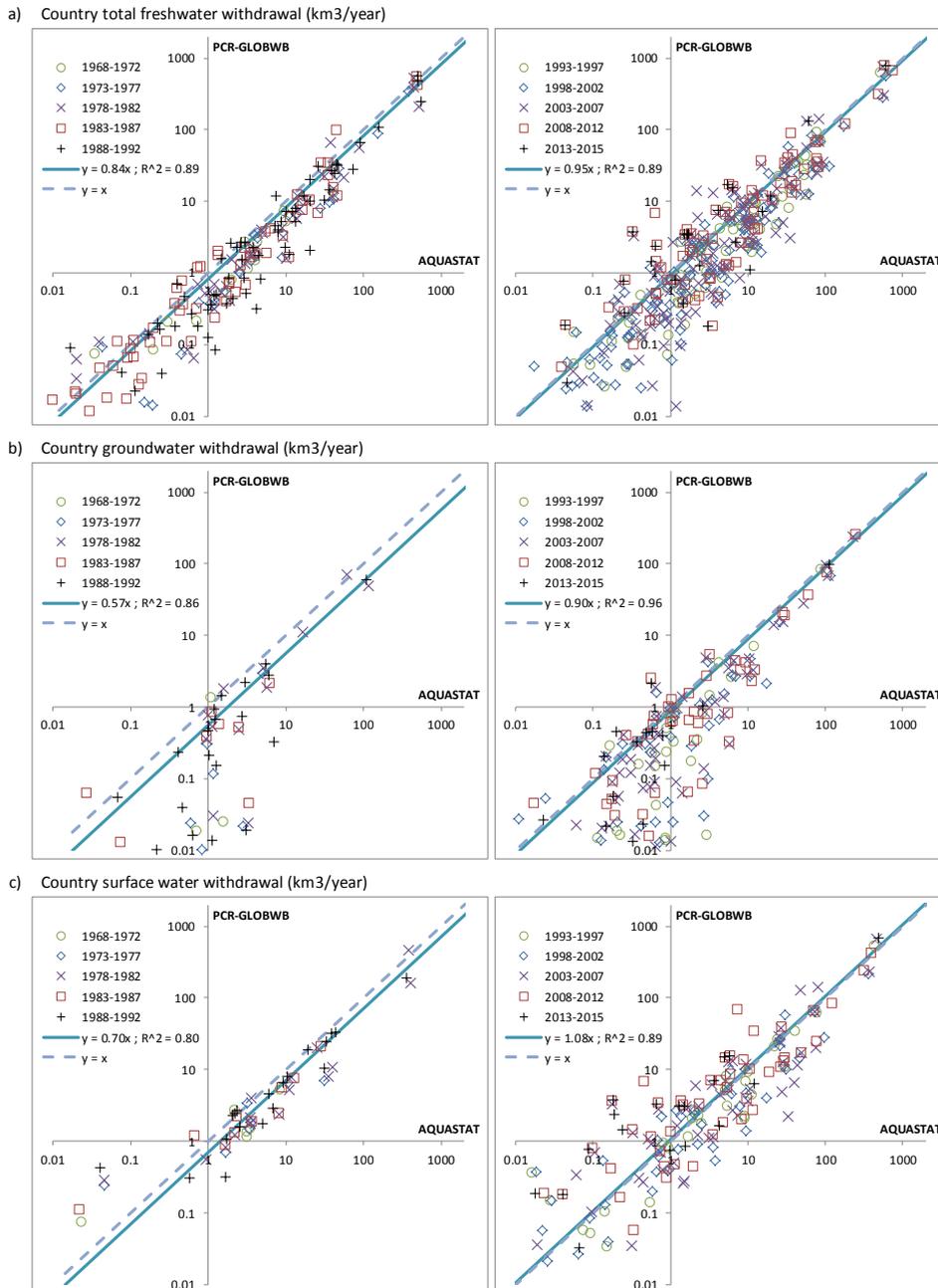


Figure 8. a. Cross-correlation between monthly TWS time series simulated PCR-GLOBWB 2.0 and the GRACE JPL PL-RL05M Mascon product over the period 2003-2015. b. Comparison of annual TWS series (inter-annual variability). Comparison is only done for the larger basins over 900,000 km², conform the 3x3 arc-degree resolution of GRACE.



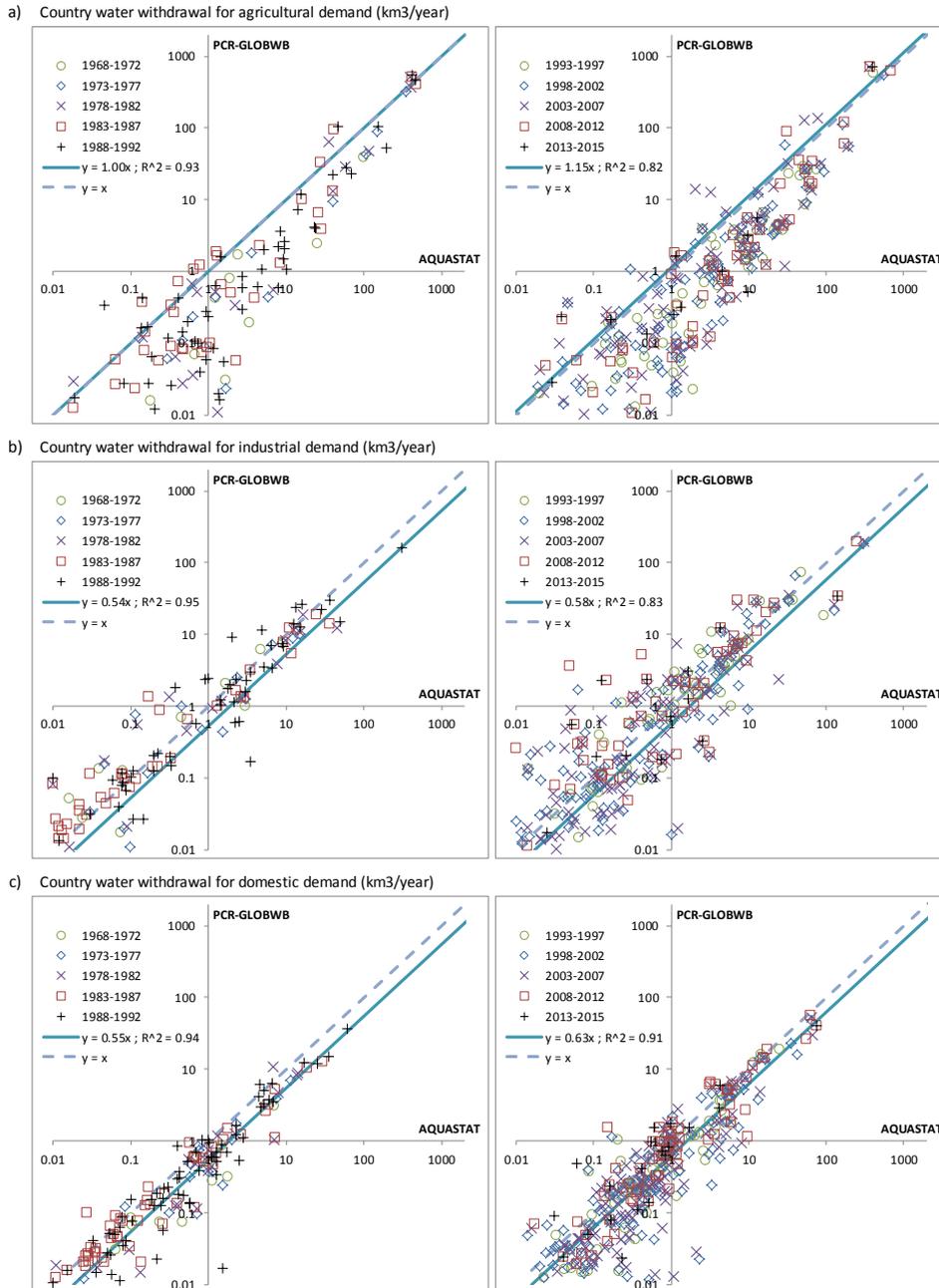
746

747 *Fig. 9: Country water withdrawal (km³/year) by source; validation of simulations with PCR-GLOBWB 2 with*

748 *reported values in AQUASTAT (FAO, 2016) for various periods; a) total water withdrawal; b) groundwater*

749 *withdrawal; c) surface water withdrawal.*

750



751

752 *Fig. 10: Country water withdrawal (km³/year) by sector; validation of simulations with PCR-GLOBWB 2 with*
 753 *reported values in AQUASTAT (FAO, 2016) for various periods; a) withdrawal for agricultural demand*
 754 *(irrigation and livestock); b) withdrawal for industrial demand; c) withdrawal for domestic demand.*

755



756 3.4.3 Water withdrawal

757

758 We compared simulated water withdrawal data from PCR-GLOBWB 2 with reported withdrawal data per
759 country from AQUASTAT (FAO, 2016). The results are shown subdivided per source (Figure 9) and per
760 sector (Figure 10). These figures show that PCR-GLOBWB 2 is able to reproduce reported withdrawal values
761 reasonably well (R^2 between 0.80 and 0.96 and regression slopes between 0.54 and 1.15). There is some
762 underestimation of groundwater withdrawal for the countries with lower withdrawal values. This may be the
763 result of not sufficiently accounting for domestic groundwater withdrawal in populated areas. Also, Figure 10
764 shows that agricultural water withdrawal is underestimated for countries with smaller withdrawal. A possible
765 cause of this may be the overestimation of irrigation efficiency.

766

767

768 4. Conclusions and future work

769

770 We presented the most recent version of the open source global hydrology and water resources model PCR-
771 GLOBWB. This version, PCR-GLOBWB 2, has a global coverage at 5 arc-minute resolution. Apart from the
772 higher resolution, the new model has an integrated water use scheme, i.e. every day sector specific water
773 demand is calculated, resulting in groundwater and surface water withdrawal, water consumption and return
774 flows. Dams and reservoirs from the GranD database (Lehner et al., 2011) are added progressively according
775 to their year of construction. PCR-GLOBWB 2 has been rewritten in Python and uses PCRaster-Python
776 functions (Karssenbergh et al., 2007). It has a modular structure, which makes the replacement and maintenance
777 of model parts easier. PCR-GLOBWB 2 can be dynamically coupled to a global 2-layer groundwater model
778 (De Graaf et al., 2017) and a one-way coupling to hydrodynamic models for large-scale inundation modelling
779 (Hoch et al., 2017b) is also available.

780

781 Comparing the 5 arc-minute with 30 arc-minute simulations using discharge data we clearly find an
782 improvement in the model performance of the higher resolution model. We find a general increase in
783 correlation, anomaly correlation and KGE, indicating that the higher resolution model is better able to capture
784 the seasonality, hydrological extremes and the general discharge characteristics. Also, PCR-GLOBWB 2 is
785 able to reproduce trends and seasonality in total water storage as observed by GRACE for most river basins. It
786 simulates the hotspots of groundwater decline that around in GRACE as well. Simulated water withdrawal, by
787 source and sector, matches reasonably well with reported water withdrawal from AQUASTAT.

788

789 Future work will concentrate on developing a full dynamic (two-way) coupling with hydrodynamic models,
790 developing 5 km and 1 km resolution (or higher) parameterizations of PCR-GLOBWB 2 using scale-consistent
791 parameterizations (e.g. using MPR; Samaniego et al., 2017), incorporating a crop growth model and solving
792 the full surface energy balance. Other foreseeable developments are using the model in probabilistic settings
793 and in data-assimilation frameworks.



794

795

796 **5. Code and data availability**

797

798 PCR-GLOBWB 2 is open source and distributed under the terms of the GNU General Public License version
799 3, or any later version, as published by the Free Software Foundation. The model code is provided through a
800 Github repository: https://github.com/UU-Hydro/PCR-GLOBWB_model (Sutanudjaja et al., 2017a,
801 <https://doi.org/10.5281/zenodo.595656>). This keeps users and developers immediately aware of any new
802 revisions. Also, it allows developers to easily collaborate, as they can download a new version, make changes,
803 and suggest and upload the newest revisions. The configuration ini-files for the global 30 arc-minutes and 5-
804 arcminute models and the associated model parameters and input files are provided on
805 <https://doi.org/10.5281/zenodo.1045338> (Sutanudjaja et al., 2017b). Development and maintenance of the
806 official version (main branch) of PCR-GLOBWB 2 is conducted at the Department of Physical Geography,
807 Utrecht University. Yet, contributions from external parties are welcome and encouraged. For news on latest
808 developments and papers published based on PCR-GLOBWB 2 we refer to <http://www.globalhydrology.nl>
809 and for the underlying PCRaster-Python code to <http://pcraster.geo.uu.nl>.

810

811

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817 the help of SURFsara Amsterdam.

818

819



820 **Appendix**

821

Table A1 - List (non-exhaustive) of state and flux variables defined in PCR-GLOBWB

Description	Symbol	Unit
Interception storage	S_{int}	m
Snow cover/storage in water equivalent thickness (excluding liquid part S_{slq})	S_{swe}	m
Liquid/melt water storage in the snow pack	S_{slq}	m
Upper and lower soil storages	S_1 and S_2	m
Surface water storage (lakes, reservoirs, rivers and inundated water)	S_{wat}	m
groundwater storage (renewable part)	S_3	m
fossil groundwater storage (non-renewable)	S_{nrw}	m
total groundwater storage = $S_3 + S_{nrw}$	S_{gwt}	m
total water storage thickness = $S_{int} + S_{swe} + S_{slq} + S_1 + S_2 + S_{gwt}$	TWS	m
potential evaporation	E_{pot}	m.day ⁻¹
evaporation flux from the intercepted precipitation	E_{int}	m.day ⁻¹
evaporation from melt water stored in the snow pack	E_{slq}	m.day ⁻¹
bare soil evaporation	E_{soil}	m.day ⁻¹
transpiration from the upper and lower soil stores	T_1 and T_2	m.day ⁻¹
total land evaporation = $E_{pot} + E_{int} + E_{slq} + E_{soil} + T_1 + T_2$	E_{land}	m.day ⁻¹
surface water evaporation	E_{wat}	m.day ⁻¹
total evaporation = $E_{land} + E_{wat}$	E_{tot}	m.day ⁻¹
direct runoff	Q_{dr}	m.day ⁻¹
interflow, shallow sub-surface flow	Q_{sf}	m.day ⁻¹
baseflow, groundwater discharge	Q_{bf}	m.day ⁻¹
specific runoff from land	Q_{loc}	m.day ⁻¹
local change in surface water storage	Q_{wat}	m.day ⁻¹
total specific runoff	Q_{tot}	m.day ⁻¹
routed channel (surface water) discharge	Q_{chn}	m ³ .sec ⁻¹
net fluxes from the upper to lower soil stores	Q_{12}	m.day ⁻¹
net groundwater recharge, fluxes from the lower soil to groundwater stores	$RCH = Q_{23}$	m.day ⁻¹
surface water infiltration to groundwater	Inf	m.day ⁻¹
desalinated water withdrawal	W_{sal}	m.day ⁻¹
surface water withdrawal	W_{wat}	m.day ⁻¹
renewable groundwater withdrawal	W_3	m.day ⁻¹
non-renewable groundwater withdrawal (groundwater depletion)	W_{nrw}	m.day ⁻¹
total groundwater withdrawal = $W_3 + W_{nrw}$	W_{gwt}	m.day ⁻¹
water withdrawal allocated for irrigation purpose	A_{irr}	m.day ⁻¹
water withdrawal allocated for livestock demand/sector	A_{liv}	m.day ⁻¹
water withdrawal allocated for agricultural sector = $A_{irr} + A_{liv}$	A_{agr}	m.day ⁻¹
domestic water withdrawal	A_{dom}	m.day ⁻¹
industrial water withdrawal	A_{ind}	m.day ⁻¹

822

Table A2 - List of model inputs and parameters

Description	Symbol	Unit	References/sources
Upper and lower soil store parameters:			
- Soil thickness	Z_1 and Z_2	m	FAO (2007) soil map; van Beek and Bierkens (2009)
- Residual soil moisture content	$\theta_{r,1}$ and $\theta_{r,2}$	$\text{m}^3 \cdot \text{m}^{-3}$	
- Soil moisture at saturation	$\theta_{s,1}$ and $\theta_{s,2}$	$\text{m}^3 \cdot \text{m}^{-3}$	
- Soil water storage capacity per soil layer: $SC = Z / (\theta_s - \theta_r)$	SC_1 and SC_2	m	
- Soil matric suctions at saturation	$\psi_{s,1}$ and $\psi_{s,2}$	m	
- Exponent in the soil water retention curve	β_1 and β_2	dimensionless	
- Saturated hydraulic conductivities of upper and lower soil stores	K_1 and K_2	$\text{m} \cdot \text{day}^{-1}$	
- Total soil water storage capacities = $SC_{\text{upp}} + SC_{\text{low}}$	W_{max}	m	
Land cover fraction: Land cover areas (including extent of irrigated areas) over cell areas	f_{lcov}	$\text{m}^2 \cdot \text{m}^{-2}$	GLCC v2.0 map (USGS, 1997); Olson (1994a, 1994b); MIRCA2000 dataset (Portmann et al., 2010), FAOSTAT (2012)
Topographical parameters	DEM	m	HydroSHEDS (Lehner et al., 2008); Hydro1k (Verdin and Greenlee, 1996); GTOPO30 (Gesch et al., 1999)
- Cell-average DEM	DEM_{avg}	m	
- Flood plain elevation	DEM_{fpl}	m	
Root fractions per soil layer	Rf_{upp} & Rf_{low}	dimensionless	Canadell et al. (1996); van Beek and Bierkens (2009)
Arno scheme (Todini, 1999; Hagemann and Gates, 2003) exponents defining soil water capacity distribution	β_{amo}	dimensionless	Canadell et al. (1996), Hagemann et al. (1999); Hagemann (2002); van Beek (2008); van Beek and Bierkens (2009)
Ratios of cell-minimum and cell-maximum soil storage to W_{max}	f_{wmin} and f_{wmax}	m	van Beek (2008); van Beek and Bierkens (2009)





825

Table A2 - List of model inputs and parameters (continued)

Description	Symbol	Unit	References/sources
Parameters related to phenology			Hagemann et al. (1999); Hagemann (2002); van Beek (2008); van Beek and Bierkens (2009)
- Crop coefficient	K_c	dimensionless	
- Interception capacity	$S_{int-max}$	m	
- Vegetation cover fraction	C_v	$m^2 \cdot m^{-2}$	
Groundwater parameters			GLHYMPS map (Gleeson et al., 2014); van Beek (2008); van Beek and Bierkens (2009)
- Aquifer transmissivity	KD	$m^2 \cdot day^{-1}$	
- Aquifer specific yield	S_y	$m^3 \cdot m^{-3}$	
- Groundwater recession coefficient	J	day^{-1}	
Meteorological forcing			van Beek (2008); CRU (Harris et al., 2014); ERA40 (Uppala et al., 2005); ERA-Interim (Dee et al., 2011)
- Total precipitation	P	$m \cdot day^{-1}$	
- Atmospheric air temperature	T_{air}	$^{\circ}C$ or K	
- Reference potential evaporation and transpiration	$E_{ref,pot}$	$m \cdot day^{-1}$	
Others:			
- Non-irrigation sectoral water demand (i.e. livestock, domestic and industrial)		$m \cdot day^{-1}$	Wada et al (2014)
- Desalinated water		$m \cdot day^{-1}$	Wada et al., (2011a); FAO (2016)
- Lakes and reservoirs			GLWD1 (Lehner and Döll, 2004); Grand (Lehner et al., 2011)

826



827

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